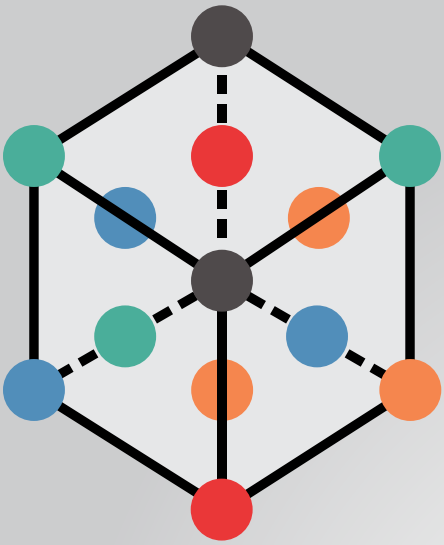

2nd WORLD CONGRESS ON

HIGH ENTROPY ALLOYS

HEA2021

December 5–8, 2021

Hilton Charlotte University Place
Charlotte, North Carolina, USA

ABSTRACT BOOK

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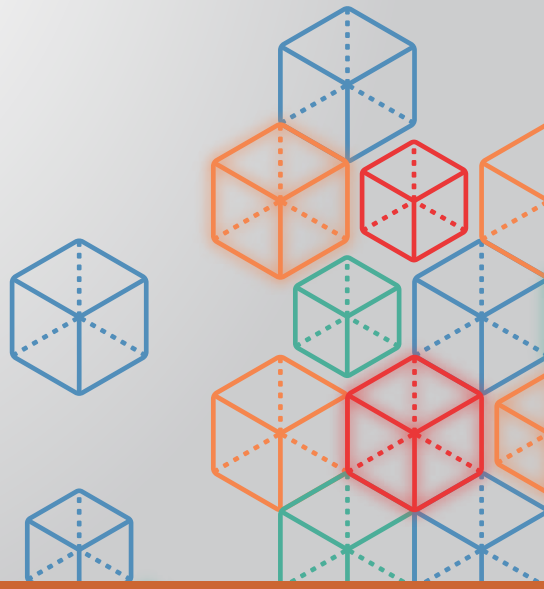

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Pre-Recorded and On-Demand Oral Presentations

Friday AM
December 3, 2021
Platform

Room: On-Demand Program Area
Location: Online Conference

Session Chair: To Be Announced

Invited

ON DEMAND: Mechanical Properties of High Entropy Single Crystal Superalloys at Elevated Temperatures: *Hideyuki Murakami*[1]; Takuma Saito[1]; An-chou Yeh[1]; [1]National Insititute for Materials Science

High entropy alloys (HEAs) have opned a vast composition field for materials design and some alloys have demonstrated excellent mechanical properties with reasonable ductility. In addition, lower mobility of alloying elements in the alloys could maintain microstructural stabilities and mechanical properties at elevated temperatures. High entropy superalloys (HESAs) have been proposed to design alloy composition to lie in the high entropy field and to have coherent gamma and gamma prime two-phase microstructure, thereby HESAs are expected to possess excellent high temperature properties. In the presentation, heat treatment, microstructure and high temperature mechanical property relationships of a HESA (Ni-8.9Fe-16.9Co-7.5Cr-0.9Mo-0.5W-10.3Al-5.8Ti-1.2Nb in at. %) are discussed. It is confirmed that change in heat treatments drastically altered the configurational features of gamma prime precipitates, which accordingly variated tensile and creep properties. It should be noted that excellent ductility of HESA is confirmed with the full standard sized single crystal tensile / creep specimens.

Invited

ON DEMAND: Exploiting the Insensitivity of Certain HEAs to Compositional Variation: *Matthew Barnett*[1]; Jithin Joseph[1]; Murugesan Annasamy[1]; Daniel Fabijanic[1]; [1]Deakin University

A cursory glance at the literature shows that a number of different HEAs occupy similar regions of property space. The present talk looks at whether or not this could be something worth exploiting. The focus is mechanical performance. A series of compositions are investigated that fall largely within the fcc phase region. Physical and numerical means are employed to probe the insensitivity of the mechanical response to compositional change. Means of quantifying insensitivity are proposed. Various manufacturing paths are examined and high temperature wear performance is considered in addition to room temperature properties. Finally, prospects and pathways for exploiting 'compositional flexibility' in recycling and manufacturing are explored.

Invited

ON DEMAND: On the Tuning of Creep Properties by Balancing Trace Elements: *Anna Manzoni*[1]; Sebastian Haas[2]; Yasemin Bahadir Yesilcicek[1]; Uwe Glatzel[2]; [1]BAM; [2]University Bayreuth

The search for a high entropy alloy that would withstand the conditions in an aeroplane turbine lead to the Al10Co25Cr8Fe15Ni33Ti6 compositionally complex alloy which combines good strength and ductility. Inspired from superalloy design the authors started to search for trace elements that would further improve the mechanical properties of the alloys. It turned out that the addition of two elements, i.e. Hf and W, would lead to a well-tunable microstructure in terms of precipitate shape and lattice misfit, as was determined via scanning and transmission electron microscopy and synchrotron x-ray diffraction. The direct link of these characteristics to the mechanical properties could be verified via creep experiments.

Invited

ON DEMAND: Developing High Entropy Alloys for Advanced Nuclear Applications: *Amy Gandy*[1]; Ed Pickering[2]; Alexander Carruthers[2]; David Armstrong[3]; Dhinisaben Patel[1]; Hamed Shahmir[1]; Bo-Shiuan Li[2]; R Mythili[4]; Chanchal Ghosh[5]; Arup Dasgupta[5]; [1]University of Sheffield; [2]University of Manchester; [3]University of Oxford; [4]Indira Gandhi Centre for Atomic Research ; [5]Indira Gandhi Centre for Atomic Research

High entropy alloys (HEAs) and other compositionally complex alloys (CCAs) are being engineered to meet the unique requirements of advanced nuclear applications. Specific to fusion and fast fission reactors, reactor core materials must withstand high fluxes of high energy neutrons, resulting in high levels of radiation induced damage and transmutation which can deleteriously impact material properties. In addition, for future commercial fusion reactors, materials are expected to meet the reduced activation criterion, designed to not be radioactive for more than 100 years following removal from the reactor core. In this talk, an overview of our alloy design process, used to target reduced activation compositions which are predicted to be radiation damage resistant, will be given. Examples of our experimental assessments of the suitability of these alloys for advanced nuclear applications, including using in-situ high temperature X-ray diffraction, and ion implantation to simulate neutron irradiation and transmutation products, will be presented.

Invited

ON DEMAND: Efficient Prediction of the Yield Strength of BCC High Entropy Alloys: *Francesco Maresca*[1]; William Curtin[2]; [1]University of Groningen; [2]EPFL

Body-centered-cubic (BCC) high entropy alloys of the (Al)-Cr-Hf-Mo-Nb-Ta-Ti-V-W-Zr family show exceptional high temperature strength. Mechanistic yet efficient computational guidance is needed to identify the most promising alloys within the immense compositional space. Here, we introduce a holistic, parameter-free strengthening theory of screw and edge dislocations in BCC alloys. In contrast with the screw-controlled pure BCC metals, in non-dilute BCC alloys both edge and screw dislocations are pinned due to strong local energy fluctuations. Both screw and edge dislocations assume wavy/kinked minimum-energy configurations where dislocation segments of characteristic length zetac are pinned at low-energy sites. Edge dislocation strengthening, that scales with misfit volumes and elastic moduli, occurs at all temperatures because of the large energy barriers associated to energy fluctuations in the random alloy. The edge theory is used to predict the high-temperature yield strength of ~10M alloys in the Al-Cr-Hf-Mo-Nb-Ta-Ti-V-W-Zr compositional space, providing guidance for manufacturing high-strength BCC HEAs.

