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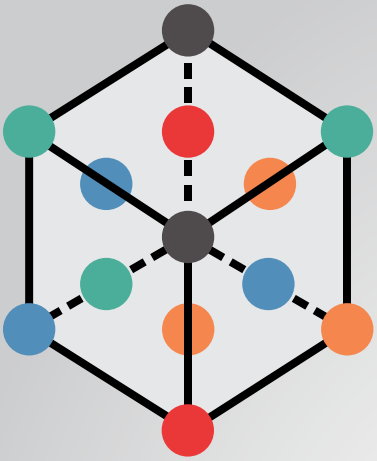

WORLD CONGRESS ON
HIGH ENTROPY ALLOYS
HEA2019

November 17–20, 2019

Hyatt at Olive 8
Seattle, Washington, USA

PRELIMINARY TECHNICAL PROGRAM

The content in this preliminary technical program was generated on September 23. However, changes are still being implemented for the final technical program. Please refer to the online session sheets for the most up-to-date information.

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Monday Plenary

Monday AM
November 18, 2019

Room: Ballroom ABC
Location: Hyatt at Olive 8

8:00 AM Plenary
Metastable High Entropy Alloys: *Dierk Raabe*[1]; [1]Max-Planck-Institut für Eisenforschung GmbH
The lecture deals with the design of high entropy alloys where metastable phase states are not coincidentally inherited from processing, but rather are engineered. Phase stability can be tuned by chemical composition (thermodynamics, e.g. partitioning), tempering (kinetics, e.g. nucleation), and microstructure (confinement, e.g. size effects). When exposed to loads metastable phases can trigger athermal transformation effects such as TRIP and TWIP. The concept works at the bulk scale and also at a spatially confined microstructure scale, such as at lattice defects. In the latter case, local stability tuning works primarily through segregation engineering, i.e. through targeted elemental partitioning to dislocation cores, stacking faults, interfaces, and precipitates with the aim to render only these confined regions metastable. Depending on stability, spatial confinement, misfit, and dispersion, both bulk and local load-driven athermal transformations can equip high entropy alloys with substantial gain in strength, ductility, and damage tolerance.

8:45 AM Question and Answer Period

8:55 AM Break

Alloy Design and Computational Modeling I

Monday AM
November 18, 2019

Room: Azure
Location: Hyatt at Olive 8

9:00 AM Keynote
Enthalpy-based Design of High Entropy Alloys: *Gregory Olson*[1]; [1]Northwestern University
The methodology of accelerated design and qualification of new alloys being advanced under the national Materials Genome Initiative is now being applied in the efficient exploitation of configurational entropy in multi-principal element (MPE) alloys. While the solution thermodynamics of solvent-rich systems is well described by binary interactions, the MPE systems involve significant contributions from ternary interactions that must be quantified for accurate prediction of phase stability. Extension of CALPHAD databases for this purpose has been facilitated by high-throughput DFT calculations of mixing enthalpies in equiatomic ternary systems. Ranking these ternary interactions also allows identification of component combinations that most effectively support the exploitation of configurational entropy for enhanced high-temperature stability of a desired phase. Predictive designs have been very effective in the solubilization of reactive components supporting enhanced resistance to aqueous corrosion or high-temperature oxidation in both FCC and BCC systems.

9:30 AM
Machine Learning-aided Accelerated Discovery of HEA for Turbomachinery Applications: *Soumalya Sarkar*[1]; Kenneth Smith[1]; John Sharon[1]; Ryan Deacon[1]; GV Srinivasan[1]; [1]United Technology Research Center
The feasible space of possible HEA, demonstrating novel thermo-mechanical properties necessary for high-efficiency turbomachinery applications, is still largely unexplored. Although some of the state-of-the-art high-throughput computational approaches have been able to scan through a large equi-molar HEA space or various HEA systems with a narrow range of composition variation under a limited set of property requirements, they haven't yet scaled up to a larger HEA space with high resolution of composition variation, which is necessary to discover non-obvious HEAs with multiple competing properties. This paper presents a machine learning-based framework which is able to converge on a set of HEA candidates given a large set of design objectives and constraints. The proposed approach demonstrates scalability to comprehensive HEA space exploration even while receiving data from variably expensive physics-based thermo-mechanical models. Experimental data from test coupons can also be incorporated in this framework to aid to the reliability of overall framework.

9:50 AM
Screening of Multi-principal Element and High-entropy Alloys by Materials Informatics: *Jeffrey Rickman*[1]; Helen Chan[1]; Martin Harmer[1]; Joshua Smeltzer[1]; Christopher Marvel[1]; Ankit Roy[1]; Ganesh Balasubramanian[1]; [1]Lehigh University
The identification of promising high-entropy alloys presents a daunting challenge given the vastness of the chemistry/composition space associated with these systems. This work describes a supervised learning strategy for the efficient screening of high-entropy alloys that combines two complementary tools, namely: (1) a multiple regression analysis and its generalization, a canonical-correlation analysis (CCA), connecting predictive metrics with material properties, and (2) a genetic algorithm (GA) that explores a multi-dimensional chemistry/composition space with a CCA-inspired fitness function. Starting with a database comprising 82 alloys for which reliable mechanical property information was available, this procedure was used to identify new alloy compositions having potentially high hardness values. These compositions were subsequently fabricated using arc-melting, and the microstructures characterized using SEM. The corresponding hardness values were measured experimentally. The results demonstrated that our informatics based methodology provides a convenient means to predict, at the 90% confidence level, complex alloy compositions with enhanced hardness.

10:10 AM Break

Ceramic HEAs I

Monday AM
November 18, 2019

Room: Cobalt
Location: Hyatt at Olive 8

9:00 AM Keynote
High Entropy Ceramics as an Emerging Class of Material: Insights from Theory and Computation: *Donald Brenner*[1]; M Lim[1]; Zs Rak[1]; S Daigle[1]; P Sarker[2]; C Toher[2]; S Curtarolo[2]; J.P. Maria[1]; [1]North Carolina State University; [2]Duke University
High entropy (HE) ceramics are an emerging material class which, like their metal counterparts, are defined by multiple equi-molar species on a crystal lattice. They are unique within the HE alloys by having multiple sublattices. HE carbides, nitrides and oxides, for example, have a rock salt structure with C, N or O on a fcc sublattice, respectively, and a fcc sublattice containing a random cation population. This talk will focus on first principles and molecular modeling studies of these materials. For oxides, the talk will include how charge compensation accommodates aliovalent elements and effects phonon thermal transport, and how random Cu placement creates a unique Jahn-Teller distortion. For HE carbides and diborides, calculations of phase stability, binding energy, bulk modulus, vacancy formation energy, and thermal conductivity will be discussed. This work was supported by MURI grant N00014-15- 1-2863.

9:30 AM
Expanding High-entropy to Ceramics: Identifying High Entropy Oxides with Perovskite, Spinel, or Pyrochlore Structure: *Veerle Keppens*[1]; Brianna Musico[1]; Candice Kinsler-Fedon[1]; David Mandrus[1]; Jiaqiang Yan[2]; T. Zac Ward[2]; [1]University of Tennessee; [2]Oak Ridge National Laboratory
The concept of entropy stabilization has recently been expanded to oxides, realizing the first high entropy oxides (HEOs) and demonstrating that configurational disorder has the potential to enable the discovery of new materials. This talk will report on our recent efforts to engineer new ceramic materials by applying the concept of entropy stabilization to complex oxides. More specifically, by adding the chemical and structural disorder inherent to entropy-stabilized materials to the competing electronic/magnetic interactions that characterize complex oxides, we provide a new strategy for the design/discovery of materials with unique properties.

9:50 AM
A Novel Ceramic Derived Processing Route for Multi-principal Element Alloys: Madison Gianelle[1]; Animesh Kundu[1]; Kevin Anderson[2]; *Helen Chan*[1]; [1]Lehigh University; [2]Naval Research Laboratory
Multi-principal element alloys (MPEAs) (a.k.a. high entropy alloys) have attracted intense research interest due to their potential for enhanced properties versus conventional alloys. To date, the vast majority of the MPEA compositions studied have been prepared by casting of a molten mixture of the elemental metals. The present work describes a novel solid state technique whereby a bulk equimolar FeCoCuNi MPEA was processed by the reduction of metal oxides. The influence of heat-treatment parameters on the resulting microstructure of the ceramic derived alloy will be presented. Compared to similar alloys fabricated by melt processing, interesting differences emerged with regard to the composition and distribution of the phases. These will be examined in the light of the different fabrication methods. The potential advantages of the ceramic derived process will be discussed, together with the extension of this technique to other MPEA compositions.

10:10 AM Break

Mechanical Properties I

Monday AM
November 18, 2019

Room: Cyan
Location: Hyatt at Olive 8

9:00 AM Keynote
Local Chemical Ordering and the Mechanical Properties of CrCoNi-based High-entropy Alloys: *Robert Ritchie*[1]; Mark Asta[1]; Andrew Minor[1]; Qian Yu[2]; Jun Ding[3]; [1]University of California, Berkeley; [2]Zhejiang University; [3]Lawrence Berkeley National Laboratory
CrCoNi-based medium/high-entropy alloys can display exceptional combinations of strength (~1 GPa), ductility (~60-90%) and toughness (>200 MPavm), properties which are further enhanced at cryogenic temperatures. In situ TEM observations identify multiple deformation mechanisms, associated with their high friction stress yet low stacking-fault energy, that act synergistically to generate damage-tolerance. The effect of local chemical ordering appears to be important here. DFT-based Monte-Carlo simulations and now MD simulations show that variations in local chemical order have a profound effect on the stacking-fault and twin-boundary energies, the TRIP effect, and the formation energy of point defects, all features that influence mechanical properties, although convincing experimental verification of the presence of such local order is rare. Here we discuss the notion of "tuning order in disorder" to achieve a science-based optimization of high-entropy alloys with specifically desired macroscale mechanical performance.

9:30 AM
Fatigue Crack Growth Behavior of CrCoFeNi: Wm Williams[1]; Martha Piness[1]; *Garrett Pataky*[1]; Paul Jablonski[2]; [1]Clemson University; [2]National Energy Technology Laboratory
Equiatomic CoCrFeNi is a single phase high entropy alloy with an fcc structure. Fatigue crack growth experiments were performed at room temperature on single edge notch samples. The experiments consisted of cyclic loading in tension with multiple R-ratios and a naturally increasing stress intensity factor. Images were taken of the samples under loading, and displacement fields were calculated using digital image correlation. The sample images and displacement fields were used to determine crack length, crack closure, and the presence of Mode II displacements. At low R-ratios, post-mortem fractography revealed significant surface roughness and microstructural features indicating high levels of roughness-induced crack closure. Of particular interest were "fin-like" features on the fracture surface, and TEM analysis was performed for further investigation. The material exhibited good fatigue crack growth resistance.

9:50 AM
Investigation on Elastic and Plastic Deformation Behaviors of Refractory High-entropy Alloy at Elevated Temperatures via In-situ Neutron Studies: Chanho Lee[1]; Gian Song[2]; Yi Chou[3]; George Kim[4]; Tingkun Liu[1]; Ke An[5]; Wei Chen[4]; Yi-Chia Chou[3]; Yanfei Gao[1]; *Peter Liaw*[1]; [1]University of Tennessee; [2]Kongju National University; [3]National Chiao Tung University; [4]Illinois Institute of Technology; [5]Oak Ridge National Laboratory
Single solid-solution phase refractory high-entropy alloys (HEAs) show remarkable mechanical properties, such as the high yield strength and excellent ductility, due to their severe lattice distortions. Hence, extensive experimental and theoretical efforts have been conducted to design and develop single-phase body-centered-cubic (BCC) refractory HEAs and verify deformation mechanisms. In this study, we have investigated the elastic- and plastic-deformation behavior of a single BCC NbTaTiV refractory HEA at elevated temperatures, using integrated in-situ neutron-diffraction experiments, density functional theory (DFT) calculations, and finite-elements methods (FEM). The in-situ neutron-diffraction results reveal a deformation transition from the isotropic to anisotropic deformations in the elastic regime at high temperatures. Furthermore, the type of mobile dislocation as a function of macrostrains are quantitatively calculated and predicted by Williamson-hall-plot profile modeling. It is found that the edge dislocations can be the dominant dislocation type for the BCC refractory HEAs during plastic deformation.

10:10 AM Break

Alloy Design and Computational Modeling II

Monday AM
November 18, 2019

Room: Azure
Location: Hyatt at Olive 8

10:40 AM Invited
Optimization of MPEA Properties with Sequential Learning: *James Saal*[1]; Chris Borg[1]; Marie-Agathe Charpagne[2]; Daniel Miracle[3]; Tresa Pollock[2]; Bryce Meredig[1]; [1]Citrine Informatics; [2]University of California, Santa Barbara; [3]Air Force Research Laboratory
The combinatorial nature of the composition space multi-principle element alloys (MPEAs) inhabit requires novel techniques to discover and design novel MPEAs with enhanced performance. Trial-and-error experimentation to exhaustively search this space would be prohibitively costly and time-consuming, and current ICME approaches rely on models which have yet to be matured for MPEA-type compositions. Given the increasing data on MPEA compositions being published, the situation is ideal for data-driven materials informatics approaches. To that end, we employ the cloud-based informatics platform, Citrination, to train machine learning models for mechanical properties and single-phase stability for MPEAs from literature data. We then use the FUELS sequential learning approach to design the most efficient series of experiments to rapidly explore composition space for high-performance MPEAs. Candidate alloys were synthesized, characterized, and used to retrain the models, culminating in improved property models and the discovery of novel MPEA systems.

11:10 AM
Data Analytics and Machine Learning to Accelerate Materials Design and Processing Development of High Entropy Alloys: Xuesong Fan[1]; Robert Jones[2]; *Baldur Steingrimsson*[3]; Kwan Yi[4]; Peter Liaw[1]; Sung Yi[2]; [1]University of Tennessee; [2]Portland State University; [3]Imagars LLC; [4]Eastern Kentucky University
This paper presents an innovative framework for application of machine learning to development of high-entropy alloys with desired properties. The nature of multi-principal elements, high mixing entropy, and mutual interactions between elements render these alloys with outstanding mechanical and functional properties, such as high hardness and elastic modulus, superior wear resistance, corrosion and temperature resistance, together with appealing electrical and magnetic properties. We present a framework for predicting the composition, yield strength, material ductility, fatigue, fracture toughness, and creep of high-entropy alloys. For each output property of interest, we identify the corresponding driving factors. These input factors may include the material composition, heat treatment, process, microstructure, temperature, strain rate, environment, and testing mode. We then carry out the prediction through a customized averaging process in the space comprising the input parameters. Discussion on incorporation of physics-based models for improved prediction accuracy and optimization of additive manufacturing processes is also included.

11:30 AM
Development of a Thermodynamic and Mobility Database Using CALPHAD for High Entropy Alloys: Huahai Mao[1]; Qing Chen[1]; *Paul Mason*[2]; [1]Thermo-Calc Software AB; [2]Thermo-Calc Software Inc.
Modeling HEAs using CALPHAD presents unique challenges compared with other alloy systems due to the lack of a single principle element. Here we describe the approach taken in developing the TCHEA thermodynamic database, which contains 26 elements, where almost all underlying binary and over 400 ternary systems have been critically evaluated to capture the composition and temperature dependence, and also the corresponding MOBHEA mobility database. Examples will be given of calculations successfully performed in the interpretation of experimental observations and design of new HEAs, for instance, to predict the phase stability and solid solubility of BCC and FCC, to understand the microstructure evolution, to estimate the density of alloys, to interpret the deformation mechanism associated with the stacking fault energy based on the estimation of energy difference between HCP and FCC , to investigate the oxidation behavior, and to design cemented carbide cutting tools using HEA as the binder phase.

11:50 AM
Assessing the Fidelity of Thermodynamic Predictions for CrFeCoNi-based High Entropy Alloys: *Nicholas Jones*[1]; K Christofidou[1]; E Pickering[2]; H Stone[1]; [1]University of Cambridge; [2]University of Manchester
One of the key challenges currently facing the HEA field is the identification of promising compositions in a time efficient manner. One option is to utilise the CALPHAD method and commercial, HEA specific thermodynamic databases are now available. However, many potential compositions lie outside the assessed ranges of these databases and, therefore, at present, predictions need to be treated with caution. To assess the fidelity of the thermodynamic predictions, here we present the outcomes from a number of systematic studies that have established the phase equilibria in selected quinary and senary CrFeCoNi-based systems. Alloys were homogenised close to their solidus temperatures before undergoing long duration thermal exposures of at least 1000 hours at temperatures between 500 and 1000°C. The resulting microstructures were characterised using advanced electron microscopy, X-ray diffraction and differential thermal analysis. The experimental results will be compared to the corresponding predictions from two different thermodynamic databases.

Fundamental Theory

Monday AM
November 18, 2019

Room: Cobalt
Location: Hyatt at Olive 8

10:40 AM Invited
The Assessment of Local Lattice Strains in Alloys Using Total Scattering: *Lewis Owen*[1]; Nicholas Jones[1]; Howard Stone[1]; Helen Playford[2]; [1]University of Cambridge; [2]ISIS Neutron and Muon Source
Of the four original core principles of the HEA field, the highly strained lattice hypothesis remains one of the least investigated and most misunderstood. One particular problem is the lack of suitable methodologies through which this local effect in alloy systems may be probed and explored. In this work, we will discuss how the total scattering technique, wherein both the Bragg and diffuse scattering data are considered simultaneously, may be used to investigate and assess local strains in alloy systems. Key practical considerations for the successful analysis of local lattice strains using this technique will be discussed, with particular reference to sample preparation, instrumental considerations and data processing effects. Further, common errors in local-strain measurements and their mitigation will be considered, and a proposed methodology for the analysis of local strains using this technique presented and demonstrated using a case example of the exemplar HEA CrMnFeCoNi.

11:10 AM
The Paracrystalline Nature of Lattice Distortion in High Entropy Alloys: *Jian Min Zuo*[1]; Yu-Tsun Shao[1]; Haw-Wen Hsiao[1]; Renliang Yuan[1]; Qun Yang[2]; [1]University of Illinois, Urbana-Champaign; [2]ShanghaiTech University
Severe lattice distortion is suggested for high entropy alloys (HEAs), however, evidence for such effect so far is lacking, and the nature of distortion is yet to be understood. Here, we reveal the distortion in selected fcc and bcc HEAs by direct electron imaging and electron nanodiffraction. Information about crystal symmetry, lattice strain and atomic distortion are data-mined and mapped from many diffraction patterns and atomic resolution images. Application to the HEAs reveals nm-sized mosaic blocks of paracrystals and fractal strain field across nanoscopic to mesoscopic scales. As lattice distortion impedes dislocation motion and contributes to strengthening, results here thus provide critical insights about the complex nature of distortion in HEAs.

11:30 AM
Lattice Distortion of High-entropy Alloys: *Michael Gao*[1]; Zongrui Pei[1]; Mike Widom[2]; Jeffrey Hawk[1]; David Alman[1]; [1]National Energy Technology Laboratory; [2]Carnegie Mellon University
Lattice distortion is one of the four core effects of high entropy alloys first envisioned by Prof. J.W. Yeh, and it plays a crucial role in intrinsic materials properties (physical, mechanical and environmental). This talk first reviews the current understanding of lattice distortion in the high entropy alloys community. The second part of the talk presents our ongoing computational modeling research to predict lattice distortion in a large number of "virtual" single-phase high entropy alloys in the structures of FCC, BCC and HCP using density functional theory. The atomic structures are generated using both special quasi-random structures and hybrid Monte Carlo/molecular dynamics. The effect of atomic position permutation is examined on example alloys. The relation between lattice distortion and electronic structures and elastic properties are discussed. Finally, the impact of lattice distortion on the intrinsic yield strength of materials is presented using continuum model and dislocation theory.

11:50 AM
Cryogenic-temperature Deformation of Boron-doped High-entropy Alloys: Hardening by Short-range Ordering: *Jae Bok Seol*[1]; Jae Wung Bae[2]; Zhiming Li[3]; Won-Seok Ko[4]; Hyoung Seop Kim[2]; [1]National Institute of Nanomaterials Technology, Center for Transformation and Microstructure, POSTECH; [2]Department of Materials Science and Engineering, Center for High Entropy Alloys, POSTECH; [3]Max-Planck-Institut für Eisenforschung GmbH; [4]School of Materials Science and Engineering, University of Ulsan
We report a strategy for improving the cryogenic strength of FCC-structured HEAs through short-range order (SRO), which is driven by soluble boron at the high-entropy grain interiors, not by interfacial boron. Introducing soluble boron into the FCC matrices provided the key benefits, i.e., creation of SROs and increase in SRO degree during cryogenic-temperature deformation, as proved by TEM diffraction and synchrotron XRD. With this new approach, we increased the cryogenic yield strengths of non-equiatomic Fe40Mn40Co10Cr10 (at %) and near-equiatomic NiFeMnCoCr alloys by ~32% to ~1.1 GPa compared to those of boron-free reference materials with similar grain sizes. We will present the main reason causing the advent of such deformation-induced SROs on planar dislocation band structures, which can be successfully visualized by common dark-field TEM conditions. Also, we will introduce a simple experiment to feasibly discern the SRO from the long-range order (LRO) states by use of common TEM method.

Alloy Design and Mechanical Properties I

Monday AM
November 18, 2019

Room: Cyan
Location: Hyatt at Olive 8

10:40 AM Invited
High Temperature Strengthening from High Entropy Precipitates: *An-Chou Yeh*[1]; Yung-Ta Chen[2]; Hideyuki Murakami[3]; Taisuke Sasaki[3]; Kazuhiro Hono[3]; Chen-Wei Li[4]; Koji Kakehi[4]; [1]National Tsing Hua University; [2]National Tsing Hua University/National Institute for Materials Science; [3]National Institute for Materials Science; [4]Tokyo Metropolitan University
This talk will present precipitation strengthening from high entropy phase in a high entropy superalloy (HESA). HESA is a Ni-rich high entropy alloy, which contains high entropy FCC matrix and medium entropy L12 precipitates. With modification of heat treatment process, additional strengthening mechanism can be induced by formation of high entropy precipitates. Detailed microstructural characterization has been conducted, including advanced atom probe tomography. Notably, high temperature tensile properties of high entropy precipitates bearing HESA can surpass not only those of the reported HEAs, but also some advanced superalloys. This work presents a possible template for the design of future high temperature alloys with improved cost-performance.

11:10 AM
Towards the Industrial Application of the AlCoCrFeNi HEA System: *Fevzi Kafexhiu*[1]; Bojan Podgornik[1]; Borut Žužek[1]; Jaka Burja[1]; [1]Institute of Metals and Technology
As in materials science in general, achievement of both high strength and high ductility constitutes a tough challenge in high-entropy alloys too. Problems with poor castability and compositional segregation of HEAs create additional limitations for industrial applications. In order to shed some light on the possibilities of adaptation of the AlCoCrFeNi HEA into large-scale industrial production, primarily, the Thermo-Calc simulations were performed on the chosen HEA system. Further, vacuum induction melting and ingot casting were used to obtain the AlCoCrFeNi HEA – eutectic alloy with a microstructure composed of alternating soft FCC and hard BCC phases. Finally, a comprehensive characterization was carried out on the as-cast- and heat-treated conditions of the AlCoCrFeNi HEA, including the XRF analysis of the longitudinal section, metallographic characterization, thermal analysis, dilatometry, hardness tests, tensile tests, impact toughness tests, tribological tests, as well as creep tests. Mutual correlation of microstructure and properties has been also attempted.

11:30 AM
Microstructure Evolution in CoCrFeMnNi High-entropy Alloy by Localized Shear Deformation: Ryohei Serada[1]; Alok Singh[2]; Ivan Gutierrez-Urrutia[2]; Koich Tsuchiya[2]; *Toshiji Mukai*[1]; [1]Kobe University; [2]National Institute for Materials Science
High entropy alloys (HEAs) have attracted attention due to their superior combination of strength and other mechanical properties as novel multi-component alloys. Understanding the deformation mechanisms in HEAs is important for their application as structural components and/or to improve their mechanical properties. In this study, microstructure evolution in a CoCrFeMnNi HEA was investigated upon localized shear deformation. The HEA was quasi-statically and dynamically deformed at room temperature by a shear experiment. Microctructure characterization by SEM/EBSD revealed formation of shear band near the localized shear region. Finite element analysis in a double shear specimen model with the similar dimensions suggested that a certain amount of equivalent plastic strain promoted the formation of the localized shear band. EBSD analysis indicated that the shear bands were subdivided by nano-twins, and an early stage of shear localization in the HEA involved the formation of twin/matrix lamellae aligned along the shear direction.

11:50 AM
Effect of Pre-strain on the Aging Response of Non-equimolar AlCoCrFeNiTi High Entropy Alloy: *Vickey Nandal*[1]; R Sarvesha[2]; Sudhanshu Singh[2]; Jayant Jain[1]; Suresh Neelakantan[1]; [1]IIT Delhi; [2]IIT Kanpur
High entropy alloys (HEAs), have attracted considerable attention of materials scientists in the past decade due to their excellent properties such as wear resistance, high temperature strength, thermal stability and potential applications in aerospace industries. In the present work, the aging response of the Al0.2Co1.5CrFeNi1.5Ti0.3 HEA with and without pre-strain has been studied. Microstructural examination reveals two distinct morphologies (cellular and spherical) of ' precipitate in both the cases. It has been observed that the amount of pre-strain has a strong influence on the fraction of these precipitate morphologies. In addition, the pre-strained HEA attains the peak aged condition at a much shorter aging time, as well an increase in the hardness values have been observed. The observed differences in the microstructural and hardness values, due to pre-strain, can be attributed to the differences in the kinetics of precipitation and their characteristics.

Alloy Design and Computational Modeling III

Monday PM
November 18, 2019

Room: Azure
Location: Hyatt at Olive 8

1:30 PM Invited
Searching of High Entropy Alloys Aided by High Throughput Calculation: *Fan Zhang*[1]; Chuan Zhang[1]; Weisheng Cao[1]; Shuanglin Chen[1]; [1]CompuTherm LLC
The search of high entropy alloys (HEAs) has become the focus of many researchers due to the promising properties of these alloys and their potential applications in various fields. Different from the traditional alloys, design of HEAs involves the use of multiple principal components. Since huge multi-dimensional composition space needs to be explored, finding the right HEA compositions becomes even more challenging. Traditional trial-and-error approach is no longer feasible due to the tremendous amount of experimental work. In this presentation, we will demonstrate that the CALPHAD method can be used as an effective approach in aiding HEA design. High-throughput calculation can be performed in the multi-dimensional composition spaces to accelerate the search of potential HEAs with user-defined optimal properties. We will also demonstrate that phase-stability diagrams coupled with density contours in the composition-temperature space provides helpful guidelines for the design of low-density HEAs with desirable combinations of properties.

2:00 PM
Enabling FAIR Data Principles for High-throughput Materials Science and Engineering: *Zachary Trautt*[1]; Brian DeCost[1]; Jason Hattrick-Simpers[1]; [1]National Institute of Standards and Technology
The large parameter space of high entropy alloys elevates the importance of high-throughput experimental methods and machine actionable data management and sharing. The "FAIR Guiding Principles for scientific data management and stewardship" [https://doi.org/10.1038/sdata.2016.18] define a set of practices governing the Findability, Accessibility, Interoperability, and Reusability of scientific data. This talk will summarize efforts at NIST and within the Materials Genome Initiative, to enable the use of FAIR Data Principles within high-throughput experimental methods throughout the data lifecycle.

2:20 PM
Multi-scale Framework for Predicting Mechanical Properties in High Entropy Alloys: Pratik Dholabhai[1]; Mike Grant[1]; Krithika Iyer[2]; Tolga Tasdizen[2]; Yongfeng Zhang[3]; *Jeffery Aguiar*[3]; [1]Rochester Institute of Technology; [2]University of Utah; [3]Idaho National Laboratory
High-entropy alloys (HEAs) are an emerging class of materials consisting of multiple principal elements. Due to entropic effects, HEAs are highly stable at elevated temperature with promising hardness, tensile strength, and corrosion resistance for potential structural applications in extreme environments. As there are an unlimited number of possible HEA compositions, discovery efforts benefit from a multifaceted data analytics approach, amendable to deep and machine learning. In this work, we focus on exploring and connecting near-equimolar compositions comprised of the main constituent elements Fe, Cr, Ni, Al, Si, and Cu with predicted mechanical properties and diffusion coefficients to salient material descriptors. Results are compiled to inform and validate multi-scale atomistic modeling to enable prediction of HEA compositions that exhibit high strength. Ultimately, this information will be used in the development of a statistically driven approach to differentiate compositions of interest during alloy design and testing for nuclear applications.

2:40 PM
Integrated Computational Materials Engineering (ICME) Design of High Performance Copmlex Concentrated Alloys: Marie Thomas[1]; Ricardo Komai[1]; *Chris Kantner*[1]; David Smathers[2]; Cameron McNamara[2]; [1]QuesTek Innovations; [2]H. C. Starck Inc.
Complex Concentrated Alloys (CCA), particularly those containing refractory elements, have the potential to surpass baseline alloy performance in both aero- and land-based high temperature applications. Since the number of CCA compositions is nearly infinite, a predictive methodology is necessary towards the optimization of a CCA. Integrated Computational Materials Engineering (ICME) tools are being developed and employed for the design of a low density, oxidation-resistant refractory CCA.A high throughput CALPHAD-informed approach has been implemented to design novel refractory CCAs (selected from 17 elements) with a large single-phase BCC region, narrow solidification window, high solidus temperature, low density and good oxidation resistance. The design constraints predicted a family of Nb-based alloys and examined the effect of Al additions. A review of the ICME design approach of complex concentrated alloys will be covered leading to the production of alloy prototypes for validation of the approach.

3:00 PM
Study of Oxidation Mechanisms in Refractory MoWTaTiZr HEA using Periodic DFT and Atomistic Thermodynamic Modelling: *Eric Osei-Agyemang*[1]; Ganesh Balasubramanian[1]; [1]Lehigh University
High entropy alloys (HEA) based on refractory elements may achieve higher temperature operations with superior creep strength compared to Ni-based superalloys. At elevated temperatures, Mo based HEAs have been observed to exhibit good thermal and mechanical properties. Recently, a refractory Mo-W-Ta-Ti-Zr HEA was observed to exhibit greatly enhanced modulus of elasticity (3x at 300K) over near atomic cases and with higher moduli above 500K over commercial alloys (2.3x at 2000K). The special quasi-random structures (SQS) model was used to generate random structures in combination with DFT to study oxidation mechanisms in Mo-W-Ta-Ti-Zr HEA. The best representative random structure is used to create different surfaces. The stable facets are subsequently reacted with oxygen to gain a detailed understanding on surface oxidation processes. A link between theoretical and experimental conditions are established by using a thermodynamic approach to establish different temperature and pressure regimes on the oxidized surfaces at different oxygen coverages.

3:20 PM Break

Alloy Design and Computational Modeling IV

Monday PM
November 18, 2019

Room: Cobalt
Location: Hyatt at Olive 8

1:30 PM Invited
Engineering Atomic-level Complexity in High Entropy and Complex Concentrated Alloys: Hyun Seok Oh[1]; Sang Jun Kim[1]; Khorgolkhuu Odbadrakh[2]; Wook Ha Ryu[1]; Kook Noh Yoon[1]; Sai Mu[2]; Fritz Körmann[3]; Yuji Ikeda[3]; Cemal Cem Tasan[4]; Dierk Raabe[3]; Takeshi Egami[2]; *Eun Soo Park*[1]; [1]Seoul National University; [2]Oak Ridge National Laboratory; [3]Max-Planck Institut für Eisenforschung GmbH; [4]Massachussetts Institute of Technology
Quantitative and well targeted design of modern alloys is extremely challenging due to their immense compositional space. When considering only 50 elements for compositional blending the number of possible alloys is practically infinite as is the associated unexplored property realm. Here, we present a simple property-targeted quantitative design approach for atomic-level complexity in high-entropy and complex concentrated alloys, based on quantum-mechanically derived atomic-level pressure approximation. It allows identification of the best suited element mix for high solid-solution strengthening using the simple electronegativity difference among the constituent elements. This approach can be used for designing alloys with customized properties, such as a simple binary NiV solid solution whose yield strength exceeds that of the Cantor high entropy alloy by nearly a factor of two. This study provides general design rules that enable effective utilization of atomic-level information to reduce the immense degrees of freedom in compositional space without sacrificing physics-related plausibility.

2:00 PM
CALPHAD-based Informatics Tools for High-entropy Alloy Design: *Chuan Zhang*[1]; Rui Feng[2]; Zongrui Pei[3]; Weisheng Cao[1]; Fan Zhang[1]; Michael C. Gao[3]; Peter K. Liaw[2]; [1]CompuTherm LLC; [2]University of Tennessee; [3]National Energy Technology Laboratory
High-entropy alloys (HEAs) attract tremendous interest in the development of new metallic materials with improved property combinations. The vastness in HEA compositional space provides us both opportunities and challenges. To accelerate the HEA development by tuning the structure-property relationship, the accurate and efficient prediction of microstructures of a material as a function of temperature, and composition is essential. As the only method to obtain multi-component phase diagrams with enough accuracy for practical applications, the CALPHAD approach is widely used in the design and development of HEAs. Recently, the CALPHAD-based high-throughput tools are also developed to efficiently explore the entire compositional space and screen potential HEAs with desired microstructures. In the present work, the application of the CALPHAD-based informatics tool for the design of high-performance Al-Cr-Fe-Mn-Ti alloys with object-oriented design strategies is presented. Experimental verifications and first-principles calculations are also carried to verify CALPHAD prediction.

2:20 PM
Determination of High-throughput Computational Modeling Approaches on Design of Al-Cr-Co-Fe-Ni Quinary High-entropy Alloys (HEAs): Songge Yang[1]; Mohammad Asadikiya[1]; Vadym Drozd[2]; *Yu Zhong*[1]; [1]Worcester Polytechnic Institute; [2]Florida International University
The high-throughput computational modeling approaches is becoming a powerful tool for accelerating the design of novel HEAs. In this paper, the combination of High-throughput calculation of phase diagram (HT-CALPHAD) and High-throughput Density functional theory (HT-DFT) is introduced for the design of Al-Cr-Co-Ni-Fe alloys. In the first part, the generation of alloying compositions of this system is based the valence electron concentration (VEC) which is an important physical factor for phase formation. More than 3000 compositions are generated for HT-CALPHAD calculations. This work also developed a screening process which can quickly screen out good compositions based on the phase stability, density, solidus temperatures, temperature ranges and cost etc. In the second part, the screened out candidates would be selected to generate the Special Quasi-random Structures (SQS) for HT-DFT calculation. The total energy and elastic properties of the SQS structures are predicted. The final candidates would be fabricated for further testing verification.

2:40 PM
Machine-learning Phase Prediction of High-entropy Alloys: Wenjiang Huang[1]; Pedro Martin[1]; *Houlong Zhuang*[1]; [1]Arizona State University
Excellent properties of high-entropy alloys (HEAs) largely depend on the selection among three phases: solid solution (SS), intermetallic compound (IM), and mixed SS and IM (SS+IM). Accurate phase prediction is therefore crucial for guiding the selection of a combination of elements to form a HEA with desirable properties. The phase selection is correlated with elemental features such as valence electron concentration and the formation enthalpy, leading to a set of parametric phase-selection rules. Here we employ machine learning (ML) algorithms to efficiently explore phase selection rules using a comprehensive experimental dataset consisting of 401 different HEAs including 174 SS, 54 IM, and 173 SS+IM phases. We adopt three different ML algorithms: K-nearest neighbors (KNN), support vector machine (SVM), and artificial neural network (ANN). Our work provides an alternative route of computational design of HEAs, which is also applicable to accelerate the discovery of other metal alloys for modernengineering applications.

3:00 PM
High Entropy Alloy Design Using Multiscale Modeling and Machine Learning Based High-throughput Computing: *Anssi Laukkanen*[1]; Tomi Suhonen[1]; Matti Lindroos[1]; Tatu Pinomaa[1]; Tom Andersson[1]; [1]VTT Technical Research Center of Finland
High entropy alloys (HEAs) promise a vast design base even with respect to basic alloy chemistry. This is extended further considering the often multiphase microstructure with its added characteristics and additional strengthening mechanisms. To explore and exploit this design space, respective design and discovery methods need to be introduced. The traditional approaches for HEA design are simple but crude, they are not expected to be able to discover the HEAs which in many applications could become the next generation materials for extreme conditions. To that effect, we introduce a workflow which merges both physics-based materials modeling in the atomistic and microstructural regimes and machine learning for optimization and discovery. Case studies are presented sampling the alloy space and optimizing the findings with respect to different property and performance metrics. Links to experimental work synthesizing the materials are included.

3:20 PM Break

Mechanical Properties II

Monday PM
November 18, 2019

Room: Cyan
Location: Hyatt at Olive 8

1:30 PM Invited
Single-crystal Mechanical Properties of Equiatomic CrMnFeCoNi High-entropy Alloy and Its Derivative Equiatomic Quaternary and Ternary Medium-entropy Alloys: *Haruyuki Inui*[1]; Kyosuke Kishida[1]; Koudai Niitsu[1]; Easo George[2]; [1]Kyoto University; [2]University of Tennessee
The plastic deformation behavior of single crystals of the FCC equatomic CrMnFeCoNi high-entropy alloy and its derivative quaternary and ternary medium-entropy alloys has been investigated in a temperature range of 10-1273 K. Deformation occurs via slip of the {111}<110> system exclusively in the whole temperature range for all alloys investigated. The CRSS values increase with decreasing temperature, especially below room temperature, so that the concept of 'stress equivalence' is obeyed. This is a clear indication that the strength of these alloys should be described by a mechanism based on solid-solution hardening. The CRSS values at 10 K seems to be well scaled by the mean-square atomic displacement from the regular FCC lattice points (calculated based on density-functional theory). Deformation twinning occurs in later stages of deformation at low temperatures below room temperature in many of these alloys. The correlation between twinning stress and the stacking-fault energy will be discussed.

2:00 PM
Orientation and Interstitial Content Dependence of Twinning in Medium and High-entropy Alloys in Comparison with Conventional Steel Single Crystals: Sezer Picak[1]; Demircan Canadinc[2]; Yuri I. Chumlyakov[3]; *Ibrahim Karaman*[1]; [1]Texas A&M University; [2]Koç University; [3] Tomsk State University, Siberian Physical Technical Institute
In this study, we investigate the role of configurational entropy on the room temperature tensile deformation response of single crystalline medium/high entropy alloys (M/HEAs), in particular in terms of activation of deformation twinning with and without interstitial carbon addition. In addition, we compare the strain hardening behavior and ductility of these materials with that of conventional steel single crystals. TEM observations revealed that two deformation mechanisms govern the strain hardening in M/HEAs, namely planar slip and twinning. It was observed that nanotwin formation was prevalent at the early stages of deformationin in almost all of the above M/HEAs, significantly enhancing the ductility, while the higher strength levels are associated with the high volume fraction of thin twins. Overall, it was concluded that higher configurational entropy does not neccessarialy warrant improved mechanical properties, as the mechanical properties of NiCoCr, SS316 and Hadfield steels are comparable or better than their HEAs counterparts.

2:20 PM
Nanomechanical Behavior of Body-centered Cubic VNbTaMoW Alloy: *Hicham Zaid*[1]; Jacob Stremfel[1]; Koichi Tanaka[1]; Angel Aleman[1]; Jenn-Ming Yang[1]; Suneel Kodambaka[1]; [1]University of California Los Angeles
We report on microstructural and mechanical characterization of a V0.2Nb0.2Mo0.2Ta0.2W0.2 bulk alloy. X-ray diffraction spectra revealed multiple reflections corresponding to a single-phase, body-centered cubic polycrystal with a lattice constant of 0.319 ± 0.001 nm. Nanoindentation tests yielded hardness and reduced elastic modulus values of 9 ± 1.4 GPa and 207 ± 19 GPa, respectively. In situ scanning electron microscopy based uniaxial compression tests conducted at room-temperature on cylindrical pillars of sizes d between 0.3 μm and 1 μm revealed that all the pillars undergo plastic deformation. We find that the yield strengths of the pillars increase with decreasing d from 3.3 GPa at d = 1 μm to 9.0 GPa at d = 0.3 μm. We attribute the observed behavior to size-dependent variations in displacement burst frequency and slip events. We expect that our results provide new insights into the nanomechanical response of body-centered cubic alloys.

2:40 PM
The Role of Twinning and HCP Phase Transformation in the Deformation of Single Crystalline High -and Medium Entropy Alloys: *Sezer Picak*[1]; Yuri I. Chumlyakov[2]; Ibrahim Karaman[1]; [1]Texas A&M University; [2]Siberian Physical Technical Institute, Tomsk State University
Tensile deformation response of Fe40Mn40Co10Cr10 high entropy alloy (HEA) and equiatomic NiCoCr medium entropy alloy (MEA) single crystals were investigated at room temperature. TEM observations revealed that up to four deformation mechanisms govern the strain hardening in these alloys, depending on the crystallographic orientation of tensile loading: planar slip, dislocation substructure controlling the nucleation of twin/hcp lamellas, twinning, and hcp phase transformation. Consequently, the interaction of these mechanisms during deformation leads to a higher work hardening rate as compared to the orientations without twinning and phase transformation. Moreover, NiCoCr single crystals attain higher fracture strains and exhibit higher ultimate tensile strengths as compared to Fe40Mn40Co10Cr10. The TEM analysis showed that nanotwins and hcp lamellas are more prevalent at the early stages of deformation in the MEA, significantly enhancing the ductility, while the higher strength levels are associated with the high volume fraction of twins/hcp lamellas with relatively small thickness.

3:00 PM
Synthesis and Mechanical Characterisation of a Single-phase bcc High-entropy Alloy: *Tim Lienig*[1]; Michael Feuerbacher[1]; Carsten Thomas[1]; [1]Forschungszentrum Juelich
In-depth understanding of structure-property relations of High-Entropy Alloys (HEAs) requires the investigation high-quality single-phase, preferably single-crystalline samples. Single-crystalline samples allow the determination of intrinsic materials properties without the influence of secondary phases or grain boundaries. We report on the synthesis of the single-phase equiatomic bcc Ti-V-Zr-Nb-Hf HEA and our advancements in the growth of a single-crystal of this material. This bcc HEA is of special interest, since it exhibits a considerably lower melting point, compared to the Senkov alloy. Poly-crystalline samples are prepared from high-purity elements by means of arc- and levitation melting and a subsequent heat treatment. Single-crystals are grown by means of the Bridgman technique. These well-defined materials are employed for the characterisation of mechanical properties and plastic deformation behaviour of the bcc HEA. By incremental testing, e.g. stress relaxations, strain-rate changes and temperature-cycling, thermodynamic activation parameters of the plastic deformation mechanism are determined.

3:20 PM Break

Computational Modeling I

Monday PM
November 18, 2019
Room: Azure
Location: Hyatt at Olive 8

3:50 PM
Crystal Plasticity in the Role of Performance Evaluation Tool in the Multiscale Design of High Entropy Alloys: *Matti Lindroos*[1]; Anssi Laukkanen[1]; Tom Andersson[1]; Tatu Pinomaa[1]; [1]VTT Research Centre of Finland
High throughput multiscale computing has been a favored choice to seek novel material solutions in the vast design space of high entropy alloys. Workflows can be established from chemistry to process and structure with the aim to produce desired properties to achieve enhanced material performance. The complexity of High Entropy Alloy (HEA) microstructures, enveloping multiphase structure and a variety of important strengthening mechanisms, requires an effective method to be capable of modeling time and length scales that can describe deformation, strengthening and failure of HEAs in the variety of applications. To address this requirement, crystal plasticity models are formulated describing microstructure level deformation behavior of HEAs. Modeling results demonstrate the complex material behavior of additively manufactured HEAs, such as phase transformations, deformation twinning, and identifying the sources of failure. The important role of crystal plasticity is established and demonstrated in the ICME workflows.

4:10 PM
Molecular Dynamic Simulations on the Mechanical Properties of CoCrFeMnNi High Entropy Alloy and the Equimolar Alloys in Its Sub-system: *Yinkai Lei*[1]; Michael Gao[1]; Youhai Wen[1]; [1]US Department of Energy National Energy Technology Laboratory
The mechanical properties of FCC CoCrFeMnNi high entropy alloy and the equimolar alloys in its sub-system are investigated by molecular dynamic simulations using a recently developed Modified-Embedded-Atom-Method potential. Four effects on the mechanical properties have been investigated, i.e. entropy effect, temperature effect, strain rate effect and grain size effect. Typical deformation mechanisms under different conditions have also been analyzed. These atomistic scale simulations provide basic understanding on the detailed deformation mechanisms in Co-Cr-Fe-Mn-Ni alloy system and how they affect the mechanical properties. The atomic structures generated from molecular dynamics are compared with those from first-principles density functional theory and hybrid Monte Carlo/ab initio molecular dynamics simulations.

4:30 PM
Artificial Intelligence for Predicting Phase Stability on High Entropy Alloys: Anus Manzoor[1]; *Dilpuneet Aidhy*[1]; [1]University of Wyoming
Using a combination of artificial intelligence (AI) and density functional theory (DFT), we elucidate the contributions of various entropies, i.e., vibrational, electronic and configurational towards predicting the phase stability of HEAs. We show that the entropy contributions could be quantitatively comparable to the mixing enthalpy; as a result, including various entropy contributions is important for correctly predicting the alloy phase stability. We also show that while the configurational entropy always favors phase stability, the role of vibrational entropy is not predictable. The configurational and vibrational entropies can either compete to destabilize or can collectively contribute to stabilize the solid solutions. As a result, even those systems that have negative mixing enthalpy can show phase instability; conversely, systems with positive mixing enthalpy can have stable phases due to the vibrational entropy contributions. Finally, we discuss our AI database that allows circumventing expensive DFT calculations towards predicting the phase stability of alloys.

4:50 PM
Compositional Design, Elongation and Dislocation Mobility in HEA Alloys: *Ridwan Sakidja*[1]; Wai-Yim Ching[2]; [1]Missouri State University; [2]University of Missouri - Kansas City
We evaluated the correlation between the computational design and the elongation as well as the dislocation mobility on a variety of HEA alloys based on external materials databases and developed the EAM potentials for a selected number of multi-component systems. The source of external materials database primarily is used on the reference from Data in Brief (2018, 2664-2678) by S.Gorsse, M.H.Nguyen, O.N.Senkov, and D.B.Miracle, combined with the secondary references to obtain the stress-strain curves (if available). We then sampled a number of multi composition systems that represent various degree of elongation and parameterized the necessary EAM interatomic potentials to observe the effect of the compositional variation toward the dislocation mobilities. The roles of the local chemical bonding within the structures are also discussed.

Ceramic HEAs II

Monday PM
November 18, 2019

Room: Cobalt
Location: Hyatt at Olive 8

3:50 PM
Selective Oxidation in a High Entropy Carbide Ultra-high Temperature Ceramic (UHTC): *Lavina Backman*[1]; Elizabeth Opila[1]; [1]University of Virginia
High entropy carbides are a novel class of UHTCs. Thermodynamic calculations using FactSage software and databases were performed for oxidation reactions of the constituent carbides in an equimolar, five-component carbide, (HfZrTiTaNb)C. The relative stability of the oxide phases formed from the constituent carbides and from binary carbide solutions were used to investigate selective oxidation. This analysis was extended to ternary and higher order alloys and carbides. The thermodynamic predictions were compared to the experimentally determined oxidation behavior of the five-component carbide at 1500°C-1700°C oxidized in 1%O_2. Experimental results verified that Group IV oxides dominated in the observed oxide scale, resulting in a Group V enriched substrate. It was concluded that, given any high entropy material, even a slight relative favorability for a given oxide formation reaction will result in selective oxidation, reducing the configurational entropy in the remaining material.

4:10 PM
Synthesis and Phase Stability of High-entropy Nitrides and Carbonitrides: *Olivia Dippo*[1]; Tyler Harrington[1]; Neda Mesgarzadeh[1]; Mahika Lunker[1]; Kenneth Vecchio[1]; [1]University of California San Diego
Ultra-high temperature ceramics (UHTCs) are critical materials for aerospace applications, such as on leading edges of supersonic aircraft. UHTCs such as transition metal carbides and nitrides have inherently favorable properties, as they are amongst some of the highest melting temperature materials. High-entropy versions of these UHTC compounds have the potential to elevate their high-temperature phase stability due to entropic stabilization. High-entropy transition metal nitrides and carbonitrides were experimentally fabricated in bulk sample form. Powder processing, bulk material densification, and single-phase character of resulting high-entropy ceramic materials were studied. Phase determination of various compositions was done using X-ray diffraction, and chemical homogeneity was characterized using energy dispersive X-ray spectroscopy. This work demonstrates the ability to continue to expand the field of high entropy alloys to include single-phase high entropy, ultra-high temperature nitrides and carbonitrides.

4:30 PM
Potential Chemical Selection Guideline for High-entropy Ceramics: *Kuo-Pin Tseng*[1]; Ming-Hung Tsai[2]; Waltraud Kriven[1]; [1]University of Illinois Urbana Champaign; [2]National Chung Hsing University
Two unique systems of high-entropy lanthanide oxides (HELO) had been synthesized by the organic-inorganic steric entrapment method to explore the chemical selection rules for solid solution phase evolution under ambient conditions. In contrast to high-entropy alloys, the metallic cations are fitted in the polyhedral sites surrounding by anions. The cation radii vary as a function of oxidation states and coordination numbers. In our HELO systems, we fixed four trivalent cations with similar radii and the fifth cation with larger size. As the radius increases, the octahedral sites become unstable and trigger the existence of a secondary phase. In the second system, a HELO was designed with smaller-sized cations as the variable. A model based on enthalpy, entropy, oxidation energies, and shear modulus was proposed. This result introduces a potential chemical selection guideline for designing structurally stable, high-entropy ceramics.

4:50 PM
Microstructure and Mechanical Properties of High Entropy Ceramic/High Entropy Alloys Composite High Entropy Material: *Zhanjiang Li*[1]; Pinqiang Dai[1]; [1]Fujian University of Technology
The (ZrTaMoTiW)C/FeCoCrNiAl composite high entropy material were fabricated by mechanical alloying and spark plasma sintering. It was found that the double-phase structured solid solution of face-centered cubic and hexagonal be obtained after 20 h milling and spark plasma sintering at 1400.With respect to the sinterability of high entropy ceramics, the addition of FeCoCrNiAl HEA can reduce sintering temperature of high entropy ceramics and the oxide impurities during sintering to enhance the sintered density. Comparing with the traditional sintering aid Co, HEA can decrease the solubility of high entropy ceramics in HEA and the solid-liquid surface energy to inhibit the grain growth. Moreover, an optimized combination mechanical properties was obtained for the (ZrTaMoTiW)C -6 wt.% FeCoCrNiAl composite high entropy material, including the relative density of 97.75±1%, the Vickers hardness of 1974.32±20HV10.

Alloy Design and Mechanical Properties II

Monday PM
November 18, 2019

Room: Cyan
Location: Hyatt at Olive 8

3:50 PM
High Speed Nanoindentation Property Mapping in Dual Phase Al_xFeCrNiMn at Elevated Temperatures: *Eric Hintsala*[1]; Youxing Chen[2]; Jacob Noble[1]; Nathan Mara[3]; Douglas Stauffer[1]; [1]Bruker Nano Surfaces; [2]University of North Carolina Charlotte; [3]University of Minnesota
There is interest in developing dual phase HEAs for reactor applications due to potentially high defect tolerance. Given the rigorous mechanical evaluation required for developing high temperature structural materials and the number of candidate HEAs, high throughput techniques are valuable. Using nanoindentation not only gives high spatial resolution of mechanical properties, but requires relatively little sample preparation versus the amount of data that can be generated. This is demonstrated in this study, where three compositions of dual phase Al_xFeCrNiMn, with x = 0, 0.3, & 1, are explored from room temperature to 400°C. Hardness and modulus values are assigned to individual phases through correlated EBSD/EDS to determine their relative temperature stability with temperature. Measurements are all made in a high vacuum chamber to reduce the role of oxide formation on measured properties. These measurements serve as a foundation upon which irradiation effects can be added.

4:10 PM
Rapid Mechanical Screening of High Entropy Alloys: Application of Spherical Punch Testing (SPT) and Spherical Indentation on Ti-V-Cr-Nb-Mo HEAs: *Ali Khosravani*[1]; Nicolas Leclerc[1]; Sepideh Hashemi[1]; Daniel Sievers[2]; Daniel Miracle[3]; Surya Kalidindi[1]; [1]Georgia Institute of Technology; [2]The Boeing Company; [3]Air Force Research Laboratory
In newly developed high entropy alloys, fast exploration of mechanical properties plays an important role in speeding up the optimization process for composition and thermo-mechanical treatments. In this work we present novel approaches for mechanical property evaluations using spherical punch tests (SPT) and spherical indentations. The former were designed to assess the ductility of newly developed Ti-V-Cr-Nb-Mo HEAs from small volume of material, while the latter are used to provide information on the grain-scale elastic and plastic properties as a function of alloy compositions. In this study, four high entropy alloys, Ti-20V-20Cr-20Nb-20Mo, Ti-25V-25Cr-15Nb-10Mo, Ti-23V-19Cr-16Nb-13Mo, and Ti-20V-25Cr-10Nb-5Mo, were studied using these methods. In addition to understanding the effects of Nb and Mo elements, SPT and nanoindentation measurements were also extended to ternary (Ti-33V-33Cr), and quaternary (Ti-25V-25Cr-25Nb) alloys. The results of this study establish the viability of the recently developed mechanical characterization methods in accelerating HEA development.