Invited

ON DEMAND: On the Corrosion and Passivation of Multi-principal Element Alloys (MPEAs): *Nick Birbilis*[1]; Sanjay Choudhary[2]; [1]Australian National University; [2]Monash University

Several multi-principal element alloys (MPEAs) are reported to exhibit excellent corrosion and pitting resistance. Owing to a scarcity of detailed physical analysis, mechanistic aspects of the passivity MPEAs have not been adequately described to date. The complex thermo-kinetic interfacial processes that govern the dissolution behavior of MPEAs are challenging to ascertain; and herein an in-situ atomic emission spectroelectrochemistry (AESEC) method was used to investigate dissolution and passivation behavior. Along with AESEC analysis, the formation and evolution of the passive films were studied using X-ray photoelectron spectroscopy (XPS), Mott-Schottky analysis and equilibrium thermodynamics. The work herein was approached in a manner to allow a visual representation of what such passive surfaces.

ON DEMAND: Density Functional Theory Study of Short-range Order in Bulk, Grain Boundary, Stacking Fault, and Surface of CrMnFeCoNi Alloy: Artur Tamm[1]; Tomorr Haxhimali[1]; *ShinYoung Kang*[1]; [1]Lawrence Livermore National Laboratory

Element distribution in high-entropy alloys influences critically the materials properties: from mechanical strength and fracture mechanisms, chemical reactivity, thermodynamic stability, to electronic structures. However, due to its short length scale (often less than nm) and complex nature tied with composition, microstructure, and processing conditions, it is challenging to experimentally probe and understand the relationship between the short-range order (SRO) and materials properties. In our first-principles based Monte Carlo study we identified the low-energy element distribution in the bulk, grain boundary (GB), stacking fault (SF) and surface of CrMnFeCoNi alloy. The predicted SRO in bulk is globally applicable to GB, SF, and surface structures, while the distinct local segregation was observed in GB, SF, and surface. The contributing factors to the local segregation and implication of SRO to the materials property will be discussed and compared with findings from other literature.

ON DEMAND: Predicting Fundamental Properties of bcc Refractory Multicomponent Alloys Using Electronic Descriptors and Statistical Learning: *Yong-Jie Hu*[1]; Christopher Tandoc[1]; Liang Qi[2]; [1]Drexel University; [2]University of Michigan

Optimizing chemistries of bcc refractory multicomponent alloys to achieve a synergy of high strength and low-temperature ductility requires reliable predictions of the correlated alloy properties across a vast compositional space. In this work, first-principles calculations were performed for 106 individual bcc solid-solution alloys to predict several strength/ductility-related fundamental alloy properties, including lattice distortions, unstable stacking fault energies, and surface energies. With the descriptors based on electronic structures of interatomic bonding, several statistical learning models were developed to efficiently and accurately predict the formation energies of these planar defects and magnitudes of lattice distortions according to alloying compositions. The developed statistical models further enabled rapid and systematic search of potential alloy candidates that are intrinsically ductile and with high yield strengths across high-order multicomponent systems.

ON DEMAND: Atomistic Simulations of Suppression of Dislocation Emission from Grain Boundaries through Free Volume in High-entropy Alloys: *Kohei Shiotani*[1]; Tomoaki Niiyama[1]; Tomotsugu Shimokawa[1]; [1]Kanazawa University

In conventional alloys, smaller excess free volume at grain boundaries (GBs) is known to increase the stress required for dislocation emission, e.g., twin boundary. In high-entropy alloys (HEAs) consisting of various elements with different atomic sizes, smaller GB free volume can be achieved even in large misorientation angles if GB segregation occurs due to large (small) atoms occupying large (small) atomic sites. In this study, we investigate the possibility of the strengthening mechanism by GB segregation in HEAs through a simple two-dimensional atomistic simulation. Thermally equilibrium atomic configurations of bicrystal models at different temperatures obtained by Monte Carlo analyses show that stronger GB segregation of the maximum and the minimum size atoms, which decreases GB free volume, occurs as the temperature becomes lower. Uniaxial deformation tests reveal the suppression of dislocation emission from segregated GBs with small free volumes. As results, GB segregation could be a strengthening mechanism in HEAs.

ON DEMAND: Investigation of Reduced Activation FCC-type High Entropy Alloys for Nuclear Applications: *Hiroshi Oka*[1]; Naoyuki Hashimoto[1]; Shigehito Isobe[1]; Mikito Ueda[1]; Shigenari Hayashi[1]; Shinichiro Yamashita[2]; Mitsuhiro Itakura[2]; Tomohito Tsuru[2]; [1]Hokkaido University; [2]Japan Atomic Energy Agency

The interest on high entropy alloys (HEAs) as next generation nuclear energy application is increasing due to its potential of irradiation resistance. For the nuclear application, Co-free HEAs are attractive because Co can be activated by neutron irradiation. Because the formation of planar defects, e.g. frank loops, introduced by irradiation are a main cause of irradiation hardening in FCC alloys, controlling stacking fault energy (SFE) is essential for designing alloys with high radiation tolerance. In this study, Cr0.8FeMnxNiy HEAs with FCC structure were investigated. The room temperature tensile tests showed that tensile strength depended on the concentrations of Mn and Ni and Cr0.8FeMn1.3Ni1.3 had the highest tensile strength, which was higher than that of conventional 316 stainless steel. The SFE was estimated by measuring the width of extended dislocations using TEM, and it is shown that the SFE increased with increasing the total concentration of Mn and Ni.

ON DEMAND: Factors Affecting Stacking Fault Energies in Concentrated Alloys Using Density Functional Theory and Machine Learning: *Gaurav Arora*[1]; Anus Manzoor[1]; Dilpuneet S. Aidhy[1]; [1]University of Wyoming

Recent experimental work has shown that addition of specific elements can lower the stacking fault energy (SFE) of certain high entropy alloys thereby breaking the strength vs ductility tradeoff. In order to design alloys with desired SFEs, understanding the mechanisms that control SFE is critical. In this work, using density functional theory (DFT) calculations, we isolate the role of atomic radii, valence electron charge, electronegativity and nearest neighbor environment on SFE in 3d, 4d and 5d doped Ni-based alloys. In particular, we find that the difference between the radius of the dopant and the matrix element is the most important factor contributing to SFE. Furthermore, we illustrate a machine learning model that is able to predict SFE in complex alloys from a database of simpler alloys thereby enabling data-science based design of alloys.

ON DEMAND: Development of an Interatomic Potential for the FeNiCrMn System: Dislocation Properties: *Ayobami Daramola*[1]; Giovanni Bonny[2]; Gilles Adjanor[3]; Christophe Domain[3]; Ghiath Monnet[3]; Anna Frackiewicz[1]; [1]Ecole des MINES SMS centre; [2]SCK CEN, Nuclear Materials Science Institute; [3]EDF—Centre de Recherche des Renardieres

FeNiCrMn alloys have attracted considerable attention in High Entropy Alloys (HEAs) research due to their various practical industrial and scientific applications. For a better fundamental understanding, the development of reliable and efficient interatomic potentials for the FeNiCrMn alloy is important. In this work, we constructed an interatomic potential for theFeNiCrMn system within the embedded atom method formalism to model dislocation movements. The FCC phase of the FeNiCrMn system was stabilized over a wide range of temperatures and compositions. The stacking fault energies and elastic constants are well reproduced for the FeNiCrMn systems in comparison with available theoretical and experimental data. The edge dislocation mobility will be presented in a wide of composition range and temperature range 300-900K. The friction stress increases essentially with the addition of Mn and increasing configurational entropy.