4:30 PM
Exploration of Compositionally Complex Al-Li-Mg-Zn Alloys, Including Discovery of a Four-component Icosahedral Quasicrystal: *Patrick Conway*[1]; Michael Ferry[2]; Kevin Laws[2]; [1]Jönköping University; [2]UNSW
With the aim of developing a single-phase light-weight HEA (LWHEA), the quaternary Al-Li-Mg-Zn alloy system is investigated with the initial selection of elements based on typical HEA formation guidelines. Beginning with an equiatomic four-component composition, AlLiMgZn, and systematically altering elemental concentrations revealed that the Mg-rich region of this quaternary space would be most promising for producing a single-phase solid solution LWHEA. Alloy compositions were refined by replicating the compositions of individual phases within the as-cast microstructure in a series of Mg-rich quaternary alloys, thereby effectively limiting the number of iterative steps and associated processing required to reach a single-phase alloy composition. Three crystal structures were identified in different compositional regions, consisting of hexagonal, monoclinic, and icosahedral quasicrystal. The underlying origin of the resultant multicomponent crystal structures and structural ordering are explored, showing a strong correlation to the electronic structure in the formation of the quasicrystal.

4:50 PM
Material Design and Process Development for Lightweight High Entropy Alloys and Composites: Xuejun Huang[1]; Jiashi Miao[1]; *Alan Luo*[1]; [1]The Ohio State University
High entropy alloys (HEAs) are a new class of materials consisting of multiple principal elements, and can offer exceptional physical and mechanical properties. CALculation of PHAse Diagrams (CALPHAD) modeling was used to explore and design lightweight AlCrTiV-based HEAs. The high hardness and high elastic modulus of these lightweight HEAs as well as their compatibility with metals/alloys make them excellent reinforcements in metal matrix composites (MMCs). Al-based MMCs reinforced with AlCrTiV-based HEA particles were prepared using mechanical alloying and powder metallurgy manufacturing techniques. Heat treatments were conducted based on CALPHAD modeling results. Advanced characterization techniques were used to identify phases and validate CALPHAD calculations for AlCrTiV-based HEAs and Al/AlCrTiV MMCs.

Tuesday Plenary

Tuesday AM
November 19, 2019

Room: Ballroom ABC
Location: Hyatt at Olive 8

8:00 AM Plenary
High Entropy Alloys Based on NiCoFeAlxTiy Hardening with Multicomponent Intermetallic Nanoparticles: Tao Yang[1]; *Chain Tsuan Liu*[1]; [1]City University of Hong Kong
This paper summarizes our recent work on the study of microstructures and mechanical properties of high-entropy alloys (HEAs) based on NiCoFeAlxTiy. The precipitation of L12-type multi-component nanoparticles strongly enhances the strength of these HEAs at ambient and cryogenic temperatures. The tensile ductility of these HEAs depends on particle sizes, heat treatments, and alloy compositions. A careful control of the precipitation reaction results in a high tensile strength more than 1.5 GPa while still retaining an extraordinary tensile ductility of 50% at room temperature. On the other hand, these precipitation-hardened HEAs exhibit a serious of embrittlement at certain elevated temperatures. Our study reveals that the mid-temperature embrittlement can be alleviated by control of the precipitation reaction on grain boundaries. A brief discussion of the possible development of new high-temperature materials will be also discussed.

8:45 AM Question and Answer Period

8:55 AM Break

Alloy Design and Environmental Resistance I

Tuesday AM
November 19, 2019

Room: Azure
Location: Hyatt at Olive 8

9:00 AM Keynote
Environmental Degradation of Multiple Principle Element Alloys: *John Scully*[1]; Angela Gerard[1]; Bi-Cheng Zhou[1]; Prasanna Balachandran[1]; Gerald Frankel[2]; Jenifer Locke[2]; Pin Lu[3]; James Saal[3]; [1]University of Virginia; [2]Ohio State University; [3]Questek Innovations LLC
Multiple principle element alloys (MPEAs) are emerging materials that have recently attracted great interest due to their many degrees of freedom in alloy design and synthesis leading to potentially attractive properties. Many unique or even heretofore unobtainable properties have been reported including resistance to various forms of degradation in harsh environments. These include promising aqueous corrosion behavior, improved oxidation resistance in high and intermediate temperature atmospheres, irradiation resistance as well as possible resistance to environmental assisted cracking. Mechanisms by which MPEAs afford excellent resistance to each of these forms of degradation are discussed. One commonality during pitting and environmental assisted cracking, which both involve film rupture repassivation events, is the rapid formation of unique protective oxides. Selected protective oxide characteristics and attributes are discussed.

9:30 AM
In vitro Biocompatibility of Novel High Entropy Alloys for Biomedical Applications: *Brandon Wagner*[1]; Olivia Chang[1]; Chanho Lee[2]; Xuesong Fan[2]; James Brechtl[3]; Peter Liaw[2]; Miqin Zhang[1]; [1]University of Washington; [2]University of Tennessee; [3] University of Tennessee
Typical biometallic implants, such as stainless steel (SS), titanium (Ti) alloys, and cobalt-chromium (Co-Cr) alloys, are limited by a high young's modulus which leads to stress shielding followed by osteopenia. Furthermore, inadequate corrosion-wear resistance results in inflammatory responses. Novel NbTaTiV and NbTaTiVZr high entropy alloys (HEAs) possessing a low young's modulus and superior corrosion-wear resistance were developed by vacuum arc-melting followed by thermal treatment. Biocompatibility of the HEAs was evaluated by investigating the cell morphology and cytotoxicity of HFF fibroblasts and MG-63 osteoblast-like cells in vitro. The cells cultured on HEAs demonstrated similar cell morphology and improved cell viability to SS and Ti alloys. The HEAs exhibited decreased corrosion potential and corrosion current density compared to SS and Ti alloy, indicating enhanced corrosion resistance. In this talk, the potential of NbTaTiV and NbTaTiVZr HEAs as a bone regenerative implant is discussed.

9:50 AM
Alloying Effects on Mechanical Properties of CoCrFeNi-based γ'-Strengthened Multi-principal Element Alloys for Elevated Temperature Applications: *Akane Suzuki*[1]; Shenyan Huang[1]; Douglas Konitzer[2]; [1]GE Research; [2]GE Aviation
Microstructure, phase stability, tensile properties, creep and oxidation resistance of CoCrFeNi-based multi-principal element alloys were explored to understand alloying effects and to assess advantages against Ni-based superalloys. Alloys containing combinations of γ'-Ni_3(Al,Ti) formers (Al and/or Ti) and a refractory element (Nb, Mo or Ta) to form additional strengthening precipitates were prepared and hot rolled to a sheet form, followed by solution and precipitation hardening treatments. Tensile and creep tests at 760 and 871°C showed presence of the γ' precipitates is the primary contributor. Laves and σ phase precipitates in alloys containing Nb and Mo, respectively, are useful in suppressing formation and coalescence of cavities along grain boundaries during creep deformation. Identifying alloy compositions that raise the γ' solvus without lowering the solidus while forming stable, fine grain boundary precipitates is the key for enhancing high temperature mechanical properties. The measured properties will be discussed in comparison with conventional wrought superalloys.

10:10 AM Break

Functional Properties I

Tuesday AM
November 19, 2019

Room: Cobalt
Location: Hyatt at Olive 8

9:00 AM Keynote
High-entropy Functional Materials: *Michael Gao*[1]; Daniel Miracle[2]; Yu Zhong[3]; David Maurice[1]; Jeffrey Hawk[1]; [1]National Energy Technology Laboratory; [2]Air Force Research Laboratory; [3]Worcester Polytechnic Institute
While most papers on high-entropy alloys (HEAs) focus on the microstructure and mechanical properties for structural materials applications, there has been growing interest in developing high-entropy functional materials. This presentation will provide a brief, timely review on select functional properties of HEAs, including soft magnetic, magnetocaloric, physical, thermoelectric, superconducting, hydrogen storage, catalyst, and (anti-wear, bond, thermal barrier) coatings. Comparisons of functional properties between HEAs and conventional low- and medium-entropy materials will be provided. Extending the HEA concept to a wide range of materials such as intermetallics, ceramics (oxides, carbides, nitrides, borides), and semiconductors through the iso-structural design approach will be discussed. Perspectives will be offered in designing high-performance high-entropy functional materials integrating high-throughput experiments and computational modeling. For example, charge neutrality consideration and integrating defect chemistry and CALPHAD will be illustrated for designing high-entropy cathode materials in the example of classic perovskite $LaMnO_{3\pm\backslash 948}$ for solid oxide fuel cell applications.

9:30 AM
Development of Sputtered HEA Thin Films and Their Functional Properties: *Jeyanthinath Mayandi*[1]; Stange Marit[2]; Espen Sagvolden[2]; Martin Fleissner Sunding[2]; Øystein Dahl[2]; Matthias[1]; Jonas Deuermeier[3]; Elvira Fortunato[3]; Ole Martin Løvvik[4]; Spyridon Diplas[5]; Terje G Finstad[1]; Patricia Almeida Carvalho[6]; [1]SMN, Department of Physics, University of Oslo, Norway; [2]SINTEF Materials and Chemistry, Norway; [3]CENIMAT, Faculdade de Ciencias e Tecnologia, Universidade Nova de Lisboa, Portugal; [4]SMN, Department of Physics and Department of chemistry, University of Oslo, Norway and SINTEF Materials and Chemistry, Norway; [5]SMN, Department of Physics and Department of chemistry, University of Oslo, Norway; [6]SINTEF Materials and Chemistry, Norway and CEFEMA, Instituto Superior Tecnico, Universidade de Lisboa, Portugal
In the last decade, high-entropy alloys (HEA) emerged as an exciting new class of materials with remarkable physical properties. It is attractive to explore the functional properties of the HEA, such as optical band gap and resistivity, relevant for scouting the potential for specific semiconductor applications. In the present work we have studied the fundamental behaviours of thin films of (i)CrFeNiCoCr, (ii) GeFeNiCoCu and (iii)MnVCrAlTi and their HEA-oxides created by reactive and nonreactive sputtering. All the samples were characterized by structural, optical and electrical methods. The resistivity of the films varied from 10-4 to more than 106 Ocm and the band gap varied from 0 to 3 eV for the different alloys. The as prepared metallic films had fcc structure while the oxides had NaCl structure. This will be discussed in terms of the structural analysis and suggested electronic model of the films.

9:50 AM
Buildind Novel Magnetic Materials Suitable for Permanent Magnets Based on "Artificial Elements" of Rare Earths and Transition Metals High Entropy Alloys: *Dimitrios Niarchos*[1]; [1]NCSR Demokritos
The most powerful PMs are based on Nd2Fe14B with small addition of Dy and (BH)max >400 kJ/m3 that can operate at temperatures up to 200 °C. For higher temperature applications SmCo5 -type magnets are used but with moderate energy products (BH)max ~ 240 kJ/m3. Today, there is an urgent need for the discovery of rare earth lean/free permanent magnets due to the critical strategic character of these metals . All these magnets are very brittle that prohibits them for wider applications.In this work we will present our efforts first to synthesize Rare-Earth based HEAs (RE-HEAs), second to synthesize Transition Metal HEAS (TM-HEAs) and subsequently the successful efforts to prepare {RE-HEAs}x-(TM-HEAs)y alloys with the same or better properties compared to the parent alloys of SmCo5, Nd2Fe14B and (Nd,Sm)-Fe12-xTx (T=Ti,Mo) alloys at much lower materials cost.

10:10 AM Break

Alloy Design and Mechanical Properties III

Tuesday AM
November 19, 2019

Room: Cyan
Location: Hyatt at Olive 8

9:00 AM Keynote
Phase Instabilities and Mechanical Properties of High-entropy Alloys (HEAs): *Easo George*[1]; [1]Oak Ridge National Laboratory
In HEAs, as in conventional alloys, phase instabilities can have beneficial or harmful effects on mechanical properties. For example, in HEAs with the FCC structure, a latent tendency for transformation to HCP anticipates twinning and/or transformation induced plasticity (TWIP/TRIP), which can enhance strength and ductility. TRIP effects have been reported also in some BCC refractory-metal HEAs. In both structures, alloy compositions can be tuned to control phase stability and, in turn, mechanical properties. Another kind of transformation occurs in single-phase HEAs most of which are actually metastable. They decompose into their thermodynamically stable phases during intermediate-temperatures anneals once nucleation and growth barriers have been overcome. Severe embrittlement is often the result, as has been shown in both FCC and BCC HEAs. In this talk I will use model HEA systems to highlight fundamental aspects of these two types of phase instabilities and their effects on mechanical properties.

9:30 AM
On the Mechanism of TRIP Behavior in Co-Cr-Ni Multi-principal Element Alloy: *Yaofeng Guo*[1]; Francisco Coury[2]; Michael Kaufman[1]; Amy Clarke[1]; [1]Colorado School of Mines; [2]Universidade Federal de São Carlos
A series of Co-Cr-Ni multi-principal element alloys (MPEAs) of single face-centered cubic (FCC) phase were designed using a combined method of solid solution strengthening and CALPHAD phase equilibria modeling. The single phase FCC MPEAs transform to a hexagonal close-packed phase during deformation at room temperature, exhibiting significant transformation-induced plasticity (TRIP). In this work, post-mortem characterization using transmission electron microscopy (TEM) was performed to study the microstructural details of deformed samples, particularly line and planar defects. Moreover, the stacking fault energy (SFE) of different MPEAs was measured and the ease of TRIP behavior was correlated with SFE. Finally, in order to elucidate the TRIP mechanism of the present alloys, in-situ observation of microstructure evolution during straining was conducted in the TEM to study the FCC-to-HCP transformation. The TRIP behavior was explained using a model of defect-assisted transformation.

9:50 AM
Microstructures and Properties of As-Cast $Al_{2.7}$CrFeMnV, $Al_{2.7}$CrFeTiV, and $Al_{2.7}$CrMnTiV High Entropy Alloys: *Keith Knipling*[1]; Richard Michi[2]; David Beaudry[3]; [1]Naval Research Laboratory; [2]Northwestern University; [3]University of Florida
High entropy alloys (HEAs) typically contain five or more principal elements in nearly equiatomic proportions, significantly expanding the composition space and achievable properties of novel metallic materials. Here we present the microstructures and mechanical properties of arc-melted $Al_{2.7}$CrFeMnV, $Al_{2.7}$CrFeTiV, and $Al_{2.7}$CrMnTiV HEAs. Metallographic analysis, powder X-ray diffraction, electron microscopy, and atom-probe tomography have revealed $Al_{2.7}$CrFeMnV to be single-phase BCC with lattice parameter (a) of 0.2968 nm. $Al_{2.7}$CrFeTiV is multiphase, with a high volume fraction of Al-rich G-phase precipitates in a BCC matrix (a = 0.3006 nm), with additional other precipitates. $Al_{2.7}$CrMnTiV contains Ti-rich FCC precipitates (a = 0.3043 nm) in a BCC matrix (a = 0.3946 nm). These experimental results are compared with the equilibrium phases predicted by thermodynamic modeling.

10:10 AM Break

Alloy Design and Environmental Resistance II

Tuesday AM
November 19, 2019

Room: Azure
Location: Hyatt at Olive 8

10:40 AM Invited
ICME Design of Corrosion Resistant HEAs for Harsh Environments: *Pin Lu*[1]; Greg Olson[1]; Tianshu Li[2]; Gerald Frankel[2]; Angela Gerard[3]; John Scully[3]; [1]Questek Innovations LLC; [2]Ohio State University; [3]University of Virginia
The integrated computational materials engineering approach is inherently suited to explore the vast, multi-dimensional high entropy alloy (HEA) compositional and processing space, and has been adopted in this work, coupled with empiricism, to design highly corrosion resistant HEAs. Using the combination of empirical and computational approaches, three non-equimolar HEA compositions were identified for their predicted ability to form a single-phase structure and to exhibit high corrosion resistance. Phase diagrams and E-pH Pourbaix diagrams for HEAs were calculated by CALPHAD. One of the HEAs, Ni38Cr21Fe20Ru13Mo6W2, has been successfully synthesized on the lab-scale and homogenized at 1250°C for 120 hours. Exceedingly high corrosion resistance of the Ni-rich HEA was demonstrated by electrochemical testing, including potentiodynamic polarization and electrochemical impedance spectroscopy, even in harsh acidic solutions. The successful validation of the computational design efforts with pre-set property goals shows that ICME is suitable for corrosion resistant HEA design, including complex non-equimolar HEAs.

11:10 AM
A Low-cost, Low-density Compositionally Complex Alloy with High Corrosion Resistance: Sean O'Brien[1]; Nick Birbilis[2]; *Rajeev Gupta*[1]; [1]The University of Akron; [2]The Australian National University
Vacuum arc melting was used to create a multiphase compositionally complex alloy (CCA) containing aluminum, iron, manganese, and silicon. The microstructure of the alloy was characterized with scanning electron microscopy (SEM) in conjunction with energy dispersive x-ray spectroscopy (EDXS). The corrosion behavior was determined by immersion and cyclic potentiodynamic polarization (CPP) testing. To characterize the surface film after immersion testing, x-ray photoelectron spectroscopy (XPS), SEM, and EDXS were implemented. The CCA exhibited a corrosion behavior similar to 304L stainless steel while maintaining significantly lesser density and cost. The alloy, after Vickers hardness testing, showed a very high hardness compared to 304L stainless steel.

11:30 AM

Anisotropic Lattice Excitation Induced by Hydrogen in CoCrFeMnNi High-entropy Alloy: *Hung-Wei Yen*[1]; Shih-Wei Chen[2]; Yan-Gu Lin[2]; Chun-Ming Wu[2]; Tsai Che-Wei[3]; Yu-Ting Mai[3]; [1]National Taiwan University; [2]National Synchrotron Radiation Research Center; [3]National Tsinghua University

CoCrFeMnNi high-entropy alloy (HEA) has been reported to own high resistance to hydrogen embrittlement. This fact was explained by the enhancement of deformation twinning when hydrogen is involved. However, the relationship between deformation twin and hydrogen in CoCrFeMnNi HEA is still unknown. The current work investigated behavior of hydrogen in CoCrFeMnNi HEA by using thermal desorption analysis, synchronicity diffraction, and neutron scattering. It was found that stored hydrogen in CoCrFeMnNi HEA leads to anisotropic lattice strain on (1 1 1) plane. Moreover, stored hydrogen in the alloy is in the form of localized hydrogen clusters. This result breaks the proposition claimed by Johnson since 1875. The metallurgical principle can be developed into an new approach to prevent from hydrogen embrittlement.

11:50 AM

Using Machine Learning to Guide Multiple Principle Element Alloy Design: *Jose Loli*[1]; Yining He[1]; Amish Chovatiya[1]; Bryan Webler[1]; Zachary Ulissi[1]; Jack Beuth[1]; Maarten De Boer[1]; [1]Carnegie Mellon University

Multiple principle element alloys (MPEAs) can exhibit exceptional resistance to wear, creep, corrosion and high temperature oxidation. The optimization of MPEAs can be daunting due to the vast number of possible compositions. If properties can be calculated as a function of composition, numerous optimization strategies to guide alloy design exist. For complex phenomena, in this work: high temperature oxidation, it is not feasible to make calculations of all parts of the problem. However, there are calculatable quantities that should correlate with oxidation resistance. Our approach here is to investigate if quantities calculated via CALPHAD software can be used to develop optimized compositions. A database of thermodynamic quantities was generated for 4 and 5 element equimolar combinations from a 12 element palette. An objective function and black-box optimization software were utilized to select 5 most promising compositions. Arc-melted buttons of these compositions are being made and characterized to test the predictions.

Functional Properties II

Tuesday AM
November 19, 2019

Room: Cobalt
Location: Hyatt at Olive 8

10:40 AM Invited

Functional Properties of High Entropy Materials with Metallic, Ionic and Covalent Bonding: *Horst Hahn*[1]; Abhishek Sarkar[2]; Ben Breitung[1]; Leonardo Velasco Estrada[1]; Qingsong Wang[1]; Ralf Witte[1]; Robert Kruk[1]; Enrique Lavernia[3]; Benjamin MacDonald[3]; Subramshu Bhattacharya[4]; [1]Karlsruhe Institute of Technology; [2]TU Darmstadt; [3]University of California Irvine; [4]IIT Madras

Mechanical properties of High Entropy Alloys (HEA) exhibiting equiatomic or near-equiatomic compositions of typically more than 5 metals as single- or multi-phase structures have been studied extensively over the past 15 years. In contrast, the functional (magnetic, electric, catalytic) properties of HEA have been studied to a much lesser extent. Recently, High Entropy Oxides (HEO) and related compounds, i.e., oxyfluorides, exhibiting ionic or covalent bonding, became popular. Several groups have reported on their functional properties, such as dielectric, magnetic, catalytic, electrochemical, etc. Examples are transition metal HEO and lithiated transition metal oxyfluorides with rocksalt structure exhibiting large Li-ion conductivity, high capacities and low degradation for electrolytes and electrodes for applications in Li-ion batteries. Rare earth HEO with fluoride structure have shown interesting magnetic properties, band gap engineering and tuning of optical properties. The talk will summarize the state-of-the-art in functional properties of HE materials with metallic, ionic and covalent bonding.

11:10 AM

Oxidation of CrFeCoNiCu Sputtered Thin Films: *Jeyanthinath Mayandi*[1]; Marit Stange[2]; Martin Fleissner Sunding[2]; Spyridon Diplas[3]; Patricia Almeida Carvalho[4]; Terje Finstad[1]; [1]SMN, Department of Physics, University of Oslo, Norway; [2]SINTEF Materials and Chemistry, Norway; [3]SMN, Department of Physics and Department of chemistry, University of Oslo, Norway; [4]SINTEF, Norway and CEFEMA, Instituto Superior Tecnico, Universidade de Lisboa, Portugal

The formation of high entropy alloys (HEAs) has the potential to influence solid solution phase stability through control of configurational entropy. For new materials with attractive properties for mechanical, magnetic, electronic and photonic applications, the oxidation behaviour and resistance is an important property (as well as interesting for synthesizing new structures). Here we have synthesized thin films of CrFeCoNiCu films of different thickness by sputtering onto insulating and optical transparent substrates in order to measure electrical and optical properties. The deposition was done by reactive DC magnetron sputtering from a sputtering targets made from an equimolar alloy of the elements. All the samples were characterized by structural and electrical optical methods. The as deposited films had fcc structure and also showed interesting electric and magneto resistive properties. The samples were annealing in air and O2 ambient in the temperature range of 300 to 500 ˚C forming an oxide layer.

11:30 AM

Metastable F.C.C. Phase and Its Influence on the Soft-magnetic Properties of FeCoNiAlxSix (0.2 < x < 0.5) Alloys: *Tanjore Jayaraman*[1]; [1]University of Michigan-Dearborn

Significant improvement in soft-magnetic properties of FeCoNiAlxSix (0.2 < x < 0.5) high-entropy alloys is achievable when the alloys are comprised of metastable f.c.c. phase. The nanocrystalline FeCoNiAl0.375Si0.375 alloy fabricated by mechanically alloying the constituent elements resulted in the formation of metastable f.c.c. phase. The metastable phase was stable up to ~800 K and thereafter it dissociated. At ambient temperature, the magnetic saturation (MS) and coercivity (HC) of the alloy was ~91 Am2/kg and ~5 kA/m, respectively. The magnetic characterization from 60 K to 900 K showed a steady decrease in MS, and the HC initially decreased and subsequently increased. The thermally-treated alloy exhibited improvement in the soft-magnetic properties while retaining the nanocrystallinity. While fabrication of the alloys by equilibrium processing facilitates the formation of two phases—b.c.c. and f.c.c., fabrication by mechanical alloying promotes the formation of metastable f.c.c. phase having relatively superior soft-magnetic properties and good thermal stability.

11:50 AM

Hydrogen Storage Properties of TiVNbCrx Multicomponent Alloys: *Renato Strozi*[1]; Guilherme Zepon[2]; Jacques Huot[1]; Walter Botta[2]; Daniel Leiva[2]; [1]Institut de recherche sur l'hydrogène; [2]Federal University of São Carlos

The effect of chromium content on the hydrogen storage properties in the TiVNbCrx (where x = 1.61, 1.0 and 0.53) multi-principal element alloys (MPEAs) was studied. CALPHAD calculation showed a relatively large BCC single-phase field since the solidification to approximately 1000C˚. The alloys were synthesized by arc-melting and characterized by X-ray diffraction and scanning electron microscopy. The hydrogen storage properties were measured using Sieverts-type apparatus. The as-cast samples presented microstructures composed of BCC, HCP Titanium rich phase and C15 Laves phase. The three alloys absorbed hydrogen rapidly under mild conditions, i.e., room temperature and 2.0 MPa of H2. XRD analysis after first hydrogenation showed that the C15 Laves phase not absorbed hydrogen and the BCC phase absorbed hydrogen by forming FCC hydride. Increasing of Cr content increases the amount of C15 Laves phase but the gravimetric hydrogen capacity decreases.

Alloy Design and Mechanical Properties IV

Tuesday AM
November 19, 2019

Room: Cyan
Location: Hyatt at Olive 8

10:40 AM Invited
Tuning the Mechanical Property of an $L1_2$-strengthened High-entropy Alloy through Microstructure Engineering: *Ming-Hung Tsai*[1]; Yan-Jie Su[1]; Yi-Ting Fan[1]; An-Chen Fan[1]; [1]National Chung Hsing University
In this work, a precipitation-hardened HEA was developed. The strengthening originates from high-density $L1_2$ particles, whose size ranges from 5 to 20 nm, depending on thermal treatment conditions. The average size, density, and volume fraction of the precipitate were analyzed quantitatively. The deformation microstructure of alloys with different mechanical properties were also analyzed and compared. It was found that planar slip band is the predominate structure at the early stages of deformation, but the activation of the second slip direction is observed at strains as low as 0.02. The interaction between dislocation and precipitates changes with precipitate size. At small precipitates sizes, dislocations shear and move through the particles. However, looping was observed in alloys with larger precipitate sizes. The effect of such transition on the deformation microstructure and mechanical properties is probed, and the conditions for optimized mechanical property is discussed.

11:10 AM
Efficient Exploration of the High Entropy Alloy Space: *Raymundo Arroyave*[1]; Tanner Kirk[1]; Richard Malak[1]; [1]Texas A&M University
High Entropy Alloys are alloys that contain multiple principal alloying elements. While many HEAs have been shown to have unique properties, their discovery has been largely done through costly and time-consuming trial-and-error approaches, with only an infinitesimally small fraction of the entire possible composition space having been explored. In this talk, we will present a recently developed framework that has mapped the problem of exploring the HEA space to a Constraint Satisfaction Problem (CSP), whose solution is, in turn, a one-class classifier implemented as a Support Vector Data Descriptor (SVDD). The resulting algorithm is used to discover regions in the HEA Composition-Temperature space that satisfy desired phase constitution requirements that essentially are mathematical representations of alloy specifications. The framework is capable of identifying regions in the HEA space with arbitrary phase constitution attributes. We demonstrate, as an example, the targeted discovery of precipitation strengthened HEAs.

11:30 AM
High Temperature, Low Cost and Light Weight High Entropy Superalloys: *Jithin Joseph*[1]; Karl Shamlaye[1]; Manisha Senadeera[2]; Santu Rana[2]; Sunil Gupta[2]; Svetha Venkatesh[2]; Matthew Barnett[1]; Daniel Fabijanic[1]; [1]Institute for Frontier Materials, Deakin University; [2]Centre for Pattern Recognition and Data Analytics, Deakin University
The single FCC phase high entropy alloys (HEAs) such as CoCrFeNi and CoCrFeMnNi showed exceptional ductility, work hardenability and fracture toughness, but are not strong enough for engineering applications at room and elevated temperatures. This study aim towards a new alloy design space for FCC HEAs strengthened by the coherent L12 ' precipitates. The exploration is made on a set of six elements using machine learning algorithm from Thermocalc (HEA3 database) based on Ni-Al-Co-Cr-Fe-Ti system. These bulk alloy compositions with a high volume fraction of ' precipitates (60%) and high concentration of Al and Ti (>16 at.%) were fabricated using direct laser deposition. HEAs such as Ni54Co20Fe5Cr5Al12Ti4 showed a high yield strength of 650 MPa at 800˚C, ' dissolution temperature of 1200˚C, excellent high-temperature coarsening resistance and low density (<7.6 g/cm3) without any detrimental TCP phases after long-term exposure at elevated temperatures is designed using this strategy.

11:50 AM
Precipitation and Strengthening in AlCoCrFeNi High Entropy Alloys as Studied by Atom Probe Tomography: *Keith Knipling*[1]; David Beaudry[2]; Peter Liaw[3]; [1]Naval Research Laboratory; [2]University of Florida; [3]The University of Tennessee, Knoxville
In this study we present the microstructures in $Al_{0.5}$CoCrFeNi (atomic fraction) HEAs in the as-cast state and after thermal aging at 700 and 1000 ˚C. The alloy solidifies into dendritic regions that have a face-centered cubic (FCC) crystal structure enriched in Co, Cr, and Fe, and interdendritic regions that are comprised of a disordered body-centered cubic (BCC, A2) phase and an ordered BCC phase (B2) formed by spinodal decomposition. During aging these regions form a variety of strengthening precipitates, including NiAl (B2 structure), Ni_3Al ($L1_2$), and a-Cr (BCC), as observed by atom probe tomography. These microstructures are correlated to the observed strength as measured by Vickers microhardness and uniaxial tensile tests and are compared to predictions made by thermodynamic modeling.

Environmental Resistance I

Tuesday PM
November 19, 2019

Room: Azure
Location: Hyatt at Olive 8

1:30 PM Invited
Oxidation Resistant Refractory High Entropy Alloys for High Temperature Structural Application: *Bronislava Gorr*[1]; Franz Mueller[1]; Steven Schellert[1]; Hans Christ[1]; Hans Chen[2]; Alexander Kauffmann[2]; Martin Heilmaier[2]; [1]University of Siegen; [2]Karlsruhe Institute of Technology (KIT)
Many High Entropy Alloys (HEAs) exhibit unusual or outstanding properties compared to those of conventional materials. In this contribution, a refractory HEA system which shows exceptionally high oxidation resistance at high temperatures is presented. The oxidation behavior of several alloys within the alloy system Ta-Mo-Cr-Ti-Al was studied in a wide temperature range from 500˚C to 1500˚C. Even at very high temperatures above 1300˚C, the oxidation kinetics of the equiatomic alloy 20Ta-20Mo-20Cr-20Ti-20Al follows the parabolic rate law yielding very moderate oxidation rates. The oxidation resistance relies mostly on the formation of the protective oxide CrTaO4 that forms at the interface oxide/substrate as a result of the inward oxygen diffusion. During initial oxidation stage, TiO2 and Al2O3, which were identified as transient corrosion products, protect the alloy from severe corrosion attacks. The underlying oxidation mechanisms as well as general perspectives of the refractory HEAs in terms of oxidation resistance are discussed.

2:00 PM
Corrosion of Single- and Multi-phase High Entropy Alloys: Sarita Sahu[1]; Tianshu Li[1]; Anup Panindre[1]; Babu Viswanathan[1]; Christopher Taylor[1]; Angela Gerard[2]; John Scully[2]; Pin Lu[3]; *Gerald Frankel*[1]; [1]Ohio State University; [2]University of Virginia; [3]Questek Innovations
The corrosion behavior of several high entropy alloys (HEAs) was studied. A single phase NiCrFeRuMoW HEA exhibited remarkable corrosion resistance, even in concentrated HCl solution, either in the as-cast or solutionized condition. Heat treatment of the solutionized HEA to precipitate second phases resulted in a large increase in hardness, and only a slight degradation in corrosion resistance. Details of the HEA microstructure and the influence on corrosion resistance will be presented. A series of single phase NiFeMnCoCr HEAs with Cr composition varying from 22 to 6%, balanced by changes in the Mn and Co contents, were also studied. Even the alloy with 6% Cr exhibited passivity and pitting in NaCl solution, behaving like a Ni-based alloy, even though the Ni content was only 38%. The pits in alloys with 6, 10, or 14%Cr were crystallographic, even when grown at high potentials, reflecting difficulty in precipitating a salt film.

2:20 PM
Oxidation Behavior of High Entropy Alloys: Experimental Results and Modeling Challenges: Aayush Sharma[1]; Mouhamad Diallo[1]; Pierre Alameda[1]; Matthew Kramer[2]; *Ganesh Balasubramanian*[3]; Pratik Ray[2]; [1]Ames Laboratory, US-DOE; [2]Ames Laboratory, US-DOE and Department of Materials Science and Engineering, Iowa State University; [3]Lehigh University
Multiprincipal element alloys (MPEAs) have attracted demonstrated significant promise for structural applications in harsh environments. While the mechanical behavior of MPEAs has been well-studied, relatively few oxidation studies are available. Furthermore, computational models of the oxidation process – especially of complex MPEAs – have received scant attention. In this presentation we shall present experimental results on the oxidation behavior of AlFeCoCrNi MPEAs and showcase the complexity of the oxidation mechanism and the effect of heat treatments and oxidation temperature on the development of the oxide scale. We will also present the fundamentals of a cellular automata model for investigating oxidation resistance of concentrated alloys. The initial model results will focus on the constituent binaries in the AlFeCoCrNi system and validated with corresponding experiments. We will also discuss the pathways for further extending this oxidation model to multicomponent systems.

2:40 PM
High Temperature Oxidation Behavior of CrMnFeCoNi and CrCoNi in Various Atmospheres: *Wencke Schulz*[1]; Christiane Stephan-Scherb[1]; Guillaume Laplanche[2]; [1]Bundesanstalt für Materialforschung und -prüfung (BAM); [2]Ruhr-Universität Bochum
The study presented here focusses on a systematic analysis of oxidation mechanisms of the well-known Cr20Mn20Fe20Co20Ni20 alloy and one of its ternary sub-system Cr33.3Co33.3Ni33.3 which were reported in the literature to exhibit attractive mechanical properties. Both alloys are single phase fcc prior to oxidation and were simultaneously exposed to different oxygen containing atmospheres at 700° C and 800° C for durations up to 288 h. Cr20Mn20Fe20Co20Ni20 showed poor oxidation resistance at high temperatures due to its high amount of manganese leading to the formation of non-protective Mn-oxide scales. In contrast, a relatively homogeneous and protective chromia layer was found to form on CrCoNi at 700° C and 800° C after each exposure time. Mass change-, SEM- and XRD analysis of the oxide layers were performed in the present study and provide a better understanding of the oxidation mechanisms as well as the impact of the alloy composition on oxidation behavior.

3:00 PM
The Origins of Excellent Passivity in Single Phase High Entropy Alloys: Angela Gerard[1]; Kang Wang[1]; Pin Lu[2]; Stephen McDonnell[1]; Wofgang Windl[3]; Dan Schreiber[4]; Bi-Cheng Zhou[1]; Sarita Sahu[3]; Tianshu Li[3]; Gerald Frankel[3]; *John Scully*[1]; [1]University of Virginia; [2]Questek Innovations LLC; [3]Ohio State University; [4]Pacific Northwest National Laboratory
Studies of passivation of several high entropy alloys (HEAs) were conducted in corrosive aqueous environments such as NaCl and H2SO4 solution. A single phase NiCrFeRuMoW HEA in the solutionized condition was spontaneously passive even in concentrated HCl solution. Good passivity at anodic potentials was traced to the formation of a disordered non-stoichiometric solid solution oxide containing all alloying elements in an oxidized state. A series of single phase NiFeMnCoCr HEAs with Cr composition varying from 6 to 22%, balanced by changes in the Mn and Co contents, was also investigated. Lower passive current densities were observed compared to the binary alloys at equivalent Cr contents. Passive films consisted of mainly oxidized Ni, Cr, and Fe with very little Co and Mn. Both thermodynamic and kinetic influences were considered to develop a better understanding of factors governing these oxide film compositions and structures.

3:20 PM Break

Alloy Design and Processing I

Tuesday PM
November 19, 2019

Room: Cobalt
Location: Hyatt at Olive 8

1:30 PM Invited
Oxidation Resistant Refractory Metal – Simple Metal Complex Concentrated Alloys: *Panagiotis Tsakiropoulos*[1]; Claire Utton[1]; Mohammad Ghadyani[1]; [1]University of Sheffield
Refractory metal intermetallic composites (RMIC) with capabilities beyond those of state-of-the-art Ni-based superalloys will require environmentally resistant coatings. The latter could be of the bond coat (BC)/thermally-grown oxide (TGO)/ceramic top-coat (TC) type with a multi-material layered BC capable of forming Al2O3 TGO. The presentation will discuss why and how parameters based on atomic size, electronegativity and the number of valence electrons per atom filled into the valence band are used to design non-pesting and alumina scale forming refractory metal – simple metal complex concentrated alloys suitable for application as BC components. The alloys 14.5Nb-27Si-22.5Ti-32.5Al-3.5Hf, 13.5Nb-23Si-23Ti-37Al-3.5Hf and 13Nb-24Si-24Ti-35Al-4Hf will be used to demonstrate alloy design and selection. The intermediate and high temperature oxidation of these alloys will also be discussed.

2:00 PM
Effect of Cr Variation on FCC Phase Fraction in AlCoCrxFeNi(x= 0 - 1) High-entropy Alloys Synthesised through Mechanical Alloying and Spark Plasma Sintering: *Rahul Bhattacharya*[1]; K. Guruvidyathri[2]; Daniel Fabijanic[1]; B S Murty[2]; [1]Institute for Frontier Materials; [2]Indian Institute of Technology Madras
The effect of Cr variation on FCC/BCC phase formation AlCoCrxFeNi (x= 0 - 1) is explored in the present work. Cr is known to be a BCC stabilizer and s-phase former. These phases were reported in AlCoCrFeNi HEA obtained through casting route. We adopted mechanical alloying and spark plasma sintering route, since it suppresses certain complex phases. It is observed that the Cr assists in FCC phase in composition domains up to 0.75 molar ratio. This FCC phase is rich in elements Fe, Co and Cr. Increasing Cr content in the alloy also influences the elemental distribution among the FCC and BCC/B2 phases, which in turn affects the thermal stability, hardness, melting point and oxidation behaviour of these HEAs. In this work, we intend to investigate the underlying thermodynamic explanation for the experimentally observed phase evolution using CALculation of PHAse Diagram (Calphad) studies as well.

2:20 PM
Rapid Alloy Development of New Promising High Entropy Alloys by Using Laser Powder Bed Fusion (3D-Printing): *Simon Ewald*[1]; Fabian Kies[2]; Johannes Henrich Schleifenbaum[1]; [1]RWTH Aachen University - Digital Additive Production; [2]RWTH Aachen University - Steel Institute
In the present study a method to screen and develop new materials by using L-PBF (3D-Printing) will be introduced. Up to now, the process of designing and developing new alloys is time-consuming and expensive. That can be significantly accelerated by the Rapid Alloy Development (RAD) approach. This approach describes a new and faster way of creating tailored alloys. New alloys can be fabricated directly by dry-mixing of elementary powders and then processed via LPBF. Thus, a large range of alloy compositions can be quickly produced, analyzed and evaluated. The Al-C-Co-Fe-Mn-Ni system is considered as the investigated material. First, promising alloy compositions are determined by using simulation tools and thermodynamic data bases. Second, different dry-mixed alloy compositions of AL-C-Co-Fe-Mn-Ni are qualified for the L-PBF process in order to screen the alloys. Finally, the various fabricated alloys are evaluated by microstructure analysis (OM, SEM, EBSD, EDX) and mechanical properties.

2:40 PM
Development of New Multi-principle Element Alloys Using Laser Additive Manufacturing: *Fabian Kies*[1]; Simon Ewald[2]; Bengt Hallstedt[3]; Christian Haase[1]; [1]Steel Institute IEHK; [2]Digital Additive Production DAP; [3]Materials Applications in Mechanical Engineering IWM
Exploring the field of multi-principle element alloys (MPEAs) by capitalizing on the flexibility of additive manufacturing (AM) provides the opportunity to design new metals with exceptional mechanical properties. So far, efficient MPEA development is held up by time-consuming manufacturing methods. Therefore, a methodology is introduced which enables flexible exploration and design of MPEAs by combining theoretical and experimental approaches. A self-compiled thermodynamic database for CALPHAD was used to identify promising composition ranges for the system, which were synthesized using elemental powder blends in AM. Materials characterization was split into light (XRD, hardness) and deep (SEM, EBSD, tensile test) screening to increase characterization speed.Precipitate types in the investigated Al-C-Co-Cr-Fe-Mn-Ni system were correctly predicted by theoretical screening. Properties identified by light screening steps translated reliably into deep screening. The applicability of the introduced methodology to identify promising MPEAs well as the resulting microstructural and mechanical properties are discussed.

3:00 PM
Study of Cavitation Erosion Behavior of AlCoCrxFeCu High-entropy Alloy Coatings Synthesized by Laser Cladding: *Danqing Yin*[1]; Guangbing Liang[1]; Shuai Fan[1]; Shanxin Li[1]; Shuai Zhou[1]; [1]Henan University of Science and Technology
AlCoCrxFeCu (x: molar ratio, x =1.0, 1.5 and 2) high-entropy alloy coatings was synthesized on 304 stainless steel with premixed high-purity Al ,Co, Cr and Cu four-component powders by laser cladding. The Fe component is obtained from melting substrate metal during laser cladding. The effect of Cr content on their phase evolution, microstructure, microhardness and cavitation erosion behavior of high-entropy alloy coatings was investigated using XRD, SEM, EDS, and ultrasonic cavitation erosion testing machine respectively. Results showed that AlCoCrxFeCu coatings was composed of BCC and FCC solid solution. The microstructure of the coatings exhibited a typical dendritic structure of high entropy alloy. The microhardness of AlCoCrxFeCu coatings increased obviously to 570 HV, which was at least 2.3 times that of substrate metal (250 HV). AlCoCrxFeCu high-entropy alloy coatings lost 9.4 mg in 10-hour ultrasonic cavitation test in distilled water, far less than 403 martensitic stainless steel.

3:20 PM Break

Alloy Design and Mechanical Properties V

Tuesday PM
November 19, 2019

Room: Cyan
Location: Hyatt at Olive 8

1:30 PM Invited
High-throughput Experimental Synthesis of Refractory High-entropy Alloys: *Dan Thoma*[1]; Michael Moorehead[1]; Michael Niezgoda[1]; Phalgun Nelaturu[1]; Adiren Couet[1]; [1]University of Wisconsin - Madison
Refractory High-Entropy Alloys (RHEAs) potentially offer enhanced properties and optimized performance in extreme conditions. Specifically, properties such as strength, radiation resistance, and corrosion resistance at high operating temperatures are of interest. To explore the compositional tailoring of RHEAs, high-throughput fabrication methods using metal additive manufacturing have been developed. Directed energy deposition, with four powder hoppers, was used for in situ alloying of elemental powders. The samples were based on Nb, Ta, Mo, and W. Over 50 alloy samples with different compositions can be fabricated in a few hours, permitting the development of high-throughput characterization methods for microstructural evolution and material properties. The methodology for elemental compositional control in the high-throughput alloying process, with an iterative technique, provides chemically uniform samples within 5% of the desired compositions. Moreover, because of the high cooling rates associated with the process, microsegregation distances have been reduced to approximately 2 microns.

2:00 PM
Microstructural and Mechanical Characterization of a Medium Entropy Alloy Produced Using Selective Laser Melting: *Tim Smith*[1]; Aaron Thompson[1]; Michael Kulis[1]; Richard Rogers[1]; Kathleen Tacina[1]; [1]Glenn Research Center
High entropy alloys (HEAs) are an interesting new class of alloys which have been shown to exhibit both notable strength and ductility for a wide range of temperature and stresses. In addition, the remarkably small difference between the solvus and liquidus temperatures for many face centered cubic HEAs makes them an excellent candidate for selective laser melting fabrication. In this study, the microstructure and mechanical properties of an equiatomic NiCoCr alloy successfully produced using selective laser melting are explored. The effect laser speed, laser power, and powder recyclability have on final part density and microstructural segregation are analyzed through both x-ray diffraction and high resolution scanning electron microscopy. These results are further validated and compared to stable phase predictions produced using a commercially available high entropy alloy mobility database. Lastly, the tensile strengths resulting from different post-processing pathways are detailed and an optimal post-build heat treatment is specified.

2:20 PM
Deformation Mechanisms of Additively Manufactured FeMnCoCrAl High Entropy Alloy with Interstitial Carbon: *Tomi Suhonen*[1]; Anssi Laukkanen[1]; Jarkko Metsäjoki[1]; Ivanchenko Mykola[1]; Juha Lagerbom[1]; [1]VTT Technical Research Centre of Finland
FeMnCoCrAl with 0.7at%C powders were gas atomized, consolidated by laser powder bed fusion and heat treated by hot isostatic pressing technique. Microstructures of different manufacturing steps were characterized (SEM-EDS-EBSD, TEM, XRD) and stress-strain behavior as well as deformation mechanisms (TWIP and TRIP) of consolidated specimens were studied with in-situ-SEM tensile tests. Engineering and true stress-strain curves as well as EBSD phase maps showing the deformation induced martensitic transformation as a function of strain are presented.

2:40 PM
Microstructural Characterization and High-temperature Mechanical Behavior of 3D Printed Eutectic High Entropy Alloy (AlCoCrFeNi2.1): *RJ Vikram*[1]; Satyam Suwas[1]; [1]Indian Institute of Science
Microstructural characterization and high-temperature mechanical behavior of 3D printed eutectic HEA (AlCoCrFeNi2.1) has been explored for the first time. The material was manufactured through laser engineered net shaping (LENS). The microstructural study revealed dual phase dendritic and eutectic structures consisting of ordered FCC (L12) and BCC. The phase fraction of L12 is more across build (X face) and BCC is more along build (Z face). Anisotropy in hardness was observed along Z and X which further resulted in yield anisotropy during compression test at room temperature. High-temperature compression study has been explored at various temperatures of 400oC, 600oC, 700oC, and 800oC. Yield strength tends to increase from room temperature till 400oC and starts dropping till 800oC. First principle calculation was done by using diffused multi-layered fault (DMLF) model by high throughput computation for estimating the planar fault energies.

3:00 PM
Weldability of High Entropy Alloys (HEA): High-throughput Exploration for Structural Alloy Design: Alexander Martin[1]; Thomas Estep[1]; *Carolin Fink*[1]; [1]Ohio State University
HEA can be tailored to have good mechanical properties, however their suitability for structural use is constrained by many others, including the ability to be joined and formed into complex shapes. Welding is a critical manufacturing process for structural components. It is essential to address the weldability of candidate HEA during the alloy development process. This can enable enhancement of weld properties, and early avoidance of adverse issues related to welding by modification of composition or microstructures during an application-driven HEA design. We propose a sequential process to screen and evaluate a large number of compositions for their metallurgical and mechanical response to the heat of welding processes. This talk will focus on how fusion-based processes affect candidate structural HEA. High-throughput thermodynamic calculations and weldability experiments are used to rapidly identify a compositional space for alloys with development potential, and quickly reject those with critical deficiencies with regard to weldability.

3:20 PM Break

Environmental Resistance II

Tuesday PM
November 19, 2019

Room: Azure
Location: Hyatt at Olive 8

3:50 PM
An In-situ TEM Observation on the Stability of High Entropy Alloys Under High Temperature Oxidation Environments: *Elaf Anber*[1]; Wayne Harlow[1]; Jean-Philippe Couzinie[2]; Mitra Taheri[1]; [1]Drexel University; [2]Université Paris Est
Recently, new developments of in-situ transmission-electron-microscopy (TEM) have led to new insights into the thermal stability mechanisms of a wider range of metals and alloys. Within this context, we propose to describe some recent results on the stability of two HEA families including refractory-based compositions and 3d transition alloys, under high temperature and oxidation environments with the use of in-situ TEM experiments. Microstructure characterizations at different annealing temperatures and oxygen partial pressures are observed and coupled with phase and orientation analysis using precession electron diffraction techniques. Overall, this work provides a foundation for understanding the stability window for candidate HEAs in extreme environments. Therefore, these results are discussed in the context of the growing literature comparing the ideal methods for stabilizing mechanisms in HEAs for use in high temperature, corrosive environments.

4:10 PM
High Temperature Oxidation of High Entropy Nb-Cr-W-Ta-V Alloy: *Shailendra Varma*[1]; Sabastian Moncayo[1]; Ramana Chintalapalle[1]; [1]University of Texas
Microstructure and high-temperature oxidation behavior of high entropy Nb-Cr-W-Ta-V alloy has been explored in this study. High temperature oxidation studies in the temperature range of 600-1400oC indicated interesting phase evolution in the alloy. The chemical composition and microstructure analysis of the oxide layer was analyzed in order to understand the mechanism involved in the oxidation process. The V-oxide appears in a perfectly whisker morphology while other oxides appear in crystalline forms with either granular, more or less, or tube/cylindrical morphologies. A more detailed account of the microstructure and oxidation behavior of the Nb-Cr-W-Ta-V alloy will be presented.

4:30 PM
Role of Oxidation on the Thermal Expansion of Refractory MoWTaTiZr High Entropy Alloy: *Eric Osei-Agyemang*[1]; Ganesh Balasubramanian[1]; [1]Lehigh University
Though Ni-based superalloys exhibit superior performance at moderate temperatures, the quest for new class of materials becomes desirable at elevated temperatures and extreme working conditions as Ni-based superalloys have low melting temperatures. High entropy alloys (HEA) from refractory elements may achieve higher temperature operations with superior creep strength. At elevated temperatures, Mo based HEAs exhibit good thermal and mechanical properties. Recently, a refractory Mo-W-Ta-Ti-Zr HEA was observed to exhibit greatly enhanced modulus of elasticity (3x at 300K) over near atomic cases with higher moduli above 500K over commercial alloys (2.3x at 2000K). The usability of the recently identified Mo-W-Ta-Ti-Zr HEA in both clean and oxidized form at extreme working conditions is required. In this study, Quasi-Harmonic Approximation method is used to estimate the coefficient of thermal expansion for clean as well as fully oxidized refractory Mo-W-Ta-Ti-Zr HEA. We discuss the effect of oxidation on mechanical properties and associated deformation mechanisms

4:50 PM
Electrochemical Preparation of Different Classes of High-entropy Materials for Advanced Applications: *Jagadeesh Sure*[1]; D. Sri Maha Vishnu[1]; Carsten Schwandt[1]; [1]University of Nizwa and University of Cambridge
For the first time, our Group has demonstrated the preparation of different classes of high-entropy materials, including alloys and carbides of four and five equi-atomic components, by electrochemical deoxidation of metal oxide mixtures in molten CaCl2. Varying the experimental conditions, in terms of starting precursor mixture, processing temperature and time, provided different materials of diverse morphologies, ranging from nano-powders to porous or dense 3D objects, as they are in demand for energy, bio and structural applications. The materials prepared were found to be hard and strong, owing to solution strengthening, and showed excellent mechanical and corrosion properties.Overall, this research has provided a bridge between the concepts of electro-deoxidation in molten salts and the concept of high-entropy materials. The novel findings promise a straightforward, low-energy and cost-affordable electrometallurgical process to produce high-entropy alloys and compounds for advanced applications in large quantities. The presentation highlights results of all these studies.

Alloy Design and Processing II

Tuesday PM
November 19, 2019

Room: Cobalt
Location: Hyatt at Olive 8

3:50 PM
Superior Tensile Properties of 1%C-CoCrFeMnNi High-entropy Alloy Additively Manufactured by Selective Laser Melting: *Hyoung Seop Kim*[1]; Jeong Min Park[1]; Jungho Choe[2]; Jung Gi Kim[1]; Jae Wung Bae[1]; Jongun Moon[1]; Sangsun Yang[2]; Kyung Tae Kim[2]; Ji-Hun Yu[2]; [1]Pohang University of Science and Technology; [2]KIMS
CoCrFeMnNi high-entropy alloys containing 1 at% carbon (C-HEAs), were additively manufactured using selective laser melting (SLM) at two different laser scanning speeds. Superior tensile properties of the as-built C-HEA (to previously reported ones) were achieved by utilizing multiple strengthening mechanisms (i.e., solid solution, grain refinement, dislocation density, and nano-precipitation). In particular, combining higher dislocation density and more nano-precipitates with the slower SLM scanning process resulted in C-HEA with enhanced yield strength and reasonable ductility.

4:10 PM

Exploration of the Solid–Solution Space in the Co–Cr–Fe–Ni System via Rapid Alloy Selection and Synthesis Methods: *Karl Shamlaye*[1]; Manisha Senadeera[1]; Santu Rana[1]; Sunil Gupta[1]; Svetha Venkatesh[1]; Daniel Fabijanic[1]; Matthew Barnett[1]; [1]Deakin University

The FCC-structured equimolar CoCrFeNi alloy has been extensively studied, yet only a small single-phase solid solution region about this composition has been found thus far. A greater solid solution range can vastly enhance alloy design, tailoring complex alloy properties by changes in the base elements. We employ machine learning algorithms to efficiently search a CALPHAD high entropy alloy thermodynamic database, screening for FCC compositions, to identify the extent of the single-phase solid solution region. Rapid synthesis of selected alloys is then done via additive manufacturing, and resulting specimens can be batch-analysed by x-ray diffraction and scanning electron microscopy. Using this high-throughput method, we show that a very wide FCC-phase region actually exists in the Co–Cr–Fe–Ni system. Thus, confidence can be built up to use similar rapid alloy selection and development methods to obtain single-phase compositions in more complex alloy systems.