ON DEMAND: Prediction of Optimal High Entropy Alloys Using New Thermodynamic Multi-objective Criteria: *Aimen Gheribi*[1]; Arthur Pelton[1]; Jean-Philippe Harvey[1]; [1]Polytechnique Montreal

We present an original formalism to identify single and dual phase regions (temperature-compositions) within the Fe-Cr-Mn-Ni-V-Ti-Al-Co-Mo system. The identification of single or dual phase regions is the first step towards the design of high entropy alloys (HEA) with interesting mechanical, thermo-physical and corrosion resistance properties. The composition ranges of new potential HEAs are calculated considering a set of multi-objective functions linked to the single (dual)-phase start temperature, the room-temperature driving force for phase assemblage evolution and the solidification range under a set of non-smooth and non-linear compositions and property constraints.The proposed approach links a constrained Gibbs energy minimization technique to an optimization algorithm implemented for solving "blackbox" objective functions and constraints. The predictive capability of the proposed approach depends on the accuracy of the thermodynamic databases considered to calculate the phase equilibria. Several examples of new first-generation HEAs potentially suitable for future industrial applications will be presented.

ON DEMAND: The Combined Effect of Irradiation and Stress on Damage in a BCC CrMnFeV High-entropy Alloy: *Hyosim Kim*[1]; Stuart Maloy[1]; Jonathan Gigax[1]; Osman El-Atwani[1]; [1]Los Alamos National Laboratory

High-entropy alloys (HEAs) have been widely studied for the past decade and have shown exceptional material properties (i.e. mechanical strength, corrosion and radiation tolerance). There is, however, a lack of coverage of HEAs subject to heavy ion/neutron irradiation to high damage levels (~200 dpa) and prototypic fast reactor environments. Furthermore, there are very few studies on the radiation response of transition metal body centered cubic (BCC) HEAs and even fewer investigating synergistic effects with radiation and other environments. In this study, the influence of tensile stress on the radiation-induced microstructural changes is investigated for BCC CrMnFeV HEA which has shown excellent mechanical properties. High dose ion irradiation (200 dpa) was conducted on the specimen at 500 °C with a tensile stress applied (50 % of yield strength) during irradiation. Post-irradiation characterization on microstructural changes such as void swelling, dislocation and grain morphologies will be presented.

ON DEMAND: Ultra-high Strength and Ductility of a Multiple Component Alloy with a Heterogeneous Microstructure of Grains and Precipitates: Weitong Wang[1]; Shengyun Yuan[1]; *Yong Zhang*[1]; [1]Nanjing University of Science and Technology

In the present study, a heterogeneous microstructure characterized by a mixture of nano-grains and ultrafine-grains embedded with ' precipitates is fabricated by cold rolling a coarse-grained Ni-Co-Cr alloy and subsequent thermal annealing. The sample with heterogeneous microstructure exhibits simultaneously higher strength and larger uniform elongation compared with the original alloy without cold rolling. Electron backscatter diffraction, transmission electron microscopy, energy dispersive X-Ray spectroscopy, and atom probe tomography are performed to investigate the microstructural evolution of the heterogeneous structure tensile loaded to various strains, with an emphasis on the evolution of defects around the interface between nano-grains and ultrafine-grains. With a thorough comparison with the original coarse-grained sample on the deformation mechanisms, the effect of the complexity of the heterogenous microstructure on the evolution of dislocation density and deformation mechanism is illustrated, which serves to reveal the mechanisms responsible the work hardening and ductility.

ON DEMAND: An Experimental Study of the Effects of Deviations from AlCoCrFeNi Alloy Composition and Heat Treatment on the Microstructure, Phase Stability and Properties of Cast High Entropy Alloys: *David Browne*[1]; Oisin Gavigan[1]; Andrew Murphy[1]; Mert Celikin[1]; [1]University College Dublin

Equal atomic parts AlCoCrFeNi and novel Al0.4CoCrFeNi1.6 and Al0.7CoCrFeNi1.3 high entropy alloy samples were fabricated, and cast into molds enabling various solidification rates. X-ray diffraction displayed single or dual phase consisting of FCC, BBC or ordered B2 phases in as-cast state. Four Al0.7CoCrFeNi1.3 samples were studied in an as cast and annealed state, with annealing performed on three of the samples at 650°C, 800°C and 950°C for annealing times of three hours. Average hardness of 277 HV across the four Al0.7CoCrFeNi1.3 samples in the as-cast condition was found to increase to within the range 545 to 1106 Hv post-annealing. Microscopy and energy dispersive X-ray spectroscopy revealed an increase in elemental segregation following annealing due to a corresponding increase in the ordering of the systems with the precipitation of Ni and Al rich B2 acicular like needle and larger globular precipitates along with the Cr rich phase being observed.

ON DEMAND: High-temperature Gas Corrosion at 800 °C in H_2O-O_2-SO_2 of CrMnFeCoNi (HEA) and CrCoNi (MEA): Wencke Schulz[1]; Stephanos Karafiludis[1]; Guillaume Laplanche[2]; Mike Schneider[2]; Christiane Stephan-Scherb[1]; *Anna Manzoni*[3]; [1](BAM) Bundesanstalt fur Materialforschung und -prufung; [2]Ruhr Universität Bochum (RUB); [3]BAM

The high-entropy alloy $Cr_{20}Mn_{20}Fe_{20}Co_{20}Ni_{20}$ (HEA) and the medium-entropy alloy $Cr_{33}Co_{33}Ni_{33}$ (MEA) exhibit excellent mechanical properties and are considered for high-temperature applications. Both materials were exposed in a mixed gas atmosphere of Ar-10% H_2O-2% O_2-0.5% SO_2 [Vol.%] at 800 °C for up to 96 h. The oxide scales formed on the quinary alloy (HEA) are systematically and significantly thicker (up to 31 µm) than those on the ternary alloy (MEA). The CrCoNi alloy developed a very thin discontinuous Cr_2O_3 layer (<1 µm). The scales on HEA-CrMnFeCoNi are composed of an outer, porous layer (Mn_3O_4 and $MnSO_4$), a thin Cr_2O_3 layer at the alloy interface and an intermediate Mn_3O_4 layer. This comparative study shows that the medium entropy CrCoNi alloy forms a protective chromia layer at 800 °C under the corrosive conditions investigated (96 h in Ar-H_2O-O_2-SO_2) and is thus more resistant to corrosive gases than the high entropy CrMnFeCoNi alloy.

ON DEMAND: On the Phase Stability, Mechanical Properties, and Deformation Mechanisms of the Equiatomic CrFeNi Medium-entropy Alloy: *Mike Schneider*[1]; Guillaume Laplanche[1]; [1]Ruhr-University Bochum

Due to its compositional simplicity and single-phase character, the CrFeNi medium entropy alloy constitutes a missing link between binary and more complex engineering alloys such as austenitic stainless steels and Fe-based superalloys. In the present study, heat treatments at various temperatures revealed that CrFeNi forms a stable FCC solid solution above ~1250 K. Compression and tensile tests were carried out for recrystallized FCC microstructures with different grain sizes between 77 K and 873 K. Additionally, tensile tests interrupted at pre-defined levels of plastic strain in combination with transmission electron microscopy were performed to reveal the active deformation mechanisms. While, in the early stages of plasticity, planar glide of dislocations dominates, deformation twinning acts as an additional mechanism as deformation progresses. From these findings, the critical resolved shear stress for twinning in CrFeNi was determined to be almost independent of temperature in accordance with modeling predictions.

ON DEMAND: Experimental Determination of Interdiffusion and Defect Kinetics in Multicomponent Systems: Susanta Kumar Nayak[1]; Somanath Danayak[1]; *Kaustubh Kulkarni*[1]; [1]Indian Institute of Technology Kanpur

'Sluggish diffusion' is probably the most debated aspect of the high entropy alloys in the literature over past one decade or so. Although rigorous experimental data on diffusion is required to settle this debate, the efforts done on the evaluation of meaningful diffusion parameters have been not much. The presentation will start with an overview of available literature on diffusion in the field of high entropy alloys and go on to explain the significance of classical interdiffusion studies in designing the compositions and applications of this class of materials. Experimental determination of interdiffusion coefficients as carried out in quinary and quaternary systems using body-diagonal diffusion couple approach will be discussed. Moreover, vacancies play important role in diffusion mechanisms in high entropy alloys and hence, the availability of data on energetics of vacancy formation and migration is crucial while addressing the issue of sluggish or non-sluggish diffusion in these alloys. The experimental determination of vacancy formation energies conducted in the binary Fe-Ni, quaternary Fe-Ni- Co-Cr and quinary Fe-Ni-Co-Cr-Mn systems will be presented. Such vacancy-formation energy data combined with experimental tracer diffusivity data available in the literature also helps in getting insights into the migration kinetics and diffusion mechanisms.

ON DEMAND: Computationally Guided High Entropy Alloy Discovery: *Kenneth Smith*[1]; John Sharon[1]; Ryan Deacon[1]; Soumalya Sarkar[1]; [1]Raytheon Technologies Research Center

Combining multiple principal elements together in single solid solution forming High Entropy Alloys (HEA) opens the possibilities to billions of new alloy combinations. To date, HEAs have demonstrated enhanced properties that can rival or exceed conventional alloys. We have used a combined computational and experimental approach to quickly assess and identify new alloy compositions. The computational approach searches composition space using machine learning informed by different computational models to identify compositions that maximize performance for different objectives while satisfying constraints. We couple the computational framework with screening experiments to validate performance as well providing a route for additional selection criteria, such as oxidation resistance that are more difficult to include directly with analytical functions. In this talk, we will describe our machine learning based framework and the experimental characterization used to assist in identifying HEA candidates.

ON DEMAND: Hydrogen Storage in Refractory High Entropy Alloys: *Claudia Zlotea*[1]; Jorge Montero[1]; Jean-Philippe Couzinié[1]; Anis Bouzidi[1]; Nayely Pineda-Romero[1]; [1]ICMPE CNRS

Hydrogen is considered as an interesting alternative to reduce fossil fuel consumption and subsequent pollution. However, one of the main challenges of using hydrogen as a clean energy carrier is its safe storage and transportation. Different metal/alloys have been investigated to store hydrogen as hydride materials. However, none of these alloys fulfil the requirements for a competitive storage media in practical applications. Consequently, breakthrough metallurgical concepts are stringently required to develop more efficient multifunctional hydrides with broad potential applications. In the present study we focus on the synthesis, the hydrogen absorption/desorption properties, and the cycling stability of the new high entropy alloys Ti-V-Zr-Nb-M where M = Mg, Al, Cr, Mn, Fe, Mo and Ta. The aim is to study the effect of the addition of M element into the initial refractory quaternary composition Ti-V-Zr-Nb on the structural, hydrogen sorption and cyclability properties.

ON DEMAND: Deformation Behaviors in Refractory High-entropy Alloys: *Chanho Lee*[1]; George Kim[2]; Yi Chou[3]; Michael Gao[4]; Ke An[5]; Gian Song[6]; Yi-Chia Chou[3]; Wei Chen[2]; Saryu Fensin[1]; Peter Liaw[7]; [1]Los Alamos National Laboratory; [2]Illinois Institute of Technology; [3]National Chiao Tung University; [4]National Energy Technology Laboratory/Leidos Research Support Team; [5]Oak Ridge National Laboratory; [6]Kongju National University; [7]University of Tennessee, Knoxville

Single-phase solid-solution refractory high-entropy-alloys (HEAs) show remarkable mechanical properties, such as high yield strength with significant softening resistance at elevated temperatures. Hence, the in-depth study of the deformation behavior for body-centered-cubic (BCC) refractory HEAs is a critical issue to explore the uncovered/unique deformation mechanisms. We have investigated the elastic- and plastic-deformation behaviors of a single BCC NbTaTiV refractory HEA at elevated temperatures, using integrated experimental efforts and theoretical calculations. The in-situ neutron-diffraction results reveal a transition of the elastic-deformation feature from isotropic to anisotropic modes at elevated temperatures. The single-crystal elastic-moduli and macroscopic Young's, shear and bulk moduli were determined from the in-situ neutron diffraction, showing the great agreement with first-principles calculations, machine-learning, and resonant-ultrasound spectroscopy results. Furthermore, the edge-dislocation-dominant plastic-deformation behaviors, which are different from conventional BCC alloys, have been quantitatively described by the Williamson-Hall plot profile modeling, which is further experimentally verified by the high-angle-annular-dark-field (HAADF) scanning-transmission-electron-microscopy (STEM).

ON DEMAND: Superior High-temperature Strength in a Refractory High-entropy Alloy: *Rui Feng*[1]; Bojun Feng[2]; Michael Gao[3]; Chuan Zhang[4]; Joerg Neuefeind[1]; Jonathan Poplawsky[1]; Yang Ren[5]; Ke An[1]; Michael Widom[2]; Peter Liaw[6]; [1]Oak Ridge National Laboratory; [2]Carnegie Mellon University; [3]National Energy Technology Laboratory; [4]Computherm, LLC; [5]Argonne National Laboratory; [6]The University of Tennessee, Knoxville

Refractory high-entropy alloys (RHEA) show promising applications at high temperatures. However, achieving high strengths at elevated temperatures above 1,173K is still challenging due to heat softening. Using intrinsic material characteristics as the alloy-design principles, a single-phase body-centered-cubic (BCC) RHEA with high-temperature strengths (beyond 1,000 MPa at 1,273 K) is designed, superior to other reported RHEAs as well as conventional superalloys. The origin of the high-temperature strength is revealed by in-situ neutron scattering, transmission-electron microscopy, and first-principles calculations. The designed RHEA's elevated-temperature strength retention up to 1,273 K arises from its large local lattice and modulus misfits, the insensitive temperature dependence of elastic constants, and the dominance of non-screw character dislocations caused by the strong solute pinning, which makes the solid-solution strengthening pronounced. The alloy-design principles and the insights in this study pave the way to design RHEAs with outstanding high-temperature strength.

ON DEMAND: Refractory Metals-based High Entropy Alloys: Phase Evolution and Radiation Damage Studies: *Poulami Chakraborty*[1]; Nilabja Sarkar[1]; Bathula Vishwanadh[1]; Raghvendra Tewari[1]; Srikumar Banerjee[2]; [1]Bhabha Atomic Research Centre; [2]Homi Bhabha National Institute

Present study reports phase evolution in equi-atomic Nb, V, Ti, Zr and Al alloy during cooling subsequent to levitation melting and laser surface melting. A large volume fraction of this alloy exhibited single phase grains having a composition of 35Nb25V25Ti10Al5Zr (all atom %). Bulk melting of an alloy of such a composition, followed by homogenisation annealing and quenching resulted in the formation of a single-phase bcc microstructure. The latter alloy, however, exhibited concomitant tendencies for clustering (phase separation into two bcc phases with differing compositions) and ordering (leading to the formation of the ordered B2 structure), which have been followed by detailed microstructural observations. These results have been rationalised in terms of thermodynamics of this multi-component system. Microstructural evolution during irradiation has also been studied with a view to examining the stability of these alloys in an intense radiation field.

ON DEMAND: Multiscale Modeling of Hydrogen Bubble Nucleation: *Tomorr Haxhimali*[1]; Artur Tamm[1]; ShinYoung Kang[1]; [1]Lawrence Livermore National Laboratory

High-entropy alloys (HEAs) have been reported as a promising system resistant to hydrogen embrittlement (HE), a century old problem affecting the mechanical stability of bridges, nuclear waste storage containers, and many other infrastructures. Using the equiatomic CrMnFeCoNi alloy as a model, we combined atomistic calculations with mesoscale phase field modeling to study its HE resistance and understand the underlying mechanisms. Density functional theory and classical molecular dynamics simulations have been performed to compute alloy-hydrogen interaction energetics, including absorption energies and migration energy barriers in bulk and grain boundaries, along with the surface cleavage energies of the alloy. Hydrogen bubble nucleation, one of the mechanisms for HE, has been simulated via a phase field model parameterized using atomistic simulation data. Hydrogen bubble nucleation kinetics and critical nuclei size in the CrMnFeCoNi alloy are predicted and compared with the pure copper system, a representative typical metal/alloy system vulnerable to HE.