4:30 PM

Vaporizing Foil Actuator Welding of Equimolar CrCoNi—weld Zone Structure and Joint Strength Characterization: *Blake Barnett*[1]; Connor Slone[1]; Anupam Vivek[1]; Michael Mills[1]; Glenn Daehn[1]; [1]Ohio State University

Medium-entropy alloys (MEA's) such as equimolar CrCoNi have shown promise of exceptional mechanical performance with good phase stability over a wide range of operating conditions. Solid-state processing technologies offer a manufacturing route for medium and high-entropy alloys that preserve microstructures and mechanical properties for enhanced performance compared to traditional thermomechanical processing techniques. Vapoirzing Foil Actuator Welding (VFAW) has been demonstrated to create solid-state welds with no changes in the phases present or production of heat-affected zones across a wide range of similar and dissimilar material couples. VFAW was utilized to form nominally solid-state autogenous CrCoNi welds, which exhibited interfacial grain refinement, as-welded ultimate tensile strength of 1.34 GPa in lap shear samples, with minimal post-weld elemental segregation. Peel testing and fractography also support failure stresses on the order of base material strength with ductile rupture failure modes.

4:50 PM

A High-throughput Laser-processing Method to Study Processing-microstructure-mechanical Property Relationship in a High Entropy Alloy: *Mu Li*[1]; Rohan Mishra[1]; Katharine Flores[1]; [1]Washington University In St. Louis

A direct laser deposition processing method was applied to construct compositional and microstructural AlxCoCrFeNi high entropy alloy libraries in an efficient and high-throughput manner. Among the compositions (x = 0.56 - 1.00) and quench rates (26 - 6400 K/s) studied, despite a crystal structure evolution from dual FCC+BCC to BCC/B2 phase, most of the samples form a dendritic structure, similar to cast counterparts. In addition to significant consistency in phase and microstructures of laser-processed HEAs with cast materials, by controlling laser parameters, change in feature sizes and even phase structures, which indicates a different solidification mechanism, can be achieved. Microstructure-led change in mechanical properties was also investigated. The microhardness vs. dendritic spacing follows a Hall-Petch relation. Ongoing work continues to discuss strengthening contributions for different boundaries. This study suggests that the high-throughput laser processing method is an ideal method for rapidly and efficiently evaluating multiprincipal element alloys.

Functional Properties III

Tuesday PM
November 19, 2019

Room: Cyan
Location: Hyatt at Olive 8

3:50 PM

Shape Memory Effect in the CrMnFeCoNi Alloy System: *Je In Lee*[1]; Koichi Tsuchiya[2]; Wataru Tasaki[2]; Hyun Seok Oh[3]; Takahiro Sawaguchi[2]; Hideyuki Murakami[2]; Eun Soo Park[3]; [1]Pusan National University/ National Instititue for Materials Science; [2]National Institute for Materials Science; [3]Seoul National University

High-entropy alloys (HEAs), which consist of multi-principal elements with near equiatomic composition, have generated substantial interest for the development of new materials with exceptional properties. Here, we demonstrate a strategy of designing HEAs with shape memory effect in the CrMnFeCoNi alloy system. We calculate the difference in Gibbs free energy between face-centered-cubic and hexagonal-close-packed phases, and find a substantial increase in thermodynamic equilibrium temperature between both phases through composition tuning, leading to thermally- and stress-induced martensitic transformations. Shape recovery temperature in non-equiatomic CrMnFeCoNi HEAs can be increased to 698 K, which is much higher than that of conventional shape memory alloys (SMAs) and comparable to that of B2-based multicomponent SMAs containing noble metals (Pd, Pt, etc.) or refractory metals (Zr, Hf, etc.). This result opens a vast field of applications of HEAs as a novel class of cost-effective high-temperature SMAs.

4:10 PM

High Entropy Shape Memory Alloys - Multi-component Intermetallic Compounds for Extended Lifetime Shape Memory Actuators: *Georgiy Firstov*[1]; Tetiana Kosorukova[1]; Andrey Timoshevskii[1]; Yuri Koval[1]; Valeriy Odnosum[1]; Christian Hinte[2]; Gregory Gerstein[2]; Hans Maier[2]; [1]G.V. Kurdyumov Institute for Metal Physics of the National Academy of Sciences o; [2]Institut für Werkstoffkunde (Materials Science) Leibniz Universität Hannover

Application of the existing shape memory alloys (SMA), NiTi in particular, has been reduced almost exclusively to the medical sector. This is a significant shortcoming of actuator potential, comparing with other materials like piezoelectrics. This is caused by functional fatigue effects of SMA, which make them unsuitable for industrial use. First and foremost, the high entropy alloy concept has been successfully combined with the possibility to initiate martensitic transformation (MT) and, consequently, shape memory behavior. So, the TiZrHfCoNiCu system exhibited a B2B19` MT. Peculiar crystal and electronic structure results in severe distortions of the lattices involved in MT and ensures high strength that favors martensitic deformation, while suppressing plastic one. Similar structure formation was confirmed for CoNiCuAlGaIn intermetallic that exhibits a $B2L1_0$ MT. Present report will include latest developments regarding major improvement in structure - properties relationship for these novel shape memory materials and their application perspective will be discussed.

4:30 PM
Mechanical Testing and Fatigue Behavior of Nickel-Titanium High Entropy Shape Memory Alloys: *Christian Hinte*[1]; David Piorunek[2]; Jan Frenzel[2]; Gregory Gerstein[1]; Mark Swider[1]; Gunther Eggeler[2]; Hans Maier[1]; [1]Leibniz Universität Hannover - Institut für Werkstoffkunde (Material science); [2]Ruhr Universität Bochum - Lehrstuhl Werkstoffwissenschaft (Material science)
In addition to unique properties such as pseudoelasticity and the shape memory effect, shape memory alloys usually also possess the negative aspect of an increased functional fatigue tendency due to degradation and thermal cycling. This has led to the development of new materials that extend the range of operating temperatures and reversibility of martensitic transformation. Based on conventional nickel-titanium high entropy alloys with the composition TiZrHfCoNiCu and their variants have been developed. In order to determine the influence of the chemical composition on the phase stability, the mechanical properties and the formation of martensite, binary to senary alloys of the material class were investigated. Static mechanical parameters were determined by means of compression tests while fatigue behaviour was characterized by 3-point bending tests. Initial mechanical tests showed high compressive strengths of up to 2500 MPa with high elongation of up to 20 %.

4:50 PM
NiTi Based High Entropy Shape Memory Alloys: *Malesela Mahlatji*[1]; Daniel Salas[1]; Kadri Atli[1]; Ibrahim Karaman[1]; [1]Texas A&M University
Quinary alloying of NiTi shape memory alloy (SMA) with Hf, Zr, and Cu has recently been demonstrated to increase the transformation temperatures, work output and strength levels through the high entropy and solid solution effects, rendering these alloys attractive for a plethora of applications. This study reports on the shape memory characteristics of Ni50-xCux (TiHfZr)50 (0 ≤ x ≤ at.% Cu ≤ 25) high entropy SMAs with equal amounts of Ti, Hf and Zr to maximize the configurational entropy. All compositions display the single-step B2-B19' martensitic transformation, with transformation temperatures reducing from 600C to 150C with increasing Cu content. In addition to the presence of oxygen stabilized Ti2Ni type precipitates in all solution heat treated compositions, aging and thermal cycling result in a complex microstructure with additional precipitate types. Identification of these precipitates as well as their effect on transformation behavior is part of ongoing work and will be presented.

Wednesday Plenary

Wednesday AM
November 20, 2019
Room: Ballroom ABC
Location: Hyatt at Olive 8

8:00 AM Plenary
Refractory Complex Concentrated Alloys for High Temperature Applications: Opportunities and Challenges: *Oleg Senkov*[1]; [1]Air Force Research Laboratory
Refractory complex concentrated alloys (RCCAs), which also include refractory high entropy alloys, are widely studied as candidates for high temperature applications. They are based on three or more refractory elements, have BCC or B2 matrix and may have non-refractory elements and secondary phases. Knowledgeable selection of alloying elements allows production of RCCAs with a wide range of densities and mechanical properties. Simultaneous presence of BCC and B2 phases in some of RCCAs may result in a coherent, superalloy-like nano-phase structure and unique mechanical properties. This new field of research still experiences many challenges, and the effects of the combinations of the alloying elements, thermal and thermo-mechanical processing conditions on the microstructure, mechanical properties and oxidation behavior need to be understood. High-temperature strengthening and deformation mechanisms operating in RCCAs need to be explored. This talk will review current RCCA efforts and will develop ideas to guide future research.

8:45 AM Question and Answer Period

8:55 AM Break

Fundamental Theory and Computational Modeling

Wednesday AM
November 20, 2019
Room: Azure
Location: Hyatt at Olive 8

9:00 AM Keynote
Emerging Computational Tools for Exploring the Refractory Compositionally Complex Alloys: *Christopher Woodward*[1]; Satish Rao[2]; Edwin Antillon[2]; A Brahim[2]; Triplicane Parthasarathy[2]; Daniel Miracle[1]; Oleg Senkov[2]; [1]Air Force Research Laboratory; [2]Air Force Research Laboratory/UES Inc.
We review a range of computational methods for predicting fundamental properties and mechanisms controlling material response in Refractory Compositionally Complex alloys. A spreadsheet model of expected density, atomic size difference, mixing enthalpy, melting temperatures, cost, and CALculation of PHAse Diagram predictions of equilibrium phases can be used to narrow the pallet of possible elements for a specific application. Electronic structure methods can also be used to predict mean field properties such as elastic constants, as well as insights into deformation mechanisms. Atomistic methods have been used to better understand deformation over a wide range of temperatures, the role of chemical short range order, and inform analytic solution strengthening models. Also, new approaches for predicting phase stability for wide range of compositionally complex alloys are in development.

9:30 AM
Insights into Refractory Multi-principal Component Alloys from Machine-learning Interatomic Potentials: *Xiangguo Li*[1]; Chi Chen[1]; Hui Zheng[1]; Shyue Ping Ong[1]; [1]University of California San Diego
Refractory multi-principal component alloys (RMPEs) show great potential in high-temperature applications due to their exceptional properties. In this work, we present a spectral neighbor analysis potential (SNAP) model for the Ta-Nb-Mo-W RMPE system by machine learning a carefully constructed computed data set of elemental and multicomponent compounds. We demonstrate that this quaternary SNAP model can achieve near-quantum accuracy in the prediction of a broad range of properties, including energies, forces, elastic properties, melting points, generalized stacking fault energies, etc. By applying this highly-accurate SNAP in atomistic simulations, we present insights into the edge dislocation motion in the Ta_{0.25}Nb_{0.25}Mo_{0.25}W_{0.25} RMPE alloy, outlining the mechanisms behind its improved mechanical properties compared to the component elements.

9:50 AM
A Machine Learning Model for Alloy Design: *Zhaohan Zhang*[1]; Mu Li[1]; Katharine Flores[1]; Rohan Mishra[1]; [1]Washington University in St.Louis
Developing fast and accurate methods to promote alloy discovery is of practical interest, especially with the vast composition space offered by multi-principal element alloys (MPEAs). While density-functional-theory (DFT)-based methods have accelerated design of binary and ternary alloys, they are not amenable for rapidly screening the vast combinatorial space of MPEAs. We develop a machine-learning model for predicting the DFT-calculated formation enthalpy of alloys and use it to identify stable alloys. The model uses easily accessible elemental properties as descriptors and has a mean absolute error (MAE) of ~ 6 meV/atom when compared to the formation enthalpy of binary alloys obtained using DFT. We use the ML model to successfully identify new binary alloys that are subsequently confirmed using DFT and experiments. We further apply it to MPEAs to predict the formation of single-phase solid solutions with bcc and fcc structures.

10:10 AM Break

Mechanical Properties and Irradiation Resistance

Wednesday AM
November 20, 2019

Room: Cobalt
Location: Hyatt at Olive 8

9:00 AM Keynote
Abnormal Strengthening Mechanism and Deformation Behavior of (TaNb)HfZrTi High-entropy Alloys: *Zhaoping Lu*[1]; [1]University of Science and Technology Beijing
High-entropy alloys (HEAs) have shown great potential to be utilized as engineering materials due to their high phase stability, large lattice distortion and complex chemical short-range ordering. The strengthening behavior and underlying mechanisms in these highly concentrated matrices attracted more and more attention due to both scientific interests and technological importance. In this talk, focuses will be placed on strengthening mechanism and deformation behavior of (TaNb)HfZrTi high-entropy alloys: 1) Interstitial solid-solution hardening; abnormal effects of interstitial oxygen atoms on deformation behavior will be discussed, 2) Transformation mediated strengthening; mechanisms of transformation-induced-plasticity will be explored, and 3) Resettable mechanical properties; effects of pre-straining on deformation behavior will be analyzed.

9:30 AM
The Design of Reduced Activation Damage Resistant High-entropy Alloys for Next-generation Nuclear Systems: *Ed Pickering*[1]; Alex Carruthers[1]; Bo-Shiuan Li[2]; Jason Burnap[3]; R Mythili[4]; Chanchal Ghosh[4]; C David[4]; A Saikumaran[4]; Raghvendra Tewari[5]; Arup Dasgupta[4]; Angus Wilkinson[2]; David Armstrong[2]; Amy Gandy[3]; [1]University of Manchester; [2]University of Oxford; [3]University of Sheffield; [4]Indira Gandhi Centre for Atomic Research; [5]Bhabha Atomic Research Centre
A potential future application of HEAs is as structural materials for advanced next-generation fission and fusion reactors, where both high temperatures and high levels of neutron irradiation are likely to be experienced. The majority of the alloys we commonly use for high-temperature structural applications, such as nickel base superalloys, are unsuitable for advanced nuclear reactor environments for two reasons: first, because they often possess an FCC crystal structure, which is susceptible to irradiation swelling, and second, because they tend to comprise significant concentrations of elements that activate strongly when irradiated and stay activated for very long periods of time. In this presentation, we discuss the design strategy and initial investigation of a number of low-activation HEAs that have been produced and analysed as part of collaboration between partners in the UK and India. Alloy microstructures, characterised using advanced high-resolution microscopy techniques, are compared to those predicted using CALPHAD software.

9:50 AM
Towards V-based High Entropy Alloys for Fusion Blanket Applications: *Paul Barron*[1]; Michael Preuss[1]; Michael Gorley[2]; Ed Pickering[1]; [1]University of Manchester; [2]Culham Centre for Fusion Energy
Conditions inside nuclear fusion reactors involve extremes of both temperature and neutron irradiation. Directly adjacent to the fusion plasma in a Tokamak reactor is the blanket. It serves to protect the Tokamak's superconducting magnets and supporting structures from high temperatures and energetic neutrons. It also captures the energy given off from the fusion reaction. To minimise radioactive waste, it is desirable that the blanket is made from materials that do not significantly activate when irradiated. By mixing elements with favourable activation properties to create high entropy alloys, it may be possible to make a material that has the properties required to withstand a fusion environment while minimising waste produced. A suite of previously unexplored V-Cr-Mn-Ti alloys have been fabricated and we have characterised the microstructures that have evolved under a range of fusion-relevant temperatures over times of up to 1000 hrs to determine potential suitability for fusion blanket structures.

10:10 AM Break

Computational Modeling II

Wednesday AM
November 20, 2019

Room: Cyan
Location: Hyatt at Olive 8

9:00 AM Keynote
Origins of High Temperature Strengthening in BCC HEAs: *William Curtin*[1]; F Maresca[1]; [1]Ecole Polytechnique Federale de Lausanne
BCC High Entropy Alloys (HEAs) consist of many elements distributed at random on the BCC lattice. The collective fluctuations in solute/dislocation interaction energies, even in dilute binary BCC alloys, lead to the spontaneous energy-lowering formation of a kinked/wavy structure for both screw and edge dislocations, respectively, over characteristic lengths ζc,screw and ζc,edge. Dislocation motion starting from the kinked/wavy structure is determined by the energetics at scale c. New general theories for both screw and edge motion in BCC alloys starting from this basic phenomenon are presented. The screw theory is sketched briefly, and shown to accurately predict strength versus composition and temperature in Nb-Mo and Nb-W binary alloys. As for BCC elements, the necessary inputs are difficult to establish, especially in more complex alloys. Key comparisons to simulations help demonstrate major features of the theory. More importantly, the edge theory shows that edge strengthening can be sufficient to compete with screw strengthening. Moreover, edges can control strengthening, especially at high temperatures, in some BCC HEAs. The edge theory, for which all inputs can be computed easily, explains (i) the exceptional retention of strength measured in MoNbTaW and MoNbTaVW at temperatures up to 1900K, and (ii) why the V-containing alloy is stronger. The edge theory can be reduced to a simplified analytic form that enables efficient computationally-guided design of new alloy compositions predicted to have high retained strengths and strength-to-weight ratios. Several new compositions are proposed. The combination of both screw and edge theories enables assessment of strengthening versus composition and temperature across the entire domain of Cr-Mo-Nb-Ta-V-W-Hf-Ti-Zr BCC HEAs.

9:30 AM
Dislocation Dynamics in $Co_{0.4}Ni_{0.4}Ru_{0.2}$ Multi-principal Element Alloys: A Phase-field-based Study: *Shuozhi Xu*[1]; Yanqing Su[1]; Irene Beyerlein[1]; [1]University of California, Santa Barbara
Dislocations are main carriers of plastic deformation in metals. In a face-centered cubic (FCC) metal, a full dislocation is usually dissociated into two partial dislocations, within an intrinsic stacking fault (ISF) in-between. In otherwise defect-free FCC pure metals, the ISF width changes slightly as a dislocation line glides or a dislocation loop expands. In multi-principal element alloys (MPEAs), however, the local chemical composition fluctuations lead to spatially varying material properties and hence a significant variation in dislocation core structures. In this work, we employ a phase-field dislocation dynamics method to simulate gliding of dislocation lines and expansion of dislocation loops in $Co_{0.4}Ni_{0.4}Ru_{0.2}$ MPEAs with an underlying FCC lattice. It is found that, the ISF width varies along the same dislocation line and fluctuates as the dislocation line glides and the dislocation loop grows. Our simulations confirm that the fluctuations in ISF width in part contribute to the strengthening of MPEAs.

9:50 AM
Ab Initio-informed Phase-field Modeling of Dislocation Core Structures in CoNiRu Multi-principal Element Alloys: *Yanqing Su*[1]; Shuozhi Xu[1]; Irene Beyerlein[1]; [1]University of California Santa Barbara
In this work, we investigate the core structure of dislocations in CoNiRu multi-principal element alloys (MPEAs) using an ab initio-informed phase-field dislocation dynamics (PFDD) method. Both equal-molar $Co_{0.33}Ni_{0.33}Ru_{0.33}$ MPEAs and non-equal-molar $Co_{0.4}Ni_{0.4}Ru_{0.2}$ MPEAs are considered. First, atomic configurations for a given composition are represented by special quasirandom structures. For all atomic configurations, material properties such as the lattice parameter, elastic constants, and gamma surfaces are obtained by density functional theory calculations. Relationships between material properties and local chemical variation are established. It follows that material properties are used as input into a PFDD model to calculate the static core structures of edge and screw dislocations. A large variation in the dislocation core size is found, with the screw dislocation experiencing a greater variation than the edge dislocation. Our results suggest that, unlike in pure metals, the core structure varies along a straight dislocation line in MPEAs.

10:10 AM Break

Fundamental Theory, Alloy Design and Mechanical Properties

Wednesday AM
November 20, 2019

Room: Azure
Location: Hyatt at Olive 8

10:40 AM Invited
It Is Not (Only) the Entropy!: *Raymundo Arroyave*[1]; Claudio Schön[2]; [1]Texas A&M University; [2]University of Sao Paulo
The basic idea of high entropy alloys (HEAs): to produce alloys without choosing one major component, adding alloying elements, is really innovative. The unusual properties and the extreme stability of these multicomponent solid solutions are reality and suggest these alloys will have a positive impact in alloy design from now on. The initial explanation for these unusual properties, however, has found considerable skepticism. The present work reviews results of ab initio simulations in model HEAs with the BCC structure, using the cluster variation method in the irregular tetrahedron approximation. It is shown that these properties can be attributed to a high value of short-range order (SRO) parameters caused by the competition between conflicting interactions, and not to the maximum configurational entropy of the multicomponent alloy. Since entropy plays only a minor role in these properties, it is evident that there is no reason to remain at the equimolar composition.

11:10 AM
Examining the Importance of the 'Entropic Effect' on the Mechanical Properties of HEAs: *Ankit Roy*[1]; Tomas Babuska[1]; Brandon Krick[1]; Pratik Ray[2]; Ganesh Balasubramanian[1]; [1]Lehigh University; [2]Department of Energy, Ames laboratory
HEAs have gained significant attention partly due to the remarkable mechanical properties demonstrated by certain compositions. While an increase in the configurational entropy by incorporating higher number of constituent elements in single-phase FCC HEAs does not guarantee enhanced mechanical properties, the role that the number and choice of elements play remains relatively inconclusive. We examine alloys formed by the binary, ternary, quaternary and quinary equiatomic combinations of refractory Mo-Ta-Ti-W-Zr multi-principal elements for their phase and mechanical properties (Young's Modulus and Vickers hardness). We find that only a subset of all possible equiatomic compositions form single phase BCC structures, and more intriguingly, the low and medium entropy alloys demonstrate enhanced properties relative to their higher-entropy counterparts. We probe the fundamental causes arising from element selection and the resulting microstructure on the mechanical properties, and understand the dependence of solid-solution hardening on the number and specificity of the elements in these HEAs.

11:30 AM
Effect of Co and Fe on the Phase Stability of CrMnFeCoNi High Entropy Alloys Following Long-duration Exposures at Intermediate Temperatures: *Maximilian Bloomfield*[1]; Kathy Christofidou[1]; Nick Jones[1]; [1]University of Cambridge
The equiatomic CrMnFeCoNi alloy is one of the most widely studied HEAs and whilst it exhibits many useful properties, the precipitation of sigma phase below 800°C makes it unsuitable for structural applications at elevated temperatures. There is, therefore, an interest in developing non-equiatomic alloys from the CrMnFeCoNi system that suppress sigma formation and offer enhanced mechanical properties. However, effective alloy design requires knowledge of how compositional variations influence phase stability. Here we report experimental studies that establish the effect of Co and Fe on the phase stability in the $CrMnFeCo_xNi$ and $CrMnFe_xCoNi$ systems, where x = 0, 0.5, 1.5, following heat treatments of at least 1000 hours at 500, 700 and 900°C. Both elements stabilise the *fcc* solid solution phase and their removal leads to the bulk formation of multiple intermetallic phases. Using this data an assessment of the fidelity of current thermodynamic predictions will be made.

11:50 AM
Atomic-scale Investigation of Deformation Substructures of High Entropy Alloy CoCrFeMnNi Subjected to High Strain Rates: *Daniel Foley*[1]; Shang-Hao Huang[1]; Elaf Anber[1]; Logan Shanahan[1]; Christopher Barr[2]; Andrew Lang[1]; Leslie Lamberson[1]; Mitra Taheri[1]; [1]Drexel University; [2]Sandia National Laboratories
The single-phase high entropy alloy (HEA) CoCrFeMnNi is an interesting material not only due to its interesting physical properties, but also because it is a unique framework to study otherwise conventional deformation mechanisms of FCC alloys. Owing to its chemical disorder, this alloy is thought to possess unique properties such as a localized, non-uniform stacking fault energy and a highly distorted lattice, both of which can be contrasted with conventional single-phase alloys. In the present study we investigate the microstructures of single-phase CoCrFeMnNi deformed at high strain rate via Kolsky compression testing. We quantitatively analyze the deformation microstructures using electron backscatter diffraction in SEM, as well as precession electron diffraction in TEM. We observe the formation of both deformation twins and microbands in dynamically loaded specimens and attribute these features in part to the unique atomic structure of HEAs.

Alloy Design I

Wednesday AM
November 20, 2019

Room: Cobalt
Location: Hyatt at Olive 8

10:40 AM Invited
Phase Inversion in Refractory High Entropy Alloys: V Soni[1]; T Alam[1]; S Dasari[1]; B Gwalani[1]; O. N. Senkov[2]; D Miracle[3]; *Rajarshi Banerjee*[1]; [1]University of North Texas; [2]UES Inc.; [3]Air Force Research Laboratory
Refractory high entropy alloys (RHEAs), consisting of a BCC+B2 microstructure, have been reported to exhibit higher strengths at elevated temperatures, as compared to conventional nickel base super alloys. However, the ductility of these alloys has often been limited due to the continuous B2 matrix in these alloys, such as for example, the Al0.5NbTa0.8Ti1.5V0.2Zr RHEA. The ductility of this alloy was dramatically improved by inverting its microstructure from "BCC precipitates in a B2 matrix", to "B2 precipitates in a BCC matrix" via isothermal annealing experiments. This microstructural evolution leading to the phase inversion, has been investigated in great detail by coupling transmission electron microscopy (TEM), atom probe tomography (APT), and some high-energy beam synchrotron experiments. With the aim to increase this BCC+B2 phase field to elevated temperatures, the microstructural stability of single phase B2 compositions, derived from these alloys, has also been investigated.

11:10 AM
Tailoring Microstructure of Refractory High Entropy Superalloy through a Bulk Combinatorial Approach: *Sangjun Kim*[1]; Hyunseok Oh[1]; Kook Noh Yoon[1]; Eun Soo Park[1]; [1]Seoul Nation University
Recently, various refractory high entropy superalloys, which have unique microstructure containing cuboidal nano-precipitates in BCC high entropy alloy (HEA), reported. They exhibited superior mechanical properties at both ambient and high temperature. However, there are many unsolved issues to attract even greater attention such as precipitation control of unwanted compounds, optimal phase selection between ordered and disordered BCC, and optimization of mechanical properties etc. In the present study, we propose how to tailor the microstructure of refractory high entropy superalloy through a bulk combinatorial approach in Ti-Hf-Nb-Al quaternary HEAs. Microstructural evolution for the non-equiatomic HEA compositions obtained by a bulk combinatorial approach were systematically investigated by considering phase transformation mechanism as well as phase equilibria. This result could provide an effective guideline for tailoring microstructure of HEAs with ordered and disordered BCC phases, and developing a promising high entropy superalloy with customized microstructure for ultra-high temperature structural application.