ON DEMAND: Novel Mechanisms for Strengthening High-entropy Alloys: *Zhiming Li*[1]; [1]Central South University

Owing to the practically infinite compositional space of the multicomponent high-entropy alloys (HEAs), unique combination of strengthening mechanisms can be invoked to achieve excellent mechanical properties. For instance, apart from the intrinsic massive solid solution strengthening effect, we have obtained a joint activation of twinning- and transformation-induced plasticity effects in a series of HEAs by rendering them metastable. In this talk, we will introduce some of the new ideas that our group has recently developed for strengthening multicomponent HEAs. One of them is about the strategy of dynamic "bidirectional transformation induced plasticity (B-TRIP)" effect triggered in our materials by local dissipative heating and local micromechanical fields, which can also be further tuned by interstitial atoms. Another is about the concept of simultaneously triggering both nanosized shearable kappa-carbides and non-shearable B2 particles (dual-nanoprecipitation) in ultrastrong lightweight HEAs. Some other novel ideas for strengthening multicomponent HEAs may also be briefly introduced.

ON DEMAND: Predict Solid Solution Formation Using Machine Learning: *Michael Gao*[1]; Zongrui Pei[1]; Junqi Yin[2]; Jeffrey Hawk[1]; David Alman[1]; [1]National Energy Technology Laboratory; [2]Oak Ridge National Laboratory

Predicting solid solution formation remains essential in the high entropy alloys research. Various empirical rules are proposed to predict the formation of single-phase solid solution, but many are based on very small datasets and hence are of very limited predictability. In this project, we perform a machine-learning (ML) study on a large dataset consisting of 1252 alloys, including binary and high-entropy alloys, and we achieve a success rate of 93% in predicting single-phase solid solution. The present ML results suggest that the molar volume and bulk modulus are the most important features, and accordingly, a new physics-based thermodynamic rule is constructed. The new rule is nonetheless slightly less accurate (73%) than the ML algorithm but employs only the elemental properties and is thus convenient in applications. Finally, the advantages and pitfalls in applying high-throughput screening and ML versus CALPHAD calculations will be discussed.

ON DEMAND: Lattice Distortion and Its Effect on Strength in Refractory High-entropy Alloys: Chanho Lee[1]; Yi Chou[2]; George Kim[3]; Michael Gao[4]; Ke An[5]; Wei Chen[3]; Jonathan Poplawsky[5]; Gian Song[6]; Yi-Chia Chou[2]; Saryu Fensin[1]; *Peter Liaw*[7]; [1]Los Alamos National Laboratory; [2]National Chiao Tung University; [3]Illinois Institute of Technology; [4]National Energy Technology Laboratory/ Leidos Research Support Team; [5]Oak Ridge National Laboratory; [6]Kongju National University; [7]University of Tennessee, Knoxville

The lattice distortion is the core effect of HEAs to enhance the strength at room as well as high temperatures. The number of constituent elements with various atomic sizes have the identical possibility to occupy at atom positions of a crystal lattice, which induces a severe distortion of the crystalline lattice. Several studies have attempted to quantitatively measure the lattice distortion with increasing the number of alloying elements, using x-ray diffraction (XRD) and neutron diffraction (ND). However, only limited alloy systems have succeeded to demonstrate the correlation between lattice distortion and mechanical properties. In this study, we have systematically investigated the evolution of lattice distortions for Nb-Ta-Ti-V-Zr systems as function of number of additional elements and its effect on mechanical properties, using experimental [atom-probe-tomography (APT at CNMS), transmission-electron microscopy (TEM)] and modeling methods [density-functional-theory (DFT)]. It is found that lattice distortions have a critical role in improving yield strength.

ON DEMAND: Synergistic Studies on the Effects of Cr Contents on Phases and Mechanical Properties of CuNiTiFeCr HEAs: *Oluwaseun Akindele*[1]; [1]Federal University of Technology Akure

Many metallic elements in near-equiatomic ratios are used to make HEAs. The elements located along lattice points in the random solid solution of a particular high entropy combination (HEA) have a personal distribution. Various HEAs have demonstrated extraordinary properties (such as high ductility, fracture resilience, specific strength, and improved mechanical efficiency at elevated temperatures). This research will investigate the Effects of chromium contents on phases and mechanical properties of CuNiTiFeCr High Entropy Alloys system. The unique inherent property of HEAs will be exploited in fabricating a system acceptable in automobiles and aerospace. The proposed methodology will involve charge calculation of the alloying elements, casting, heat treatment and characterization (optical and mechanical). The morphologies and alloys structure will be characterized using an optical microscope, a SEM and a TEM. Micro-Raman spectrometer will be used to determine the efficiency of the fabrication technique for the alloys production and XRD, the elemental composition.

ON DEMAND: Multiphase, Multispecies Simulation of High Entropy Alloys for Brazing Applications: *Bogdan Nenchev*[1]; Chinnapat Panwisawas[1]; Hongbiao Dong[1]; Russell Goodall[2]; Dan Luo[2]; Nick Ludford[3]; [1]University of Leicester; [2]University of Sheffield; [3]TWI Ltd.

High Entropy Alloys (HEAs) are alloys consisting of multiple principal elements where configurational entropy of mixing dominates the thermodynamics of solidification. HEAs can find applications as brazing fillers by tailoring the material properties using computational alloy design. To tackle the challenge of the vast compositional space, the complexity of alloy composition and the large contrast in thermo-physical properties achieved, a combination of materials and computational modelling is crucial. In this work, finite element and level-set techniques were employed to study the wetting, spreading, and thermal-fluid behaviour of multiple HEA alloys. Melting and solidification multiphase flow coupled with heat transfer and diffusion models was constructed to simulate the laser brazing process of Inconel 718 to BNI2, FeCoNiMnCu, and CoCrCuFeNi alloys. A combination of experimental studies and thermodynamic simulations was utilised to obtain the required thermo-physical properties. Computational modelling is shown to be of paramount importance in the understanding the brazing performance.

Pre-Recorded and On-Demand Poster Presentations

Friday AM
December 3, 2021
Platform

Room: On-Demand Program Area
Location: Online Conference

Session Chair: To Be Announced

ON DEMAND: Designing New Corrosion Resistant Materials with Exceptional Strength-ductility Synergy and Good Weldability Using High Entropy Approach: *S. Nene*[1]; Rajiv Mishra[2]; [1]Indian Institute of Technology Jodhpur; [2]University of North Texas

Multiphase high entropy alloy (HEA) design provides abundant compositional space for developing newer materials having unexpected properties. However, good weldability is an important requirement for applications that require building a structural system. Thus we are pursuing new HEA design and processing approach wherein all other essential/desirable properties would be synergized with good weldability. As HEAs tend to limit solute partitioning or promote disordered solid solutions, a question emerges regarding formation of intermetallic compounds (IMCs) in the weld. Can IMCs be minimized in welds? With this notion, new metastable HEAs were designed and their preliminary weldability was evaluated through bead-on-plate friction stir welding (FSW). As-FSW HEAs showed exceptional combination of mechanical properties and corrosion resistance, the work was extended to dissimilar butt FSW of HEA/Al-7050 alloy. Initial results showed lower reactivity at the weld interface. The results are compared to dissimilar welds of Al alloy/stainless steel combinations.