11:30 AM
Grain Boundary Segregation Behavior of Mechanically-alloyed Refractory High Entropy Alloys: *Joshua Smeltzer*[1]; B. Hornbuckle[2]; Anit Giri[2]; Christopher Marvel[1]; Kristopher Darling[2]; Jeffrey Rickman[1]; Helen Chan[1]; Martin Harmer[1]; [1]Lehigh University; [2]U.S. Army Research Laboratory
Grain boundaries are known to affect bulk material behavior and dictate mechanical, thermal, and electrical properties. However, the role of grain boundaries in high entropy alloys is relatively unexplored as there are several open questions regarding the thermodynamic and kinetic behavior of grain boundaries in these complex microstructures. Here, a refractory alloy with equimolar Ta, W, Mo, and Nb concentrations was synthesized via high energy ball milling, and transition metal additives were strategically added to modify grain boundary structure and composition to alter thermal (*e.g.* grain growth) and mechanical properties (*e.g.* hardness). Microstructures were examined using aberration-corrected scanning transmission electron microscopy and grain boundaries were characterized via atomic-resolution imaging and energy dispersive spectroscopy. Understanding the role of grain boundary structure and composition in these materials allows for improved design of alloys with superior properties, and hence viability in extreme environment applications.

11:50 AM
Microstructural Evolution of Refractory Metal Additions to the CrFeCoNi High Entropy Alloys: *Katerina Christofidou*[1]; James Miller[1]; Ed Pickering[2]; Howard Stone[1]; Nick Jones[1]; [1]University of Cambridge; [2]University of Manchester
Transition metal high entropy alloys have been the subject of multiple studies due to their potential suitability for structural applications. In particular, the CrFeCoNi alloy has been shown to be single phase at all temperatures, and hence is an appropriate alloy for further development. However, as alloying with other transition elements has only resulted in limited strengthening benefits, it is necessary to consider alternative strategies. Herein, the additions of Nb and Mo are considered due to their potency as solid solution strengthening elements. Alloys containing additions and co-additions of Nb and Mo of up to 10 at.% were cast, homogenised and aged for 1000 hours at temperatures between 500–900°C. The resulting microstructures were characterised using microscopy and diffraction methods and the hardness of the alloys was examined to determine the efficacy of the alloying strategy. These observations have been further explored using thermodynamic modeling.

Mechanical Properties and Processing I

Wednesday AM
November 20, 2019

Room: Cyan
Location: Hyatt at Olive 8

10:40 AM Invited
Slip Systems and Dislocation Mobility in Refractory Multi-principal Element Alloys: Fulin Wang[1]; Paul Rottmann[1]; Leah Mills[1]; Jean-Charles Stinville[1]; Glenn Balbus[1]; Oleg Senkov[2]; Dan Gianola[1]; *Tresa Pollock*[1]; [1]University of California, Santa Barbara; [2]Air Force Research Laboratory
New techniques for examination of dislocation mobility and grain-scale activation of slip systems have been employed to study the plastic behavior of equiatomic MoNbTi and HfNbTaTiZr multi-principal element (MPE) alloys in comparison to pure Nb and Ta. Dislocation dynamics have been studied via in-situ straining with custom MEMs devices combined with scanning transmission electron microscopy (TSEM) detectors in a scanning electron microscope platform. Differences in the relative motion of edge vs. screw segments in MPE alloys in comparison to BCCs have been investigated. Complementary TEM studies of indentation-induced debris will be discussed. Additionally, a new digital image correlation technique that employs Heaviside functions to detect slip discontinuities and examine the onset, relative activity and planarity of individual slip planes within individual grains during monotonic straining has been applied. Differences in the pure BCCs compared to the equiatomic MPEs will be discussed.

11:10 AM
Modeling and Experimental Validation of Refractory CCA Solidification and Homogenization: *David Smathers*[1]; Cameron McNamara[1]; Marie Thomas[2]; Chris Kantner[2]; [1]H. C. Starck Inc.; [2]QuesTek Innovations
A CALPHAD-informed Integrated Computational Materials Engineering (ICME) has been used to identify novel refractory Complex Complimentary Alloy (CCA) compositions of interest. However, the design and scale-up of these alloys is still a significant challenge, and practical production of CCAs towards a specific commercial product has yet to be demonstrated. This paper describes results from an experimental program to evaluate their melting, solidification, and homogenization characteristics. Additionally, homogenization results are compared to simulation to assess the accuracy of predictive tools. Prototype 15 lb. ingots of 5 Nb-based CCA compositions identified using high throughput methods were vacuum arc melted, processed and evaluated to understand challenges associated with the scale-up of this class of alloy from button to lab ingot. In addition to characterizing the solidification behavior and as-cast microstructure, the impact of aluminum content on the various homogenization cycles was studied for each alloy and compared to DICTRA simulations.

11:30 AM
Heat Treatment and Property Optimization Study of Refractory Complex Concentrated Alloys: *Cameron McNamara*[1]; David Smathers[1]; Marie Thomas[2]; Chris Kantner[2]; [1]H. C. Starck Inc.; [2]QuesTek Innovations
Complex Concentrated Alloys (CCAs), particularly those containing refractory elements, have the potential to surpass current high temperature alloy performance. A CALPHAD-informed Integrated Computational Materials Engineering (ICME) approach has been used to identify novel refractory CCA compositions of interest for these applications. This paper describes results from an experimental program evaluating the effect of solution treatment and artificial aging on microstructure and mechanical properties of five Nb-based alloys. Prototype 15-lb ingots were cast, homogenized, and thermo-mechanically processed to produce material for this study. Solution and aging experiments were performed to validate calculated phase behavior and suggest temperature ranges in which to optimize processing and mechanical properties. Microstructural characterization and mechanical testing were performed to develop the process-structure-property relationship for these refractory CCAs.

11:50 AM

Synthesizing Refractory High Entropy Alloys (HEAs) of 3rd Generation by Selective Electron Beam Melting (SEBM) Using Elemental Powders Blend: *Alexander Katz-Demyanetz*[1]; Vladimir Popov[1]; Eyal Eshed[1]; Aleksey Kovalevsky[1]; Natalya Larianovsky[1]; Andrey Koptyug[2]; Menachem Bamberger[3]; [1]Technion Research and Development Foundation; [2]Sports Tech Research Centre, Mid Sweden University; [3]Department of Materials Science and Engineering, Technion - Israel Institute of Technology

Despite the high potential of HEAs, their implementation is complicated because of necessity to use vacuum arc melting, which may be difficult because of the difference in melting points and vapor pressures of the alloying elements at high temperatures. Furthermore, the castability of such liquid blend in insufficient to obtain a homogeneous material. The alternative trials to synthesize refractory HEAs is Additive Manufacturing thermal routes like EBM and SLM, at which pre-alloyed powders made by powder metallurgy route are used as raw material. The current work reports on synthesizing Al0.5CrMoNbTa0.5 alloy by SEBM from elemental powders blend. Samples characterization was done by SEM/EPMA, XRD. Though no completely homogeneous microstructure was achieved, the as-printed material was composed of the zones with two multi-component solid solutions, confirming in situ alloying. The main conclusion is that the production of Al0.5CrMoNbTa0.5 alloy from elemental powders blend using SEBM technique is achievable.

Alloy Design and Mechanical Properties (RHEAs)

Wednesday PM
November 20, 2019

Room: Azure
Location: Hyatt at Olive 8

1:30 PM Invited

On the Deformation Mechanisms of a B2 Refractory Complex Concentrated Alloy: *Jean-Philippe Couzinie*[1]; Oleg Senkov[2]; Vishal Soni[3]; Raj Banerjee[3]; Dan Miracle[2]; [1]Université Paris Est, ICMPE (UMR 7182) CNRS-UPEC; [2]Materials and Manufacturing Directorate, Air Force Research Laboratory, Wright-Patterson AFB; [3]Advanced Materials and Manufacturing Processes Institute, University of North Texas

Among the most promising candidates for high temperature structural applications, refractory complex concentrated alloys are serious candidates achieving - in some specific cases - superior mechanical properties to some nickel-based superalloys. In that respect, the most impressive results are currently obtained for B2 or BCC/B2 microstructures which may retain high specific strengths up to 120 MPa.cm^3.g^{-1} at 1000°C. Thus, and to gain more insights into such enhanced properties, the present work aims at studying the behavior of a TiZr-rich B2 single phase material. After induction melting and appropriate heat treatments, the alloy is subjected to uniaxial compressive testing under quasi static conditions at room temperature. Attention will be drawn to the relationships between mechanical properties and underlying deformation mechanisms analyzed by post-mortem transmission electron microscopy observations. Results will also be discussed and compared with other classical B2 compounds.

2:00 PM

Mechanical Properties of Single-phase Refractory High Entropy Alloys: *Francisco Coury*[1]; Michael Kaufman[2]; Amy Clarke[2]; [1]Universidade Federal de São Carlos; [2]Colorado School of Mines

Refractory High Entropy Alloys (RHEAs) are a new and promising class of metallic alloys for structural applications at elevated temperatures. RHEA alloy development is challenging, due to the vast composition space characteristic of these multicomponent alloys. Predictive models are paramount for their development, so alloy design does not need to rely on trial-and-error experimentation. Unfortunately, the fundamentals that determine the solid-solution strengthening of RHEAs are not fully understood. In this work, compression stress-strain curves of seven RHEAs were generated at temperatures from room temperature to 1000 °C. The results are interpreted using a combination of models available for conventional body centered cubic (BCC) alloys. The temperature dependence of these alloys is interpreted to gain insight on the fundamentals of solid solution strengthening on the multicomponent field of BCC RHEAs.

2:20 PM

Precipitation Behaviour and Mechanical Properties of Complex Concentrated Alloy in the AlMoTaTi System: *Daniel Schliephake*[1]; Alexander Medvedev[2]; Andrey Molotnikov[1]; Xinhua Wu[1]; [1]Monash University; [2]RMIT

The development of refractory complex concentrated alloys (RCCAs) attracts a lot of attention to replace Nickel based superalloys as structural high-temperature materials. Recently, a superalloy like microstructure was found in several systems, including alloys based on the AlMoNbTaTiZr system. However, instead of forming fcc/L12 phases, the microstructure consists of bcc/B2. While having promising mechanical properties at temperatures around 1000°C, some alloy compositions even show room temperature ductility in compression. However, the effect of each alloying element on the microstructure and the mechanical properties is still not clear, yet. This talk aims to shed some light on the effect of different alloying elements and heat treatment conditions on the microstructure and mechanical properties in the AlMoTaTi system. Therefore, alloys with varying composition were produced by repetitive arc-melting and heat treated at temperatures up to 1600°C. For microstructural characterization, SEM/TEM were used. Hardness testing and compression testing determined mechanical properties.

2:40 PM

Development and Study of a TiNbMoAlSi Complex Concentrated Alloy with a Body-centered Cubic and Orthorhombic Microstructure: *Antoine Lacour-Gogny-Goubert*[1]; Zhao Huvelin[1]; Philippe Vermaut[2]; Ivan Guillot[3]; Jean-Philippe Couzinié[3]; [1]ONERA; [2]Chimie ParisTech; [3]ICMPE

Refractory complex concentrated alloys (RCCAs) are potential substitutes for nickel or TiAl alloys for high temperature application in aircraft engines, between 800°C and 1000°C. In particular, the Ti-Nb-Al ternary system shows good properties, both microstructural (precipitation of a strengthening, stable orthorhombic phase) and mechanical (good room temperature ductility and high temperature resistance), but its use is limited above 800°C. In order to increase the service temperature of these alloys the effect of refractory elements addition to the ternary system was explored. Following a design method based on diffusion couples, a RCCA TiNbMoAlSi with a body-centered cubic matrix plus orthorhombic precipitates microstructure was elaborated. The microstructural (transmission electron microscopy) and mechanical (compression) properties of this alloy were then assessed in order to ascertain the effect of Mo addition. Moreover, differential thermal analysis was done to determine if Mo addition could extend the stability domain of the O phase at higher temperature.

3:00 PM

Understanding the Microstructure of Refractory Metal High Entropy Superalloys: *Tamsin Whitfield*[1]; Ed Pickering[2]; Howard Stone[1]; Colin Jones[3]; Nick Jones[1]; [1]University of Cambridge; [2]University of Manchester; [3]Rolls-Royce plc.

Refractory Metal High Entropy Superalloys (RMHES) have been proposed as potential successors for Ni-based superalloys in ultra-high temperature applications. These alloys have microstructures containing crystallographically related ordered and disordered phases, good high temperature compressive yield strengths and competitive densities. However, further development of these materials requires a more complete understanding of their underlying metallurgy, in particular the evolution of their microstructure. Understanding the microstructural development of these materials is particularly challenging due to their inherent compositional complexity and relatively little is currently known about the influence of compositional modifications. Here we report on the influence that systematic compositional variations have on the microstructural evolution and phase equilibria of simplified ternary and quaternary RMHES systems. The results provide a knowledge base that will underpin the development of more complex RMHES in the future.

3:20 PM Break

HEA Thin Films

Wednesday PM
November 20, 2019

Room: Cobalt
Location: Hyatt at Olive 8

1:30 PM Invited
Discovery and Optimization of High Entropy Alloys Using Combinatorial and High-throughput Methods: A. Savan[1]; Y. J. Li[1]; T. Löffler[1]; A. Garzón Manjón[2]; M. Meischein[1]; L. Banko[1]; A. Kostka[1]; J. Pfetzing-Micklich[1]; S. Thienhaus[1]; C. Scheu[2]; W. Schuhmann[1]; *Alfred Ludwig*[1]; [1]Ruhr-Universität Bochum; [2]Max-Planck-Institut für Eisenforschung GmbH
The challenge to discover, investigate and optimize new high entropy alloys (HEA) with interesting properties out of their almost unlimited multinary element composition space is addressed by combinatorial fabrication of materials libraries, their high-throughput characterization, and materials informatics for multidimensional data analysis. Thin film HEA libraries are fabricated by co-deposition from five magnetron sputter sources. Resulting composition spreads comprise significant fractions of all possible quinary compositions of the respective system. By using high-throughput x-ray diffraction, the compositional limits of the solid solution existence range and multiphase regions are identified. Functional properties are mapped by high-throughput characterization tools. Furthermore, single-phase HEA may decompose into multiple phases at elevated temperatures or reactive environments: We present an accelerated methodology to investigate HEA phase stability using a combinatorial processing platform and atom probe tomography. By using combinatorial sputtering into ionic liquids nanoparticle libraries are fabricated and we recently discovered excellent electrocatalytic properties of HEA nanoparticles.

2:00 PM
Superhard Nanostructured Thin Films Based on Refractory Type HEA Nitrides: *Joerg Kaspar*[1]; Martin Kuczyk[1]; Tim Krülle[1]; Otmar Zimmer[1]; Martina Zimmermann[2]; Christoph Leyens[1]; [1]Fraunhofer IWS; [2]TU Dresden
Despite a great industrial demand for superhard (hardness > 40 GPa) yet tough thin films with high thermal stability (T > 1000˚C) such films can currently not be synthesized. By combining the material strategy of HEA nitrides with the design concepts of nanostructured thin films it is assumed that new horizons in the combination of these three criteria can be achieved. In the current work preliminary results for the synthesizing of refractory type HEA nitride system (TiVZrNbMo)N and (TiVZrNbHf)N thin films by means of arc deposition technique are presented. The deposited films were thoroughly characterized by structural analysis (SEM, TEM, EDS, XRD) and first attempts on creating a nano-structuring (nano-layers and nano-composites) proved to be successful. Basic screening tests with regard to the mechanical properties could demonstrate that refractory type HEA nitride thin films are very promising candidates for wear protection under severe conditions.

2:20 PM
Outstanding Radiation Resistance of Tungsten-based High Entropy Alloys: *Osman El-Atwani*[1]; Stuart Maloy[1]; Arun Devaraj[2]; Damian Sobieraj[3]; Jan Wrobel[3]; Duc Nguyen-Manh[4]; Jonathan Gigax[1]; Enrique Martinez[1]; [1]Los Alamos National Laboratory; [2]Pacific Northwest National Laboratory; [3]Warsaw University of Technology; [4]United Kingdom Atomic Energy Authority
A novel nanocrystalline W-based refractory high entropy alloy with outstanding radiation resistance has been developed. The alloy was grown as thin films and showed unique 4 nm lamella-like structure. TEM and XRD show an underlying BCC structure with black spots appearing after thermal annealing at elevated temperatures. TEM and APT correlated the black spots with Cr and V precipitation. After heavy ion irradiation, these precipitates evolve to quasi-spherical particles with no sign of irradiation-created dislocation loops even after 8 dpa at either RT or 1073 K. Nanomechanical testing shows a large hardness of 14 GPa in pristine samples, with a slight increase after thermal annealing and almost negligible irradiation hardening. Theoretical modeling based on ab initio methodologies combined with Monte Carlo techniques predicts the formation of Cr and V rich second phase particles and points at equal mobilities of point defects as the origin of the exceptional radiation tolerance.

2:40 PM
High-throughput Aging Investigation of High-entropy Alloys for Advanced Nuclear Applications: *Michael Moorehead*[1]; Mohamed Elbakhshwan[1]; Calvin Parkin[1]; Kumar Sridharan[1]; Chuan Zhang[2]; Alan Savan[3]; Alfred Ludwig[3]; Dan Thoma[1]; Adrien Couet[1]; [1]University of Wisconsin - Madison; [2]Computherm LLC; [3]Ruhr-Universität Bochum
While high-entropy alloys (HEAs) have gained interest for advanced nuclear applications, many single-phase HEAs undergo phase separation or form precipitates at intermediate temperatures which can lead to undesirable property changes. Long-term aging experiments for select compositions in the Cr-Fe-Mn-Ni and Nb-Ta-Ti-V systems at 700 ˚C have confirmed this. However, performing such experiments for entire HEA composition spaces, conventionally, is intractable. To overcome this, high-throughput synthesis techniques of these two HEA systems, including in situ alloying via additive manufacturing and combinatorial thin-film co-deposition have been employed. Using these techniques, compositional arrays have been produced on build plates and wafers which have been subjected to thermal aging at temperatures relevant to advanced nuclear reactors. X-ray diffraction has been used to examine the compositional arrays for second phases while X-ray spectroscopy and electron microscopy have been used to estimate compositions and phase fractions. These results are used to inform CALPHAD modeling for HEAs.

3:00 PM
Combinatorial Thin Film Approach to Develop Refractory BCC HEAs with Improved Ductility: *Taohid Bin Nur Tuhser*[1]; Daryl Chrzan[2]; Andrew Minor[2]; Mark Asta[2]; Thomas Balk[1]; [1]University of kentucky; [2]Lawrence Berkeley National Laboratory
The optimum balance between ductility and hardness of refractory high entropy alloys (RHEAs) is strongly dependent on alloy composition, which need not be exactly equiatomic. In this study, 2D composition gradients of VNbMoTaW and VNbMoTaWHf thin films were made by magnetron sputtering. Replacing Mo with Nb in the same system is expected to improve ductility. X-ray diffraction and energy dispersive x-ray spectroscopy were used to develop a map of alloy phase space. More than 30 local compositions were reported with respective crystal structures, from each thin film. We identified a set of compositions with a single-phase BCC structure. Also, the BCC crystal structure was retained while replacing Mo with Nb. Bulk samples of selected compositions were prepared using vacuum arc melting. Mechanical properties, including hardness and ductility, were investigated with these bulk samples to establish appropriate composition-structure-property relationships.

3:20 PM Break

Mechanical Properties and Processing II

Wednesday PM
November 20, 2019

Room: Cyan
Location: Hyatt at Olive 8

1:30 PM Invited
Novel Equiatomic and Non-equiatomic Refractory High Entropy Alloys Exhibiting Tensile Ductility Even in As-cast State: *C. Tasan*[1]; S.L. Wei[1]; S.J. Kim[2]; E.S. Park[2]; Y.J. Zhang[3]; T. Furuhara[3]; [1]Massachusetts Institute of Technology; [2]Seoul National University; [3]Tohoku University
After the recognition that conventional superalloys have reached their limits in high-temperature applications, there has been growing interest in developing alternative metallic-based structural alloys. Owing to their unique characteristics such as high melting point and excellent softening resistance, refractory metals have attracted significant focus in high-entropy alloys (HEAs) design. However, the investigation of novel refractory HEAs is largely retarded by the traditional trial-and-error alloy design framework, particularly within the non-equiatomic composition regime. To this end, here we present that by making use of the natural thermodynamic mixing characteristics, a series of non-equiatomic refractory HEAs can be developed. We show that these non-equiatomic HEAs exhibit desirable strength-ductility synergy and promising high-temperature performances.

2:00 PM
Study of Deformation Characteristics CoCrFeMnNi and Associated Alloys at Very Low Temperatures: *Aditya Srinivasan*[1]; Theresa Hanemann[2]; Klaus-Peter Weiss[2]; Christian Reinhart[3]; Guillaume Laplanche; Sabine Schlabach[1]; Dorothee-Vinga Szabo[1]; David Geißler[4]; Jens Freudenberger[4]; Martin Heilmaier[1]; Alexander Kauffmann[1]; [1]Institute for Applied Materials, Karlsruhe Institute of Technology; [2]Institute for Technical Physics, Karlsruhe Institute of Technology; [3]Ruhr-University Bochum ; [4]IFW Dresden
The deformation of the Cantor alloy and single phase FCC subsets of the system was carried out at cryogenic temperatures. Through tensile tests conducted in the temperature interval between 4.2 K and 77 K, the observed serrated plastic flow was found to be largely unaffected by extrinsic experimental parameters. The serrations were evaluated statistically and the stress drop variation with progressive deformation shows a tendency towards an increased influence of dislocation-related events. Additionally, the misinterpreted effect of deformation twinning at these low temperatures has been addressed. Characteristic features of deformation seen at these temperatures, vis à vis, appearance of aforementioned deformation twinning, appearance of epsilon martensite (or the lack of in certain cases) and the corresponding effect on deformation was studied by comparing the alloys that exhibited these features. This was done utilizing characterization methods such as EBSD, BSE imaging and TEM.

2:20 PM
Assessing the Impact of Severe Warm-rolling on Microstructure and Properties of AlCoCrFeNi2.1 Eutectic High Entropy Alloy: Seelam Reddy[1]; Upender Sunkari[1]; Adrianna Lozinko[2]; Sheng Guo[2]; *Pinaki Bhattacharjee*[1]; [1]Indian Institute of Technology; [2]Chalmers University of Technology
The impact of warm-rolling on microstructure and properties of a AlCoCrFeNi2.1 eutectic HEA (EHEA) was investigated. The EHEA consisting of the lamellar arrangement of L12 and B2 phases was deformed at 673 K up to 90% reduction in thickness and subsequently annealed at temperatures ranging from 1073 K to 1473 K. Increasing deformation resulted in the gradual reorientation of the lamellae in the rolling direction (RD). Ultra-fine lamellar microstructure evolved after heavy deformation with the development of a fiber (ND//<110>) texture in the L12 and typical RD //<110> and ND//<111> fiber components in the B2 phase. Annealing considerably influenced the development of an ultrafine micro-duplex structure, characteristic recrystallization texture and mechanical properties of the EHEA. The results were finally compared and contrasted with those of the EHEA processed by other thermo-mechanical processing routes for adequately highlighting the impact of warm-rolling.

2:40 PM
Enhanced Mechanical Properties in CrMnFeCoNi High Entropy Alloy by Harmonic Structure Design: *Kei Ameyama*[1]; Zhe Zhang[2]; Naoto Togawa[1]; Bhupendra Sharma[1]; Mie Kawabata[1]; Xu Chen[2]; [1]Ritsumeikan University; [2]Tianjin University
Heterogeneous nanograined structures have been proposed to achieve unprecedented mechanical properties. In the present work, harmonic structure designed CrMnFeCoNi high entropy alloys were produced by mechanical milling and subsequent spark plasma sintering. A co-relationship between various microstructural characteristics and mechanical properties were established. Due to the peculiar microstructural characteristics, the harmonic structured CrMnFeCoNi high entropy alloys demonstrated a winning combination of high strength, large uniform elongation, and large total elongation to failure, simultaneously. It was also found that the harmonic structure with shell volume fraction of approximately 50%-60% was recommended to be the optimized microstructural characteristics for CrMnFeCoNi high entropy alloy.

3:00 PM
3D Ink-extrusion Additive Manufacturing of CoCrFeNi High-entropy Alloy Micro-lattices: *Christoph Kenel*[1]; Nicola Casati[2]; David Dunand[1]; [1]Northwestern University; [2]Paul Scherrer Institut
Additive manufacturing of high-entropy alloys combines their mechanical properties with the geometrical freedom and complexity required by modern designs. Here, a non-beam approach to additive manufacturing of high-entropy alloys is developed based on 3D extrusion of inks containing a blend of oxide nanopowders (Co_3O_4+Cr_2O_3+Fe_2O_3+NiO), followed by co-reduction to metals, inter-diffusion and sintering to near-full density CoCrFeNi in H_2. A complex phase evolution path is observed by in-situ X-ray diffraction in extruded filaments when the oxide phases undergo reduction and the resulting metals inter-diffuse, ultimately forming face-centered-cubic equiatomic CoCrFeNi alloy. Linked to the phase evolution is a complex structural evolution, from loosely packed oxide particles in the green body to fully-annealed, metallic CoCrFeNi with 99.6 ± 0.1% relative density. CoCrFeNi micro-lattices are created with strut diameters as low as 100 µm and excellent mechanical properties at ambient and cryogenic temperatures.

3:20 PM Break

Processing and Application

Wednesday PM
November 20, 2019

Room: Azure
Location: Hyatt at Olive 8

3:50 PM
Additive Manufacturing of High Entropy and Compositionally Complex Alloys: Joerg Kaspar[1]; *Martina Zimmermann*[2]; Liliana Kotte[1]; Martin Kuczyk[1]; Lukas Stepien[1]; Christoph Leyens[1]; [1]Fraunhofer IWS; [2]TU Dresden
Recent research work on HEA and CCA is related to material primarily processed by the melting & casting route. Since alloy synthesis is very complex and in most cases very costly, additive manufacturing (AM) offers new perspectives by allowing to deposit the costly material solely where the favorable properties are needed, thus paving the way for HEA and CCA utilization on an industrial scale. The present contribution demonstrates the potential of different kinds of AM (laser metal deposition, fused filament fabrication, binder jetting) to synthesize transition metal and refractory type HEAs. One major objective is to explore how the synthesis route influences the structure and properties, demonstrated for CrMnFeCoNi in the as-cladded and the heat treated condition. For single phase bcc TiZrNbHfTa and two-phase AlxCrMnFeCoNi it is shown that laser metal deposition is capable of generating crack free coatings with high chemical homogeneity and without macroscopic segregations, exhibiting high hardness.

4:10 PM

Mechanical Properties and Joining of Additively Manufactured Ti-Nb-Zr-Ta Alloy Parts with HEA Fillers: *Eugene Ivanov*[1]; Alexander Shapiro[2]; [1]Tosoh SMD, Inc.; [2]Titanium Brazing, Inc.

Strips and rods of Ti-35Nb-7Zr-5Ta alloy (TNZT) suitable for aerospace structures were made by additive manufacturing using gas-atomized fully-alloyed powder. Vacuum brazing of TNZT was carried out at 920°C by TiBraze200 (Ti-20Zr-20Cu-20Ni wt.%) and at 1080°C by TiBraze200Nb (Ti-11Zr-11Cu-16Ni-17Nb at.%) filler metals. Microstructures and mechanical properties of base metal and brazed joints are reported. Microstructures and phase compositions were studied by optical and scanning electron microscopies using EDX analysis. Density of resulting TNZT strips is >99.9% of theoretical value, tensile strength and yield strength are R0.2 = Proof Strength 484 MPa, Rm = Tensile strength 519 MPa with 24% elongation. The TNZT alloy after additive manufacturing is a beta phase, while the joint metal is characterizable as a high entropy alloy (HEA) joint. Shear strengths of brazed joints are up to 144.4 MPa for TiBraze200 and up to 196.3 MPa for TiBraze200Nb. Strength of TNZT-alloy-to-alumina-ceramic brazed joints is ~128 MPa.

4:30 PM

Ti-Zr-Nb-Cu-Ni and Co-Cr-Ni-Si-Mo/Nb High-entropy Alloys as Brazing Filler Metals: *Alexander Shapiro*[1]; Eugene Ivanov[2]; [1]Titanium Brazing, Inc.; [2]Tosoh SMD, Inc.

High-entropy alloys are attractive as brazing materials that usually exhibit significantly higher yield strength and ductility. Heat resistance of brazed joints is limited by the content of the eutectic phase that is typically used in the filler metals to decrease brazing temperature. Designing and applying high-entropy filler metals for joining superalloys, refractory metals, carbon-fiber composites can resolve many technical problems in the manufacture of new power sources, jet and rocket engines, high-temperature electronic devices, etc. We present new Ti4Zr1Nb1Cu1.5Ni1.5, Co3Ni1Si1Mo1Cr1.3 and Co3Ni1Si1Nb1Cr1.3 high-entropy alloys having relatively low brazing temperature in the range of 1050-1200°C but exhibiting high heat resistance in the service temperature range of 600-800°C. Shear strength of Ti-6Al-4V alloy, as well as of Molybdenum, was tested at 600°C and 800°C. Microstructure of brazed joints was studied by optical and scanning electron microscopy. Application in vacuum brazing, effect of the post-braze diffusion treatment, and future developments are also discussed.

Alloy Design II

Wednesday PM
November 20, 2019

Room: Cobalt
Location: Hyatt at Olive 8

3:50 PM

Competition Between L1$_2$ and B2/L2$_1$ Precipitation in FCC Based Complex Concentrated Alloys: Multi-scale Microstructures and Tuning Mechanical Properties: S Dasari[1]; B Gwalani[1]; V Soni[1]; S Gorsse[2]; *Rajarshi Banerjee*[1]; [1]University of North Texas; [2]CNRS, ICMCB, UPR 9048

Thermo-mechanical processing can substantially influence the phase transformation pathways in complex concentrated alloys (CCAs). These pathways lead to different combinations of phases, at multiple length scales, within these alloys. This presentation will focus on investigating and rationalizing how such transformation pathways can dramatically alter the microstructure and mechanical properties in face-centered cubic (FCC) based HEAs. Example systems to be considered include FCC-based 3d transition series alloys, such as Al0.3CoCrFeNi, Al0.5Co1.5CrFeNi1.5, and Al0.2Ti0.3Co1.5CrFeNi1.5. All these alloys inherently exhibit a competition between the precipitation of different ordered intermetallic phases, such as the L12, B2, and L21, within the FCC solid solution matrix. The thermodynamic rationale underlying such competition is the complex interplay between the driving force and the nucleation barrier associated with these phases. The resultant microstructural diversity within the same HEA can lead to dramatically different mechanical properties, as aspect which can be used for tuning their properties for various applications.

4:10 PM

Improving Ductility of Dual-phase High-entropy Alloys for High-temperature Structural Applications: *Young-Sang Na*[1]; Ka-Ram Lim[1]; Hyun-Jun Kwon[1]; Jong-Woo Won[1]; [1]Korea Institute of Materials Science

The untapped potential of high-entropy alloys (HEAs) has attracted considerable interest in recent years. HEAs are expected to offer a new route to form highly stable and simple solid solution structures (as compared to intermetallic compounds) in multicomponent alloys, and they also have considerable potential in the extreme conditions such as cryogenic temperatures, high temperatures and corrosive environments. Among many HEAs, AlCoCrFeNi alloy shows outstanding specific strength over the temperature range of 400 - 600°C, since it has dual-phase structure (A2+B2) and high coherency between the two phases. However, its ductility is very poor even at high temperatures. To enhance ductility, we have controlled the volume fraction and the chemical composition of each phase by combining experimental and computational approaches. In the present study, mechanical properties of newly developed alloys have been examined from a microstructural point of view.

TEM Techniques in HEAs

Wednesday PM
November 20, 2019

Room: Cyan
Location: Hyatt at Olive 8

3:50 PM

-factor Quantitative Chemical Microanalysis of Multi-phase Complex Concentrated Alloys: *Christopher Marvel*[1]; Joshua Smeltzer[1]; Anit Giri[2]; B Hornbuckle[2]; Kristopher Darling[2]; Martin Harmer[1]; [1]Lehigh University; [2]U.S. Army Combat Capabilities Development Command Army Research Laboratory

Complex concentrated alloys (CCA) have intricate and oftentimes unpredictable microstructures, and depending on the processing procedures conducted to synthesize CCA like mechanical alloying, there is a high probability that the multi-phase microstructures will consist of both ceramic and metallic phases. To best correlate microstructure to properties, there is a need to confidently identify microstructural phases. This talk will introduce and demonstrate that -factor microanalysis, a quantitative transmission electron microscopy (TEM) energy dispersive spectroscopy (EDS) framework which non-trivially corrects for X-ray absorption, is a powerful tool to correlate microstructure to properties, especially when used in tandem with aberration-corrected atomic-resolution imaging. -factor microanalysis is specifically demonstrated to characterize a nanostructured mechanically alloyed refractory CCA that includes ceramic nitride phases. Overall, -factor microanalysis enabled full phase identification which would otherwise been difficult due to severe X-ray absorption of nitrogen K-line X-rays. Other potential uses and practical aspects of -factor microanalysis will be presented.

4:10 PM
Weak-beam Dark-field STEM Study of Dislocation Microstructure in NiCoCr Medium Entropy Alloy: *Jiashi Miao*[1]; Michael Mills[1]; [1]Ohio State University
Equiatomic NiCoCr medium entropy alloy has exceptional mechanical properties, including high ductility, large work hardening rates and superior fracture toughness at both room temperature and cryogenic temperature. Such excellent properties are closely related to its dislocation microstructure under deformation. In this study, a newly developed defect imaging mode: weak-beam dark-field scanning transmission electron microscopy (WB DF STEM) was used to characterize dislocation dissociation, slip and cross-slip, dislocation decorrelation and interactions in this alloy. The new WB DF STEM imaging technique can offer bend-contour and thickness-fringe free dislocation images with resolution similar to those captured using conventional WB DF TEM imaging. The mechanisms of deformation twinning and deformation induced face centered cubic (FCC) to hexagonal close-packed (HCP) trasnformation in this alloy were revealed by using WB DF STEM imaging in combination with atomic-resolution STEM imaging.

4:30 PM
Ultrastrong High-entropy Alloy Micro-fiber Strengthened by High Density Dislocations: *Dongyue Li*[1]; Yong Zhang[1]; [1]University of Science and Technology Beijing
High entropy alloy (HEA) is a novel and versatile alloy with attractive mechanical properties and simple phase structure. However, single-phase face-centered cubic (FCC) HEAs are generally quite ductile, while the ultimate tensile strength at room temperature is relatively weak. In current study, Al0.3CoCrFeNi HEA micro-fiber of 60 μm in diameter was fabricated by hot drawing. This FCC based fiber exhibits an ultimate tensile strength above 2.8 GPa at ambient temperature, which was more than five times increase to that of the as-cast ingots. Additionally, the mechanical properties of the micro-fiber improve at cryogenic temperatures. The deformation mechanism was further revealed by in-situ transmission electron microscope. It demonstrates that high density dislocations and nano-structured grains effectively strengthen the fiber.

Poster Session

Monday PM
November 18, 2019

Room: Ballroom DE
Location: Hyatt at Olive 8

A Design Strategy for Developing Lightweight TWIP High Entropy Alloy: *Min Seok Kim*[1]; Kook Noh Yoon[1]; Hyun Seok Oh[2]; Eun Soo Park[1]; [1]Seoul National University; [2]Massachusetts Institute of Technology

Combination of high strength and ductility is a long standing issue for structural materials. Furthermore, weight reduction has recently become an urgent issue as environmental problems become more severe. In the present study, we tried to develop an unique lightweight high entropy alloys (HEAs) with twin-induced plasticity (TWIP) behavior. It is well known that deformation mechanism of material can be systematically changed from slip to twin as stacking fault energy (SFE) decreases. Thus, we first designed dual phase HEA using the CALPHAD approach to lower the SFE down to dual phase region. And then we added aluminum, which is known for SFE elevating and light-weight element. As a result, we could achieve good mechanical properties and light weight in the newly developed HEA by controlling SFE in the TWIP region. This result can be applicable to various 3d transition metal based alloys that require good mechanical properties and weight lightening.

Cold Working of $Al_{0.3}$CoCrFeNi High Entropy Alloy: *Christopher Reynolds*[1]; Deep Choudhuri[1]; Marcus Young[1]; Jeff Lloyd[2]; [1]University of North Texas; [2]US Army Research Laboratory

While mechanical properties, such as tensile fracture strength and ductility, as a function of microstructure have been previously explored in $Al_{0.3}$CoCrFeNi high entropy alloy, few studies have examined the workability of this HEA system and, specifically, no detailed study relating structure and properties during different extents of cold work. In this study, an $Al_{0.3}$CoCrFeNi HEA is cold worked to 99.49% reduction in thickness. Starting from an $Al_{0.3}$CoCrFeNi HEA an annealed billet of 6.67 × 3.26 mm^2 in dimensions, the sample was cold rolled to a rod with diameter of 1 mm. The rod was then cold drawn to a wire with a diameter of 375 μm. Cold working beyond 375 μm resulted in cracking. The $Al_{0.3}$CoCrFeNi HEA samples throughout the cold working process were characterized using scanning electron microscopy (SEM) with energy dispersive spectroscopy (EDS), Vickers hardness testing, and synchrotron radiation X-ray diffraction.

Creep Properties of High Entropy Alloys Having a Single FCC Crystal Structure at Elevated Temperature: *Min-Gu Jo*[1]; Jin-Yoo Suh[2]; Woo-Sang Jung[2]; Heung Nam Han[1]; [1]Seoul National University; [2]Korea Institute of Science and Technology

In this study, creep test was carried out at temperature ranging from 650 to 725 under the stress range of 50~200 MPa with CrMnFeCoNi quinary and CrFeCoNi quaternary high entropy alloys. Before and after creep test, SEM-EDS/EBSD and X-ray diffraction analyses were performed to discuss microstructural development, and tensile properties and Vickers hardness were evaluated. Both alloys showed the single face-centered cubic crystal structure and similar mechanical properties at room temperature and elevated temperatures but significantly different creep rupture life. The quaternary CrFeCoNi high entropy alloy showed much longer creep rupture life than the CrMnFeCoNi alloy. The reason for this difference will be discussed in terms of the fcc phase stability and the degree of solid solution strengthening.

Development of High Entropy Alloy with Nano-laminated Martensite/Austenite Structure: *Min Seok Kim*[1]; Kook Noh Yoon[1]; Hyun Seok Oh[2]; Eun Soo Park[1]; [1]Seoul National University; [2]Massachusetts Institute of Technology

Strength and ductility are the most important physical properties in evaluating structural materials. Unfortunately, common strengthening strategies in most conventional alloys cause sacrifice of ductility inevitably. This trend is well known to 'strength-ductility trade-off dilemma'. Recently, however, high-entropy alloy (HEA) which is constituted with several major elements is regarded as a good candidate that can overcome the strength-ductility trade-off. In the present study, we attempt to design the unique HEA microstructure with nano-thickness austenite film in hard martensite phase matrix. First of all, we made fully martensite HEA. Secondly, low temperature tempering process was performed for partial austenitization of the martensite. As a result, the HEA exhibited a novel 'composite-like' microstructure with metastability of the austenite film in martensite HEA matrix, which resulted in good ductility and strength balance. This result can provide a guideline on how to overcome strength-ductility trade off by tailoring microstructure in HEA.

Dislocation Emission from Grain Boundaries in High Entropy Alloys Through Atomic Simulations: *Tomotsugu Shimokawa*[1]; Kohei Shiotani[1]; Tomoaki Niiyama[1]; [1]Kanazawa University

Grain boundaries are interfaces between two grains with different crystal misorientation angles and free atomic volumes at the boundaries vary in size from small to large. Because high entropy alloys (HEAs) consist of various kinds of atoms with different atomic radii, there is a possibility that grain boundaries in HEAs is composed of specific atoms based on the relationship between the atomic free volume at grain boundaries and the atomic radii and such grain boundaries influence mechanical properties of HEAs. In this study, we first construct grain boundaries in two-dimensional HEA models through Monte Carlo simulations and then the investigate grain boundary characteristics focusing on atomic free volumes at grain boundaries. Finally, we examine the influence of the grain boundaries characteristics in HEAs on dislocation emission from the grain boundaries by performing tensile and compressive deformation tests through molecular dynamics simulations.

Dissimilar Infrared Brazing of CoCrFeMnNi Equiatomic High Entropy Alloy and 316 Stainless Steel Using Nickel-based Braze Alloys: *Chieh Lin*[1]; Ren-Kae Shiue[1]; Shyi-Kaan Wu[1]; Yu-Sy Lin[1]; [1]National Taiwan University

Dissimilar infrared brazing of CoCrFeMnNi equiatomic high entropy alloy (HEA) and 316 stainless steel using BNi-2 and MBF601 fillers has been investigated. The wettability of both fillers at 50 °C above their liquidus temperatures on both substrates is great. The BNi-2 brazed joints are dominated by Ni-rich matrix with borides in the center of brazed zone and tiny borides at the interface between the braze and substrate. The MBF601 brazed joints are comprised of phosphide and Fe/Ni-based matrix. The joint brazed with the BNi-2 filler at 1020 °C for 300s has the highest shear strength of 392 MPa and the cracks with cleavage dominated-fracture are propagated through the borides in the Ni-rich matrix. Both fillers show the potential in dissimilar brazing the CoCrFeMnNi HEA and 316 stainless steel.

Effect of Local Chemical Ordering on Mechanical Properties in High Entropy Alloys: *Kook Noh Yoon*[1]; Hyunseok Oh[2]; Zhang Jing[1]; Baptiste Gault[3]; Dierk Raabe[3]; Eun Soo Park[1]; [1]Seoul National University; [2]Massachusetts Institute of Technology; [3]Max-Planck-Institut für Eisenforschung GmbH
High entropy alloys (HEAs) are constituted with multi-principal elements in single solid solution. Thus, it is important to understand the local environment around the specific constituents. In particular, the local chemical ordering (LCO) can be formed by a stronger driving force to make preferential bonding depending on the constituents. Moreover, some of simulation results are proposed that stacking fault energy (SFE) of HEAs is locally tunable by forming these LCOs. In the present study, we systematically evaluate the influence of LCO formation on mechanical properties in FCC HEAs with different SFEs. The LCO formation was carefully controlled by solidification history and annealing conditions, and then was confirmed by intensive structural analysis. As a result, we report the meaningful changes of mechanical properties depending on LCOs in HEAs with same composition. This work will give us a new pathway to optimize the mechanical property of HEAs by controlling atomic-scale structure.

Effects of Cu Precipitation on Mechanical, Anti-corrosion and Antibacterial Properties in a Medium-entropy Super-austenitic Stainless Steel: *Shih-Che Chen*[1]; Tzu-En Chen[1]; Zen-Hao Lai[1]; Yueh-Lien Lee[1]; Hung-Wei Yen[1]; [1]National Taiwan University
In this study, a new medium-entropy super-austenitic stainless steel with mixing entropy of ~1.3R was developed. The effects of Cu precipitation on mechanical properties, corrosion resistance and antibacterial performance after solution and aging treatments were investigated by transmission electron microscopy, electrochemical corrosion, and antibacterial test. The results showed that, after solution treatment, the single-phase austenitic steel was obtained and it has good corrosion resistance and excellent combination of strength and ductility due to high strain hardenability by shear-band-induced plasticity. After aging treatment, coherent Cu-rich precipitates with sizes of about 2-5 nm were observed homogeneously distributed in the austenite matrix, leading to a higher strength without much scarification of uniform elongation. Moreover, Cu precipitation greatly enhanced antibacterial ability but slightly declined corrosion resistance of the steel. Based on our current results, high-entropy concepts can be successfully applied to design new multifunctional super-austenitic stainless steel.

Establishing Processing-microstructure-property Paradigm in Complex Concentrated CoCuFeMnNi High Entropy Alloy: *Reshma Sonkusare*[1]; Aditya Swain[1]; Krishanu Biswas[1]; Nilesh Gurao[1]; Sumanta Samal[2]; [1]India Institute of Technology Kanpur; [2]India Institute of Technology Indore
The present investigation focuses on hot deformation behavior of CoCuFeMnNi complex concentrated alloy, studied via isothermal compression tests on Gleeble-3800 thermo-mechanical simulator. Processing maps shows optimum thermo-mechanical processing conditions to be T = 1173 K, = 10-3 s-1 and T = 1273 K, = 10-2 s-1. Microstructural investigation using SEM-EBSD reveal phase separation between Cu-rich and Cu-lean regions. Cu-rich FCC phase at the grain boundaries undergoes DDRX while the Cu-lean phase undergoes DRV. The average activation volume (44-250 b3) suggest cross slip to be the rate controlling mechanism and activation energy of 394 kJ/mol, indicate contribution from both mechanical and thermal component. Neutron diffraction measurement shows [110] type of texture, which is characteristic FCC compression texture and was verified by viscoplastic self consistent simulations. Numerical simulations using FEM are able to correctly predict hot deformation behaviour establishing the processing-microstructure-property paradigm in CoCuFeMnNi complex concentrated alloy.

Evolution of Precipitation Hardening in Al0.2CoCrFeNi High Entropy Alloy Studied by Synchrotron Small-angle X-ray Scattering: *Yung-Chien Huang*[1]; Cheng-Si Tsao[2]; Shyi-Kaan Wu[1]; Chieh Lin[1]; [1]National Taiwan University; [2]Institute of Nuclear Energy Research
The synchrotron small-angle X-ray scattering (SAXS) technique was used to reveal the evolution and growth kinetics of nano-precipitates in 80% cold-rolled Al0.2CoCrFeNi high-entropy alloy aged at 550 °C for different times. The Vickers microhardness measurements demonstrate two hardness peaks occur during aging treatment of 550 °C. The first hardness peak occurs at 15 min aging with the rapid hardness increment from 410 Hv to 470 Hv. The hardness then drops to the local lowest value of 450 Hv at 1 hr aging, and gradually increases to 485 Hv at 25 hrs aging where the second hardness peak appears. The growth kinetics of nano-precipitation are quantitatively resolved using SAXS in terms of the temporal evolutions of size and volume fraction. TEM observations of the nano-precipitates also show a complementary investigation with SAXS results.

FCC to $L1_2$ Ordering Transformation in Equimolar FeCoNiV High Entropy Alloy: *Shubin Wang*[1]; Da Shu[1]; Fuyang Tian[2]; Yongbing Dai[1]; Baode Sun[1]; [1]School of Materials Science and Engineering, Shanghai Jiao Tong University; [2] Institute for Applied Physics, University of Science and Technology Beijing
The ordered $L1_2$ phase generally appears as dispersed precipitates in high entropy alloys (HEAs). In this work, a single $L1_2$ ordered intermetallic is obtained in the annealed equimolar FeCoNiV alloy. This FCC to $L1_2$ ordering transformation causes the lattice contraction and anti-phase boundaries formation. It also decreases the low-temperatrue magnetic moment and leads to a high linear strain hardening rate (up to 5.0 GPa). The ab initio calculations based on the EMTO-CPA predict that the $L1_2$ phase becomes more stable with respect to FCC phase below 849 ˚C with V atoms preferring to occupy the cubic corner sites of $L1_2$ sublattice. This sublattice atomic occupation can be traced back to the short-range order (V atoms prefer to bond with the Fe, Co and Ni atoms) in liquid FeCoNiV alloy. The present work demonstrates a new design strategy of HEAs which focus on multicomponent but ductile intermetallic compounds.

Fracture and Fatigue Resistance of High Entropy Alloys: *John Lewandowski*[1]; Mohsen Seifi[2]; Peter Liaw[3]; [1]Case Western Reserve University; [2]ASTM International; [3]University of Tennessee, Knoxville
Fracture toughness and fatigue crack growth of various high entropy alloys were determined. Two multi-phase alloys, in addition to single phase FCC Al0.3CoCrFeNi HEA were prepared and tested. Notched/fatigue precracked toughness values were significantly higher for the FCC single phase HEA compared to the multi-phase HEA and higher than those reported in the literature. Fatigue experiments exhibited high thresholds that decreased significantly with an increase in load ratio, with low Paris regime exponents. Fatigue thresholds at all R were much higher than most conventional alloys. Fatigue fracture surfaces of the multi-phase samples revealed ductile and brittle features at various regions of the fatigue curve, with some evidence of fatigue striations in the Paris regime. The FCC single-phase samples only exhibited ductile features, also with some evidence of fatigue striations in the Paris regime. The results will be compared to data obtained on other HEA's.

High Energy Synchrotron Radiation X-ray Diffraction Measurements on $Al_{0.3}$CoCrFeNi High Entropy Alloy during in situ Annealing: *Christopher Reynolds*[1]; Deep Choudhuri[1]; Zachary Herl[1]; Marcus Young[1]; Jeffrey Lloyd[2]; [1]University of North Texas, Department of Material Science and Engineering; [2]US Army Research Laboratory

High entropy alloys (HEAs) offer the ability to tailor microstructures based on specific properties. One family of alloys of interest is Al_xCoCrFeNi, where x varies from 0.0 to 2.0 wt. %, here specifically $Al_{0.3}$CoCrFeNi HEA. The purpose of our study is to compare phases observed using high energy synchrotron radiation X-ray diffraction measurements during in situ annealing with the equilibrium phases predicted by the phase diagram generated using CALPHAD. The $Al_{0.3}$CoCrFeNi HEA sample was cold rolled and then in situ annealed, which consisted of heated to 800 °C, held for three hours, and then cooled back down. In addition to examining the phase changes with temperature, the crystal lattice strains associated with temperature changes are also presented and compared with scanning electron microscopy images of the sample at the various stages of processing. In this context, the phase evolution and dissolution are discussed and compared with the CALPHAD predictions.

Hydrogen Sorption in MgTiNbCr0.5Mn0.5Ni0.5 High Entropy Alloy Synthesized Using High Energy Ball Milling (HEBM): *Felipe Marques*[1]; Haroldo Pinto[2]; Walter Botta[1]; Guilherme Zepon[1]; [1]Federal University of São Carlos; [2]University of São Paulo

A new HEA, namely MgTiNbCr0.5Mn0.5Ni0.5, was synthesized by HEBM for 24 hours in two conditions: i) under 0.07 MPa of argon ii) under 3.0 MPa of hydrogen. In the former, the HEA presented BCC solid solution combined with metallic manganese and chromium; in the later, the HEA exhibited major FCC high entropy hydride phase (MH2 with CaF2-type structure) with small fraction of metallic chromium. Both samples were subjected to in situ synchrotron radiation X-ray diffraction to analyze phase transitions during hydrogen absorption/desorption. It was found that the BCC phase absorbed hydrogen by solid solution with a change of structure volume of \916V=5.42 Å^3(15.3%) without phase transition. Yet, the high entropy hydride undergone phase transition from FCC to BCC during hydrogen desorption at 400 °C. This results show that this HEA is able to store hydrogen reversibly, although the transition from BCC to FCC during absorption still need further investigation.

Investigating the Mechanical Response of Refractory High-entropy Alloys Using Ion Irradiation and Micromechanical Testing: *Bo-Shiuan Li*[1]; Anna Kareer[1]; Angus Wilkinson[1]; Amy Gandy[2]; Alexander Carruthers[3]; Ed Pickering[3]; David Armstrong[1]; [1]University of Oxford; [2]University of Sheffield; [3]University of Manchester

Refractory high-entropy alloys (RHEAs) are an alternative type of HEAs that possess BCC matrix and superior high-temperature strength compared to their FCC predecessors, making them ideal structural materials for extreme nuclear environment. As part of the UK-India collaboration on developing nuclear-friendly HEAs, three quaternary TiV(Nb, Zr, Cr)Ta equiatomic RHEAs were manufactured via arc melting. Micromechanical tests of three as-cast RHEAs showed no hardening after irradiation. The samples were then homogenised at 1400 °C for 100 hrs to ensure thermal stability of microstructure. Large fraction of the brittle C15 Laves phase Ta(V, Cr)2, were found in the TiCVrTa, due to the slow cooling rate during homogenisation. To ensure excellent strength and ductility at reactor condition, future heat treatment will focus on reducing the fraction of the Laves phase. High-temperature micromechanical tests in conjunction with high-resolution microscopy will be used to shed light on the microstructural origin of the irradiation resistance.

Investigation of CoCrCuFeNi Alloys in the Semisolid State: *Caio de Freitas*[1]; Kaio Niitsu Campo[1]; Rubens Caram[1]; [1]University of Campinas

The equiatomic CoCrCuFeNi alloy is composed by two phases of distinct melting points, opening the possibility of employing the semisolid technology, which offers advantages over conventional casting and forging. It is believed that the increase of Cu in the CoCrCuFeNi alloy leads to a higher volume fraction of the Cu-rich phase with lower melting point. Therefore, the present work aimed to study the influence of Cu on the microstructure of CoCrCuFeNi alloys in the semisolid state. For this purpose, samples with different Cu contents were submitted to isothermal heat treatments between the solidus and liquidus. The results showed that it is possible to effectively control the volume fraction of the existing phases by modifying the alloy composition. Accordingly, higher liquid fractions at a same temperature can be obtained with increased Cu content. Furthermore, all samples presented fine and globular primary particles, demonstrating their favorable characteristics for semisolid processing.

Is the Cantor Alloy (CrMnFeCoNi) the Most Stable Combination within CrMnFeCoNiCu?: *Artashes Ter-Isahakyan*[1]; Thomas Balk[1]; [1]University of Kentucky

The Cantor alloy originates from a set of experiments conducted on combinations of equiatomic CrMnFeCoNi-Nb/Ge/Cu/Ti/V systems prepared by non-equilibrium processing.However,the use of non-equilibrium processing may provide only a conditional basis of compositional ratios. Consequently, observed compositions may be stable phases but metastable under a different set of conditions regarding composition, temperature, and cooling rate. True equilibrium processing requires cooling rates that are complementary to a geological time scale.This is unrealistic, but the slower the cooling rate, the closer one approaches equilibrium conditions. In this work, we describe a method applicable to HEAs, where controlled processing conditions decide the most probable and stable composition. We demonstrate this by cooling an equiatomic CrMnFeCoNiCu from the melt over a period of 3 days, which results in large Cr-rich precipitates and a nearly Cr-free matrix. From this juncture, we argue that the most stable composition lies in the MnFeCoNiCu system rather than the CrMnFeCoNi system.