ON DEMAND: The Effect of Titanium and Silicon on the Phase Equilibrium in the Co-Cr-Fe-Mn-Ni System: *Syuki Yamanaka*[1]; Satoshi Takizawa[1]; Ken-ichi Ikeda[1]; Seiji Miura[1]; [1]Hokkaido University

The equiatomic CoCrFeMnNi high-entropy alloy (Cantor alloy), which is an fcc single solid solution alloy, is expected as a next-generation structural material because of its excellent ductility. For further improvement of its mechanical properties, it is a natural way to introduce second phases to the Cantor-based fcc matrix by extra-element addition. For the design of multi-phase alloys, phase diagrams are required which clearly express the relationship between the Cantor-based fcc phase and the second phase stabilized by extra-element addition. The phase equilibrium on Ti or Si-added Cantor alloys which was produced by arc melting and homogenized at 1000°C were investigated. From the result of XRD and EPMA, it was found that Ti addition stabilized the s, A12(aMn), and C14-Laves phases, while Si addition stabilized the A13 phase (ßMn). Based on fragmental information in its sub-system phase diagram, it is suggested that both A12 and A13 phases are derived from pure-Mn.

ON DEMAND: Short-range Order Influence on the Quality of Interatomic Potential Built Using Machine Learning Technique for High Entropy Alloys: *Ivan Lobzenko*[1]; Tomohito Tsuru[1]; [1]Japan Atomic Energy Agency

Nowadays quantum mechanical approach is essential part of computer modeling of materials. Nevertheless, long time scale and large systems are still inaccessible for that method because of high demand of computational resources. That is why classical molecular dynamics is the method of choice for modelling such processes as dislocation movement or crack propagation. This work is devoted to development of high accuracy interatomic potentials for high entropy alloys. To begin with, we have built potentials for medium entropy ternary alloys MoNbTa and ZrNbTa. The technique of machine learning of neural network was used. It allows effective fitting of the data set calculated using quantum mechanical approach. The composition of the data set is discussed. To ensure high quality of the potential the structures with a short-range order were added to the data set. For that purpose, Monte Carlo simulations of special quasirandom structures were carried out.

ON DEMAND: DED Additively Manufactured HEAs Optimized via Parametric Study of Functionally Graded Materials: Calvin Downey[1]; *Luis Nunez*[1]; Isabella Van Rooyen[1]; [1]Idaho National Laboratory

The nuclear industry requires advanced materials that possess mechanical strength, corrosion resistance, and irradiation resistance. High entropy alloys (HEAs) such as FeCoCrNi perform well in these categories and can present a single phase (SP) FCC structure, seen to demonstrate superior irradiation resistance compared to multi-phase and BCC structures. Past investigations of HEAs revealed significant challenges in manufacturing the SP structures with conventional casting methods. Additive manufacturing (AM) presents novel HEA fabrication technologies such as Laser-engineered-net-shaping (LENS). Process control in LENS, such as laser heat input and in-situ material composition, make this method unique to overcome issues with conventional HEA manufacturing. This study investigates LENS fabricated compositionally functionally graded materials (FGM). FGM samples are produced for compositional phase control along with parametric studies of FeCoCrNi HEA-like structures. Scanning electron microscopy, energy dispersive x-ray spectroscopy, and microhardness tests will determine microstructure, elemental distribution, and preliminary mechanical behavior.

ON DEMAND: Computational Design of Co-free Complex Concentrated Alloys (CCA) for Nuclear Applications: *Dinesh Ram*[1]; Anna Fraczkiewicz[2]; Franck Tancret[1]; [1]Université de Nantes, Institut des Matériaux de Nantes – Jean Rouxel (IMN), CNRS UMR 6502; [2]MINES Saint-Étienne, Centre SMS / LGF UMR CNRS 5307

Structural materials in a nuclear environment require a set of highly demanding properties. "High entropy matrix" alloys are suspected to impede irradiation damage hence we attempt the computational conception of novel cobalt-free "complex concentrated alloys." An approach relying on combinatorial exploration and optimization, both with as well as on predictive models that correlate composition, structure, and properties (CALPHAD, solid-solution, and precipitation hardening models, machine-learning) is proposed. Target microstructures are based on +' mixtures commonly found in Ni-superalloys. Genetic algorithm multi-objective optimizations in this phase region were set up on the Ni-Cr-Fe-Mn-Mo-Nb-W-Al-Ti system, using the models developed. However, the designed alloys present a moderate configurational entropy. A systematic CALPHAD exploration of the +' dual-phase region of the subsystem Ni-Cr-Fe-Mn-Al-Ti indicates that the conception of CCAs in this compositional area is thermodynamically restricted. An outlook into alternative strategies of different reinforcing-phases and strengthening mechanisms to design Co-free CCAs is therefore also proposed.

ON DEMAND: Solidification Behavior and Mechanical Properties of a MnFeCoNiCu HEA for Filler Applications: *Benjamin Schneiderman*[1]; Andrew Chuang[2]; Peter Kenesei[2]; Olivia DeNonno[1]; Jonah Klemm-Toole[1]; Zhenzhen Yu[1]; [1]Colorado School of Mines; [2]Advanced Photon Source

The characteristic properties of HEAs, including their tendency to favor single-phase solid solutions, the potential for sluggish diffusion, and the vast composition space available for exploration, make these alloys attractive candidates for filler materials in similar and dissimilar material joining applications. A non-equiatomic MnFeCoNiCu HEA was developed for joining and repair of Ni-base superalloy 600. An in-situ synchrotron-based study of the HEA solidification behavior indicated that classical concepts governing solidification were at play for this HEA. In this analysis, a novel, comprehensive approach to analyzing diffraction data—combining a hard-sphere approximation, thermodynamic simulations, thermal expansion measurement and microstructural characterization—was developed to circumvent the challenges posed by performing a conventional Rietveld refinement on a concentrated solid solution structure. Tension testing on brazed joints indicated that the HEA filler offers comparable strength and superior ductility relative to a conventional boron-suppressed filler at both room temperature and elevated temperature.

ON DEMAND: Precipitation Strengthened High Strength Al0.2CoCrFeNiMo0.5 High Entropy Alloy: *Yasam Palguna*[1]; Rajesh Korla[1]; [1]Indian Institute of Technology Hyderabad

From past one decades, there is a growing interest on High Entropy Alloys (HEAs) because of their superior structural and physical properties compared to conventional alloys. The present work focuses on the precipitation hardening behavior of Al0.2CoCrFeNiMo0.5 wrought high entropy alloy, prepared through induction melting followed by hot forging and thermomechanical processing. Samples are solutionized at 1200oC followed by cold rolled up to 80% reduction in thickness. Cold rolled samples are annealed at different temperatures in the range of 200 to 1200oC for 1hr followed by water quenching and the resultant microstructure evolution are studied using XRD, FE-SEM and TEM. Fine precipitates with BCC structure were observed in samples annealed at temperatures beyond 700oC. Hardness and tensile experiments were performed as a function of annealing temperature and peak hardness and strength were observed in the sample annealed at 700oC, beyond which the hardness was decreasing with increasing annealing temperature.

ON DEMAND: High-throughput Screening of Structural High Entropy Alloys Using a Machine Learning Approach: *Novana Hutasoit*[1]; Pragalathan Apputhurai[1]; [1]Swinburne University of Technology

High entropy alloys consist of five or more elements pose a hyper-dimension compositional space that screening the potential chemical composition through conventional synthesis-test route is time-wise impractical. Therefore, turning to the machine learning method is deemed adequate to establish algorithms capable of identifying chemical composition space that yields high entropy alloys with a set of desired mechanical properties. In this study, data-driven machine learning is explored. The chemical composition and mechanical properties of high entropy alloys; and physical properties of each element composing high entropy alloys reported in the are literature are retrieved and archived in a database. A decision-tree-based ensemble machine learning algorithm using the input of features constructed from elemental composition and properties exhibits a capability to predict the mechanical properties of given high entropy alloys chemical composition. The algorithm developed in this study aid in the development of high entropy alloys with tailored mechanical properties.

ON DEMAND: Optimized Tailoring of Phase Constitution Leading to Exceptional Oxidation Behavior in AlCoCrFeNi HEAs: *Rahul Bhattacharya*[1]; Murugesan Annasamy[1]; [1]Institute for Frontier Materials

Oxidation behavior of AlCoCrFeNi HEA depends on its constituent elements, their varying content, FCC/BCC/B2/Sigma phase fractions. It has been observed that the as-cast AlCoCrFeNi microstructure comprises Fe-Cr-rich BCC + Al-Ni-rich B2. On exposure to heat, FCC, Sigma, and various other phases are formed. In our present work, we have first stabilized the phase constitution of the base alloy to Ni-Al rich B2 + Fe-Co-rich FCC by subjecting the as-cast pellet to an annealing treatment in a vacuum atmosphere at 1150C for 5h. This stabilized simple B2+FCC microstructure is introduced to isothermal continuous oxidation at 1150C. A stable, adherent, alpha-alumina oxide layer is achieved in just 3 minutes of exposure which grows to protect the underlying base alloy from further oxidation. The specific weight gain rate is remarkably low. Characterization tools like STEM, TEM, SEM, EBSD, XRD, TGA, and DSC have been deployed to study the oxidation behavior.

ON DEMAND: Effect of Crystal Orientation on Creep Deformation Behavior of a Single Crystal High Entropy Superalloy: *Takuma Saito*[1]; Akira Ishida[1]; Michinari Yuyama[1]; Yuji Takata[1]; Kyoko Kawagishi[1]; An-Chou Yeh[2]; Hideyuki Murakami[1]; [1]National Institute for Material Science; [2]National Tsing Hua University

There is a continuous effort to elucidate the relationship between microstructure and high temperature mechanical properties of high-entropy superalloys (HESAs), which possess similar gamma and gamma prime two phase structure to Ni-based superalloys, while their compositions are quite different. However effect of crystal orientation on the creep deformation behavior of single crystal HESAs has not been reported yet. This study focuses on the effect of crystal orientation on creep deformation of single crystal HESAs. Single crystal bars of HESA (Ni-8.9Fe-16.9Co-7.5Cr-0.9Mo-0.5W-10.3Al-5.8Ti-1.2Nb in at.%) having approximately 70 vol.% of gamma prime precipitates were fabricated. Crystal orientation of each bar was checked by the X-ray Laue analysis then two specimens with characteristic crystal orientations were selected. Tensile creep tests were performed at 760 °C and 520 MPa and their creep deformation and rupture behavior depending on the crystal orientation was discussed based on the microstructural observation by SEM, TEM and EBSD analyses.

ON DEMAND: Analysis of Mutli-hit Events in Atom Probe Tomography of Refractory High Entropy Alloys: *Patrick Callahan*[1]; Keith Knipling[1]; [1]US Naval Research Laboratory

Atom probe tomography enables the accurate determination of both the composition and morphology of microstructural features from ~250×250×1000 nm3 volumes from targeted regions of samples. This fine scale resolution in both chemistry and length scale enables study of a number of phenomena, including short range order and clustering, which still require more study in high entropy alloys. This work will present an analysis of multi-hit detection events in two refractory HEAs, MoNbTi and HfNbTaTiZr, and how they affect quantitative measurements in APT studies of these refractory alloys. We will also discuss order and atomic-scale clustering in these refractory high entropy alloys as well as oxide formation and oxide observation by laser assisted APT in these alloys.

ON DEMAND: Nanomechanical Testing of In-situ Synthesized Laser-deposited High Entropy Alloys for Aerospace Applications: *Modupeola Dada*[1]; Patricia Popoola[1]; Ntombi Mathe[2]; [1]Tshwane University of Technology; [2]Council for Scientific and Industrial Research

This study examines the nanomechanical properties of in-situ doped Vanadium in AlCoCrFeNiCu and AlCoCrFeNiTi High Entropy Alloys and investigates the effect of V doping on the mechanical properties of AlCoCrFeNiCu and AlCoCrFeNiTi alloys via in-situ laser metal deposition as opposed to the traditional method of mixing powders via a ball mill prone to contamination and segregation. We explore the capability of in situ reactive alloying by delivering the V and high entropy alloy powders from multiple powder feeders through regulating their feed rate ratios into the nozzles. The preliminary nanohardness and microstructural morphologies of the alloys were characterized using nanoindentation tester, XRD and SEM, respectively. The results showed satelliting the larger parent High entropy alloys powder and the smaller V powder fraction using double powder feedstock had a homogeneous distribution with high solidification and dendritic structures. The AlCoCrFeNiCu-Vx showed higher hardness values than AlCoCrFeNiTiVx alloy attributed to the compositional blend.

Monday Plenary

Monday AM
December 6, 2021
Place

Room: University Ballroom CDE
Location: Hilton Charlotte University

Session Chair: To Be Announced

Introductory Comments

Plenary

The Interplay between Phase Transformation and Mechanical Properties in High Entropy Alloys: *Maryam Ghazisaeidi*[1]; [1]The Ohio State University

Phase prediction in multicomponent alloys remains one of the most fundamental challenges. Navigating the vast compositional space of these alloys requires a predictive capability to efficiently guide alloy discovery and microstructure design. Recently we have developed a Multicell Monte Carlo (MC)^2 method, based on first-principles calculations, to study phase formation in multicomponent alloys. This method is particularly powerful when applied to multicomponent systems, for which phase diagrams do not exist. First, I introduce the (MC)^2 method and present its successful prediction of the stable phases of known binary systems. Next, I will present the application of (MC)^2 to high entropy alloys and discuss the effect of emerging stable phases on deformation mechanisms and consequently the overall mechanical behavior.

Break

Session I

Monday AM
December 6, 2021
Place

Room: University Ballroom AB
Location: Hilton Charlotte University

Session Chair: To Be Announced

Introductory Comments

Invited

Solution Thermodynamics Guided Tuning of Local Chemical Ordering in High Entropy Alloys: Implications for Mechanical Properties: Sriswaroop Dasari[1]; Abhishek Sharma[1]; Chao Jiang[2]; Bharat Gwalani[3]; Srivilliputhur Srinivasan[1]; *Rajarshi Banerjee*[1]; [1]University of North Texas; [2]Idaho National Laboratory; [3]Pacific Northwest National Laboratory

Understanding the atomic distributions in random solid solutions and their propensity for local chemical ordering in high entropy alloys (HEAs) has been the subject of intensive recent research. This work presents a simple thermodynamics-based framework, starting from enthalpies of mixing of binary pairs, to guide the design of complex multi-component systems with targeted mechanical properties by controlling the nature and extent of chemical ordering in HEAs. Our framework illustrates how chemical ordering of a nearly random equiatomic CoFeNi solid solution can be tuned by controlled additions of Al and Ti. By coupling high resolution electron microscopy, atom probe tomography, hybrid Monte-Carlo, Special Quasirandom Structures, and density functional theory calculations, we show the presence of short-range ordered domains that are precursors of long-range ordered precipitates and how they inform mechanical properties. We further establish that progressively increasing local order surprisingly boosts the tensile yield strengths of the parent CoFeNi alloy by a factor of four and substantially improves ductility, potentially breaking the so-called strength-ductility tradeoff dilemma in materials.