Kinetic Monte Carlo Study of a Vacancy Diffusion Driven Ordering in High-entropy Alloys: *Zeqi Shen*[1]; Jun-Ping Du[2]; Shuhei Shinzato[1]; Peijun Yu[3]; Shigenobu Ogata[1]; [1]Osaka University; [2]Kyoto University; [3]City University of Hong Kong

High entropy alloys (HEAs), which contain five or more principle elements, have attracted increasingly attention in science and technology applications due to its superior mechanical performance. Recent theoretical studies suggest that the chemical arrangement of the elements on the crystalline lattice is not fully random, but partially ordered, and it probably is a short ranged. Recently, effects of the short-range order (SRO) on the material properties, such as the stacking fault energy, have been investigated. However, the formation process and stability of SRO are still unclear. Here, we use kinetic Monte Carlo (kMC) method and study the vacancy diffusion driven short-range ordering process, temperature dependent SRO formation rate, and thermodynamic stability of constructed SRO. We find that, the stability of SRO is critically related to the interatomic interactions and temperature. Below a critical temperature, SRO is starting to be constructed along the vacancy diffusion pathway.

Local Plasticity and Interfacial Effects in Cubic HEA Studied by Correlative Methods: *Vaclav Ocelik*[1]; Indranil Basu[1]; Jeff De Hosson[1]; [1]University of Groningen

Nanoindentation, phase analysis, EBSD and local stress analysis were applied on AlCoCrFeNi HEA. Microstructure comprises strain-free fcc phase and strongly deformed bcc phase. bcc grains shows microstructure after spinodal decomposition, alternating of ordered Ni and Al rich B2 phase and disordered Cr rich A2 phase. Indentation in the bcc grain revealed strain bursts occurring in random and stochastic manners. The observed plastic behavior was associated with dislocation hardening arising from a combination of the spinodally modulated microstructure and order hardening. Certain indents revealed a strain induced transition from bcc to fcc. The geometry of bcc-fcc interface governs an appearance of additional yield excursions during nanoindentation near interface boundary. bcc-fcc boundary strengthening of the order of 4 GPa was estimated. The influence of image forces due to presence of a bcc-fcc interface is quantified and correlated to the measured stress and hardness gradients in both bcc and fcc grains.

Microstructural Evolution of TRIPLEX Structure in TiVNbTaW High Entropy Alloy Fabricated by Spark Plasma Sintering: *Sangjun Kim*[1]; Jinyeon Kim[1]; Da Hye Song[2]; Jin Kyu Lee[2]; Eun Soo Park[1]; [1]Seoul Nation University; [2]Kongju National University

Recently, BCC high entropy alloys (HEAs) composed by Group-4 to Group-6 elements were reported to exhibit superior mechanical properties up to high temperature above 1273 K comparing conventional Ni-based superalloy. However, RHEAs is their industrial application is limited due to the high melting point and poor ductility in room temperature. In this study, TiVNbTaW RHEA powder with single BCC phase was prepared by high-energy ball milling and the fabricated powder were sintered using spark plasma sintering. Sintered TiVNbTaW high entropy alloy exhibited TRIPLEX nanostructure consisting of (Nb,Ta)-rich BCC, W-rich BCC and TiO FCC phase, which was formed during the sintering process by decomposition of single BCC phase in as-milled powder. Microstructural evolution of TRIPLEX nanostructure was analyzed in terms of metastable thermodynamic equilibrium and segregation of solute in a complex multi-principle system. This result could provide an effective guideline for tailoring the nanostructure of RHEAs fabricated by powder metallurgy.

Microstructure and Superconductivity in Equiatomic Hf-Nb-Ta-Ti-V High Entropy Alloy: *Nilabja Kanti Sarkar*[1]; Raghvendra Tewari[1]; [1]Bhabha Atomic Research Centre

High entropy alloys (HEA) due to highly distorted lattice are expected to show unusual superconducting behaviour.We report synthesis, microstructural and superconducting properties characterization of a novel equiatomic high-entropy alloy with nominal composition of $Hf_{20}Nb_{20}Ta_{20}Ti_{20}V_{20}$.Detailed microstructural characterization of the alloy showed dendritic morphology with preferential segregation tendency of Hf, Ti and V in inter-dendritic regions.XRD analysis revealed the presence of single bcc pattern indicating both the phases are having the same bcc phase. However TEM investigation indicates the presence of small amount of omega like secondary phase in HEA matrix.Transport properties and magnetization measurements established that the HEA is a type-II superconductor with a T_c of 5.5K, lower critical field (H_{c1}) of 20.0±8 mT and upper critical field (H_{c2}) of 6.63±0.05 T.Analysis of low temperature specific heat data suggests that the HEA is a moderately coupled superconductor which can be well described with the single-gap BCS model.

Microstructure Evolutions of $AlCoCrFeNiTi_{0.5}$ High-entropy Alloy at Elevated Temperatures: *Tao-Tsung Shun*[1]; Cheng-Ju Chiang[1]; [1]Feng Chia University

Microstructure evolutions of an as-cast $AlCoCrFeNiTi_{0.5}$ high-entropy alloy after heat treatments 72 h at 500-1100 were investigated. The alloy shows a dendritic structure which dendrite is a spinodal structure composed of (Cr,Fe)-rich BCC phase and (Al,Ni)-rich ordered BCC phase, and the interdendrite comprises (Cr,Fe)-rich BCC, Heusler-type (Ni,Al,Ti)-rich β', and σ phases. After heat treatments, the BCC phase transforms into σ phase in interdendrite at 600, the shape of BCC phase in dendrite changes from plate to particle at 800, and the spinodal structure vanishes in dendrite replaced by an ordered BCC phase at 1000; meanwhile, both β' and σ phases in interdendrire transform into a BCC phase at 1000. Furthermore, profuse DO_3 nanoparticles with 20 nm in size precipitate in BCC phase at 1000. These nanoparticles coarsen to 50 nm at 1100 and parts of them grow into 150 nm squares which are rich in Cr, Fe, Co, and Ni.

Multi-cell Monte Carlo for Phase Prediction of High Entropy Alloys: *You Rao*[1]; Changning Niu[1]; Wolfgang Windl[1]; Maryam Ghazisaeidi[1]; [1]Ohio State University

Prediction of stable phases of high entropy alloys is of great importance in understanding the thermodynamics of the alloys, especially for multicomponent systems whose phase diagrams have not been established. Atomic simulations often come across the difficulty in dealing with the point defects due to atom transfer and the increased computational cost with the increase of complexity. We propose a robust multi-cell Monte Carlo algorithm from first principles for simulating phase coexistence in crystalline solids where the free atomic transfer is achieved via the application of a molar fraction from the lever rule that virtually controls the percentage in each cell in the simulation. This algorithm has been applied to a quaternary high entropy alloy case and has successfully predicted the separation to a bcc phase and an hcp phase.

Nanocrystalline, Two Phase High-entropy Alloy: Strengthening by Grain Boundaris Versus Second-phase Particle: *Jeong-Min Park*[1]; Dong-Hyun Lee[2]; Zhaoping Lu[3]; Jin-Yoo Suh[4]; Megumi Kawasaki[5]; Upadrasta Ramamurty[6]; Jae-il Jang[1]; [1]Hanyang University; [2]Max-Planck-Institut für Eisenforschung GmbH; [3]University of Science and Technology Beijing; [4] Korea Institute of Science and Technology; [5]Oregon State University; [6]Nanyang Technological University

Recent studies reported that the mechanical properties of high-entropy alloys (HEAs) can be further improved by grain refinement or precipitation hardening. Thus, one can expect a synergetic effect on mechanical performance by combining these two strengthening mechanisms. In this study, (CoCrFeNi)94Ti2Al4 HEA with and without L12-Ni3(Ti,Al) second-phase particles was subjected to high-pressure torsion (HPT) to examine the possibility of deriving the benefits of particle and grain boundary strengthening simultaneously. The mechanical behavior and microstructural stability of second-phase strengthened HEA processed by HPT was investigated through a series of experiments using nanoindentation tests and transmission electron microscopy analysis. The obtained results were analyzed in terms of the changes in microstructure, strain rate sensitivity, and activation volume with HPT turns.* This work was supported by the National Research Foundation of Korea (NRF) grants funded by the Ministry of Science and ICT (No. 2015R1A5A1037627 and No. 2017R1A2B4012255).

Overcoming Mechanostability and Thermal Shielding Trade off via Concatenated Dendritic High Entropy Alloy Foam: *Kook Noh Yoon*[1]; Khurram Yaqoob[2]; Je In Lee[3]; Jinyeon Kim[4]; Su Hyeon Kim[5]; DongEung Kim[6]; Eun Soo Park[1]; [1]Seoul National University; [2]National University of Sciences and Technology; [3]National Institute for Materials Science; [4]Northwestern University; [5]Korea Institute of Materials Science; [6]korea institute industrial technology

Thermal shield materials (TSMs) have been designed for saving energy by insulation or protecting human being from extreme environments. For these purposes, the TSMs should be much stronger and insulative. Although metals exhibit high strength and excellent ductility, they by themselves have not been considered as an appropriate candidate for TSMs due to their high thermal conductivity (). Therefore, to utilize metallic materials on TSMs, it has been processed into porous structure. Understandably, the pores can effectively hinder the heat transfer through materials; however, they degrade the mechanical property inevitably. In the present study, we first report concatenated dendritic HEA foam which is fabricated by dealloying process in phase separating FeCoCrNi-Cu HEAs. The HEA foams exhibit ultra-low , while maintaining the mechanostability of HEAs. Therefore, HEA foam can overcome the trade-off dilemma of conventional metal foams, which might open the door of new era of thermal protection utilizing metals.

Partial Melting and Microstructural Evaluation of CrCuFeMnNi High-entropy Alloys for Semisolid Processing: *Kaio Niitsu Campo*[1]; Caio Chaussê de Freitas[1]; Rubens Caram[1]; [1]University of Campinas

Semisolid processing can be advantageously used in multiphase high-entropy alloys (HEAs) to produce components with complex geometries. In association with 3d transition metals, Cu can lead to phase separation and formation of phases with lower melting temperatures, which can be conveniently explored in semisolid technology. Accordingly, this study aimed to analyze the effect of Cu content on the melting behavior, phase formation, and semisolid microstructural evolution of CrCuFeMnNi alloys. The melting process was evaluated by DSC, whereas microstructural characterization involved SEM and XRD investigations. The melting spectrum revealed three peaks related to the main phases in the microstructure. As expected, the Cu-rich phase had the lowest melting temperature, allowing the partial melting experiments to be carried out at 1080 ˚C. The liquid fraction increased with Cu content, while fine and globular solid phases were obtained. Therefore, it is suggested that CrCuFeMnNi alloys can be properly processed in the semisolid state.

Physical Properties of Sputtered CrFeCoNiCu Thin Films on Quartz Substrate: *Jeyanthinath Mayandi*[1]; Marit Stange[2]; Martin Fleissner Sunding[2]; Matthias Schrade[1]; Jonas Deuermeier[3]; Elvira Fortunato[3]; Ole Martin Løvvik[4]; Spyridon Diplas[5]; Patricia Almeida Carvalho[6]; Terje G Finstad[1]; [1]SMN, Department of Physics, University of Oslo, Norway; [2]SINTEF Materials and Chemistry, Norway; [3]CENIMAT, Faculdade de Ciencias e Tecnologia, Universidade Nova de Lisboa, Portugal; [4]SMN, Department of Physics, University of Oslo, Norway and SINTEF Materials and Chemistry, Norway; [5]SMN, Department of Physics and Department of chemistry, University of Oslo, Norway; [6]SINTEF Materials and Chemistry, Norway and CEFEMA, Instituto Superior Tecnico, Universidade de Lisboa, Portugal

Equiatomic high entropy alloys (HEA) have attracted considerable interest due to their exceptional properties, which might be closely related to their extreme disorder induced by chemical complexity. We have sputtered thin films of CrFeCoNiCu onto insulating and optically transparent substrates in order to measure electrical and optical functional properties. After several optimizations desired sputtering conditions were obtained for the deposition of CrFeCoNiCu onto fused quartz wafers. All the samples were characterized by structural, chemical and electrical methods. The as prepared films had fcc-type structure. Hall measurements were performed from 10 K to 600K. The resistivity was a factor 104 higher than the elemental metals and the temperature dependence was different. The sign of the Hall coefficient indicates that the film was dominated by holes, while the Seebeck coefficient was negative and dominated by electrons. The electric properties will be discussed in terms of a model considering electronic structure and scattering.

Predicting Phase and Mechanical Properties of Refractory HEAs Using Machine Learning: *Ankit Roy*[1]; Ganesh Balasubramanian[1]; [1]Lehigh University

HEAs have witnessed an exponential rise in interest over the last decade and have attracted significant attention due to their potential for achieving unique properties. While on one hand the Edisonian approach that opens infinite possibilities of combining various elements to synthesize HEAs is time-consuming, on the other hand, the experimental recipes may not necessarily lead to specific solid-solution phases required for the strengthening mechanisms. Thus, an inverse design strategy is required to address this challenge. We develop a machine learning tool, trained to correlate structural metrics with alloy properties, to identify designer compositions with targeted mechanical properties and crystallographic phases from refractory multi-principal elements. In particular, we employ an artificial neural network scheme and engineer the dataset with the Hume-Rothery rules, lattice features and physical properties. The model predictions for the phases and Young's moduli for equiatomic alloys composed of Mo-Ta-Ti-W-Zr elements show reasonable agreement with experimental measurements.

Radiation-induced Damage of CrMnFeNi-based High-entropy Alloys: *Zhouran Zhang*[1]; Patrick Grant[1]; David Armstrong[1]; [1]Oxford University

CrMnFeCoNi HEA has been extensively investigated and exhibits many promising properties. Early experiments of CrMnFeCoNi and Cr0.66MnFeNi HEA under ion implantation indicated their potentials as structural materials in nuclear applications. CrMnFeCoNi, Cr0.66MnFeNi and yttrium-doped CrMnFeCoNi HEA were irradiated with 2 MeV V and Ni ions at temperature of 500oC and at 0.4 and 2.7 displacements per atom (dpa). Using advanced characterisation techniques, radiation-induced damage was investigated. All alloys show significant depletion of Mn, minor depletion of Cr, significant enrichment of Ni and slight enrichment of Fe along grain boundaries at 2.7 dpa. The segregation of y-doped CrMnFeCoNi is less pronounced. Both V and Ni ions were used in order to investigate the effect of particle type on radiation damage. Nano indentation tests showed that the irradiated specimens showed no obvious hardening at 0.4 dpa but an increase of ~10% and ~15% at 2.7 dpa in y-free and y-doped CrMnFeCoNi HEA.

Sintering of HfNbTaTiZr Alloy: *Frantisek Lukac*[1]; Monika Vilémová[1]; Radek Mušálek[1]; Štefan Csáki[1]; Jan Cížek[1]; Jakub Cížek[2]; [1]Institute of Plasma Physics of the Czech Academy of Sciences; [2]Charles University, Mathematics and Physics Faculty

Refractory alloys are often produced by sintering process due to the advantage of relatively low processing temperature and time and high heating rates. Mechanical properties of powder metallurgy products sintered by spark plasma sintering method used in this work are drastically different from other processing routes due to smaller grain size, different phase composition, porosity, oxide content and microstructure depending on powder preparation. Firstly, single phase HfNbTaTiZr alloy with various grain size was produced from gas atomized powder using various sintering parameters. Secondly, sintering of mechanically alloyed powder produced by high energy ball milling process resulted in disintegration of high entropy bcc phase into marble-like microstructure of nanocrystalline sized grains comprised of different intermetallic phases. High deformation induced in this powder acts as diffusion accelerator and therefore thermal treatment during sintering produces promising properties. Besides quantitative phase composition analysis, defects concentration measured by positron annihilation is emphasized in this work.

Strain Hardening Behavior of Equi-atomic CoCrFeMnNi High-entropy Alloy at Low and Room Temperature: *ChuChun Chueh*[1]; [1]National Tsing Hua University
The effect of lattice distortion on mechanical properties and deformation mechanism was investigated at –145 °C and room temperature. In the present study, tensile tests of pure Ni, Ni-2at.% W (medium lattice distortion), Ni-4at.% W (severe lattice distortion which is compatible with CrFeNi and CoCrFeMnNi), equi-atomic CrFeNi and equi-atomic CoCrFeMnNi high entropy alloy were conducted. Strain hardening behavior was investigated by strain hardening rate, hardening exponent evolution and Crussard-Jaoul analysis. The tensile tests showed that all of these had better mechanical properties at lower temperature. CoCrFeMnNi is due to the deformation twin, therefore, Ni, Ni-2at.% W and Ni-4at.% W are because the less dynamic recovery, which cause the increase of work hardening rate according to Considère criterion. As for the deformation mechanism, in addition to lattice distortion, factors such as stacking fault energy, critical twinning stress and lattice distortion distributions were used to explain the differences of strain hardening behavior.

Studies on Wear Behavior of High Entropy Alloy Synthesized by Mechanical Alloying and Spark Plasma Sintering: *Shree Krishna*[1]; Sonali Tanwar[1]; Debjani Chakraborty[1]; Jyotsna Majumadar[1]; [1]Indian Institute of Technology
In the present study, CoCrFeMnTi based high entropy alloy has been synthesized by mechanical alloying and subsequently, consolidated by spark plasma sintering at the pressure of 50 MPa and at a temperature of 9000C. The developed powders and coupons have been subjected to a detailed microstructure, elemental and phase analysis by using Scanning electron microscope, energy dispersive spectroscopy and X-ray diffraction techniques. The mechanical properties of the coupons have been evaluated in terms of Vickers microhardness testing and wear behavior at varying loads. The wear rate, wear depth and coefficient of friction were also determined accompanied by the SEM images of wear track and debris and possible wear mechanism were also proposed. At the end wear behavior of the alloy was compared with High speed steel of M2 grade which shows supremacy in term of wear resistance.

Study of Lattice Distortion Effect on the Mechanical Property of BCC Alloy: From Low-entropy to High-entropy Alloys: *Ying-Chih Wu*[1]; [1]National Tsing Hua University
The mechanical properties of BCC-series alloys subjected to various annealing temperature were investigated. The influence of severe lattice distortion effect to material's hardness and tensile properties were analyzed. In this study, Ta, HfNbTa, HfNbTaTiZr BCC-series alloys with different degree of entropy were fabricated by vacuum arc melting and subjected to cold working. The cold worked specimens were annealed under different temperature for one hour and water quenched. With fixed annealing period, relation between microstructure and mechanical properties showed special tendency. The number of elements involved dominates the overall mechanical properties since the lattice distortion degree increases with elements number. The present research concluded this extraordinary trend and made a comparison with conventional alloys, hence helped figure out the origin of its outstanding properties through deformation behavior. With this study, it is hoped to have a better understand and an extensive utilize of refractory high entropy alloy.

Synthesis and Characterization of TixAlSixMoW Light-weight High Entropy Alloys: Mechanical and Electrochemical Studies: *Lehlogonolo Kanyane*[1]; Patricia Popoola[1]; Nicolus Malatji[1]; [1]Tshwane University of Technology
High entropy alloys (HEAs) materials possess outstanding mechanical and corrosion properties for advanced engineering applications such as aerospace, chemical plants and furnace parts. In this work, TiAlMoSiW, Ti0.25AlMoSi0.25W0.1 and Ti0.3AlMoSi0.3W0.1 HEAs are developed via spark plasma sintering. The developed HEAs are consolidated at 1000oC with holding time of 8 min and applied pressure of 50MPa. SPS technique is known to offer enhanced densification and controlled grain growth of the alloy with minimal porosities. Scanning electron microscope coupled with energy dispersive spectrometer (SEM/EDS) and X-ray diffractometer (XRD) are used to analyze the morphological evolution and phases formed respectively. Microhardness and tribological properties of the synthesized alloys were analyzed by means of diamond base micro hardness tester and tribometer (Rtec) respectively. Corrosion resistant properties of the synthesized HEAs was evaluated by means of 101 AUTOLAB potentiostat. The synthesized HEAs shows a good mechanical properties and high corrosion resistance properties.

Synthesis of Equiatomic CoCrFeMnTi and CoCrFeMnNiTi Based High Entropy Alloys by Powder Metallurgy Route: *Turin Datta*[1]; Jyotsna Dutta Majumdar[1]; Debjani Chakrabarty[1]; [1]Indian Institute of Technology Kharagpur
The traditional conventional alloying strategy was taken to a newer height when the concept of high entropy alloy was emerged in which more than five elements are added in equiatomic or near-equiatomic proportions which increases the high configurational entropy of mixing and stabilizing solid solution based microstructure. In this work, 3D transition elements based equiatomic nanocrystalline high entropy alloys having composition CoCrFeMnTi and CoCrFeMnNiTi has been synthesized using the non-equilibrium, solid-state route, known as mechanical alloying. The phase evolution as a function of milling time has been evaluated by X-Ray Diffraction technique. The nanocrystalline behavior of the alloys has been confirmed by transmission electron microscopy (TEM) and selected area diffraction pattern (SAED) technique. Futher, to understand the high temperature stability of the alloys, both CoCrFeMnTi and CoCrFeMnNiTi has been heat treated at 800 degree celsius for 24 hours and its XRD phase evolution has been carried out.

The Hardness of Al-Cr-Si-Ti Nitride Coatings: *Ching-Yin Lee*[1]; [1]National Tsing Hua University
The high-entropy nitride coatings comprised of various constituents Al, Cr, Si, Ti was deposited on Si substrate by Radio Frequency magnetron sputtering process. The Al-Cr-Si-Ti multi-component target introduced in this study was fabricated by vacuum arc melting. Different coatings were fabricated with different composition of target designed by Taguchi method. The hardness of AlCrSiTi nitride films with different composition was investigated and then analyzed by factor effects. The result showed that with increasing content of Al as well as Si, the hardness of the nitride film decreased, whereas as the Ti element decreased, the hardness of the nitride film did not change significantly. We got the best integrate property optimized film H with a hardness of 32 GPa. This research demonstrates that the $(AlCrSiTi)_{100-x}N_x$ nitride films have a potential for application of the protective hard coating on cutting tools.

The Role of Short-range-order on Strengthening of NiCoCr: Theory and Experiments: B Yin[1]; S Yoshida[2]; N Tsuji[2]; *William Curtin*[1]; [1]Ecole Polytechnique Federale de Lausanne; [2]Kyoto University

The FCC medium entropy alloy NiCoCr has received considerable attention for its high yield strength, high toughness especially at low temperature, twinning behavior, low stacking fault energy, and presence of, and possible effects of, chemical Short Range Order (SRO). Here, we derive the misfit volumes of the elements Ni, Co, and Cr in the equi-composition alloy from high-precision measurements of the lattice constants at compositions around the central equi-composition. We show that standard spin-polarized DFT predicts incorrect volumes for Co and Cr, which leads to incorrect misfit volumes in the random state. Further deviations between DFT and experimental lattice constants of NiCoCr occur when SRO is introduced. We then use the measured misfit volumes and measured elastic constants as input to a theoretical model for the yield strength based on a random alloy with no SRO. The theory predicts the CRSS for NiCoCr in good agreement with recent single-crystal measurements. Further validation of the theory is obtained for the yield strength of Ni-Cr binary alloys that do not possess SRO and NiCoV. Furthermore, the hardness values for NiCoCr after 16 days of annealing at 700 °C and 1100 °C are measured to be equal. All of these findings point to the negligible role of SRO in the strengthening of NiCoCr. This indicates that either SRO itself is negligible or that the level of SRO in these alloys does not make a major contribution to strengthening.

Toughness Enhancing Deformation Mechanisms in the CoCrNi Family of MPEAs: *John Copley*[1]; Francisco Coury[2]; Jonah Klemm-Toole[1]; Jinling Gao[3]; Yaofeng Guo[1]; Kester Clarke[1]; Benjamin Ellyson[1]; Chandler Becker[1]; Brian Milligan[1]; Christopher Frinfrock[1]; Chloe Johnson[1]; Niranjan Parab[4]; Kamel Fezzaa[4]; Tao Sun[4]; Wayne Chen[3]; Amy Clarke[1]; [1]Colorado School of Mines; [2]UFSCar; [3]Purdue University; [4]Argonne National Laboratory

Multi-Principal Element Alloys (MPEAs), which have evolved from studies of High Entropy Alloys (HEAs), are a new and promising class of materials that have potential in structural applications. Some MPEAs, especially those from the CoCrNi family, have shown promise as high toughness materials, even at cryogenic temperatures. These MPEAs gain their high toughness from deformation mechanisms such as transformation and twinning induced plasticity (TRIP and TWIP respectively), which increase work hardening and consequently, toughness. Studies of the deformation behavior of CoCrNi MPEAs may enable the design of high toughness structural alloys. As the compositional landscape for MPEAs is vast, high-throughput methods for determining the TRIP/TWIP viability of alloys are required. This requires a better understanding of the alloying, strain rate and thermal effects on TRIP/TWIP behavior. To this end, a series of CoCrNi alloys were prepared and tested under various conditions to examine these effects on the deformation mechanisms exhibited.

Microstructural Evolution of CoCrFeMnNi under Tribological Load with Varying Stress Field: Antje Dollmann[1]; Alexander Kauffmann[2]; *Martin Heilmaier*[2]; Christian Greiner[2]; [1]Karlsruhe Institute of Technology; [2]Karlsruhe Institute of Technology

The high strength and corrosion resistance of High Entropy Alloys (HEAs) is expected to be advantageous for tribological applications. As the microstructure of a material under a tribological load is highly dynamic and has a complex interplay with the tribological properties, understanding the fundamental mechanisms of deformation and microstructure change is challenging. The focus of the present work is to reveal the fundamental deformation mechanisms governing the mechanical response of CoCrFeMnNi to the high shear loading of a sliding contact after single strokes with varying tangential and normal loads. While changes of normal load are easy to be realized, changes in tangential load were provoked by varying adhesive forces with counter body modifications. By STEM and Kikuchi Diffraction Patterns, the resulting deformation layer was analysed. The obtained microstructural data was used to evaluate the effect of stress field modifications on HEAs in terms of their potential use in tribological contacts.

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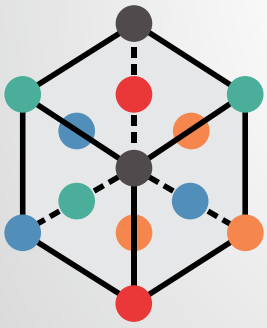

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