Determination of Transformation Pathways and Microstructural Evolution in Multi-principal Element Alloys using Coupled Materials Characterization and Phase Field Modeling: *Hamish Fraser*[1]; Zachary Kloenne[1]; Kamalnath Kadirvel[1]; Jean-Philippe Couzinie[1]; Jacob Jensen[1]; Yunzhi Wang[1]; [1]Ohio State University

A recently developed refractory MPEA, AlMo0.5NbTa0.5TiZr, exhibits an interesting microstructure with an ordered B2 phase being the matrix and a disordered bcc phase being the precipitate, unlike the conventional Ni-based superalloys where the ordered phase (') is the precipitate and the disordered phase is the matrix (). Specific heat-treatments have been employed which have been designed to yield mechanistic details of the phase transformation pathway leading to the final microstructure. Based on these experiments, it appears that the pathway includes conditional spinodal decomposition, phase separation, and congruent ordering and disordering transformations. These experimental results are being used to develop a phase field model of the phase transformation pathway of this alloy, and this model is being employed to provide predictions of heat-treatments that will result in optimized microstructures. The progress made will be presented at the conference.

Phase Field Modeling of Transformation Pathways in Multi-phase HEAs: Kamalnath Kadirvel[1]; Jacob Jensen[1]; Zachary Kloenne[1]; Hamish Fraser[1]; Sang Kim[2]; Eun Park[2]; Yunzhi Wang[1]; *Shalini Koneru*[1]; [1]Ohio State University; [2]Seoul National University

Multi-phase HEAs has gained a lot of interest owing to its excellent high temperature properties. It is crucial to understand the phase transformation pathways (PTPs) in these alloys in order to tailor their microstructures for desired properties. In this work, we investigated various possible PTPs in HEAs whose microstructures consist of B2 and bcc phases through phase-field modelling, including order-disorder transitions, conditional spinodal decomposition, and precipitation by nucleation and growth. We systematically investigated the effects of volume fractions of individual phases, lattice misfit and modulus mismatch between the phases and the free energy curves of the individual phases on the PTPs and two-phase microstructures. A microstructure map is created that will assist in multi-phase HEA microstructure design through adjusting alloy composition and heat-treatment schedule. This work is supported by AFOSR under grant FA9550-20-1-0015.

Break

Machine Learning-assisted Phase Prediction for High Entropy Alloys and Feature Analysis: *Kyungtae Lee*[1]; Timothy Hartnett[1]; Mukil Ayyasamy[1]; Prasanna Balachandran[1]; [1]University of Virginia

High entropy alloys (HEAs) are typically solid solutions of face centered cubic, body centered cubic, or hexagonally closed packed phases. The goal of this work is to develop a machine learning approach to optimally guide the HEA design with the targeted phase(s) in the microstructure. Our input dataset for ML models is prepared by merging several datasets from previous reports about the HEA phase prediction. The dataset ranges from binary to multi-component alloys, categorized by seven different phases. We represent each alloy using 125 features that were mainly generated based on the physical and chemical properties of elements that make up the alloy. Redundant features were removed using correlation analysis. Two machine learning algorithms such as random forest and ensemble of support vector machines are considered for the classification learning task, showing predictability close to 90%. Global and local feature importance analysis uncovers insights into the HEA phase formation problem.

Machine Learning Assisted Ab Initio Thermodynamics: From BCC unaries to HEAs: *Prashanth Srinivasan*[1]; Fritz Körmann[2]; Blazej Grabowski[1]; [1]University of Stuttgart; [2]Max Planck Institut für Eisenforschung

Machine-learnt interatomic potentials such as MTPs (Shapeev, 2016) trained to high-temperature DFT data predict energies and forces of atomic configurations highly accurately. In combination with thermodynamic integration (TUTILD, Duff, 2015), one can calculate total free energies of HEAs to 1 meV accuracy (Grabowski, 2019, Ferrari, 2020) up to melting point, including vibrational contributions with anharmonicity. We demonstrate this for various refractory BCCs ranging from unaries to five-component HEAs and break-down the total free energies to individual contributions. Certain BCC unaries have a small positive anharmonic contribution (beyond quasi-harmonic) whereas the others have a large negative anharmonicity, which is also reflected in the HEAs that constitute them. This is in contrast to FCCs (Glensk, 2015) where there is always a positively increasing contribution with temperature. We narrow this feature to DOS and first- and second neighbor forces and illustrate differences in bonding behavior in different BCCs.

New Physics-based Features for Machine Learning Oxidation Properties of Refractory Complex Concentrated Alloys: *Logan Ware*[1]; Haydn Schroader[1]; Tinuade Daboiku[2]; Emily Cheng[3]; Todd Butler[4]; Andrew Detor[3]; Michael Titus[1]; [1]Purdue University; [2]UES Inc.; [3]GE Research; [4]Air Force Research Laboratory

Predicting and improving the high temperature oxidation performance of refractory complex concentrated alloys (RCCAs) remains a barrier to their adoption for ultra-high temperature structural components. Recent work has shown many internal and external oxides form at ultra-high temperatures in these alloys, including multi-component complex oxides. The formation of some complex oxides has been correlated with improved oxidation performance, but the conditions for favorable oxide formation are still unknown. In this presentation we report a high-throughput methodology utilizing ab-initio calculations to predict the thermodynamic driving force for oxide formation as a function of oxygen activity. This method is easily extensible and performs comparably to commercial thermodynamic modeling software at predicting oxide phases in RCCAs. From these predictions, we then extract physics-based features for use in machine learning models to estimate the oxidation properties of each alloy, and find these features to be better equipped to predict oxidation performance than rule-of-mixture features.

Machine Learning Derived Periodic Table for High Entropy Alloys: *Scott Broderick*[1]; Krishna Rajan[1]; Stephen Giles[2]; Debasis Sengupta[2]; [1]University at Buffalo; [2]CFD Research Corporation

This work uses a graph representation approach to capture the thermodynamic and structural complexity of high entropy alloys (HEAs). This approach has been used for materials discovery based on first principles, but now we are using it to design engineering alloys. We identify the potential existence of new combinations of phases not previously identified by tracking the connections in the network, which are analogous to tie lines in a traditional phase diagram representation. In this way, mechanical properties are rationally designed through proposed chemical design rules across the entire HEA search space, resulting in a machine learning based representation of a periodic table based on HEA properties. This approach provides chemical substitution rules where phase design rules have not previously been possible due to the number of components and the complex governing physics, allowing us to propose new chemistries with enhanced yield strength and ductility.

Phase Classification of High Entropy Alloy Using Machine Learning: *Stephen Giles*[1]; Debasis Sengupta[1]; [1]CFD Research Corp

Properties of high entropy alloys (HEAs) are highly dependent on the microstructure and phases that it forms during processing. Therefore, classification of phases, such as single-phase and multiple-phase, or solid solution and intermetallics, is critical in developing HEAs with desired properties. However, due to the large compositional and elemental space, only a fraction of the possible HEAs so far have been explored experimentally, primarily by trial-and-error. Thus far, various simple "rules of thumb" have been suggested which can predict the phase behavior of HEAs with varying degrees of success. In this work, we use machine learning techniques to predict phases of refractory HEAs (RHEAs). This work uses both supervised and unsupervised techniques combined with feature selection to develop machine learning models for accurate phase prediction. We further demonstrate the utility of our intelligent, data-driven model to elucidate the phase behavior of novel RHEAs predicted to have superior high-temperature yield strength.

Session II

Monday AM
December 6, 2021
Place

Room: University Ballroom CDE
Location: Hilton Charlotte University

Session Chair: To Be Announced

Introductory Comments

Invited

A High-throughput Strategy to Study Phase Stability and Mechanical Properties in Complex Concentrated Alloys: Mu Li[1]; Zhaohan Zhang[1]; Rohan Mishra[1]; *Katharine Flores*[1]; [1]Washington University in St. Louis

Although the design of high entropy alloys often focuses on identifying equiatomic solid solution alloys, expanding these complex concentrated alloys (CCAs) to include multiphase microstructures offers the opportunity to further enhance properties. However, information about the stability of competing intermetallic phases is still lacking. Here, we examine phase stability in Nb-Ti-V-Zr as a function of composition. Starting with an equiatomic NbVZr alloy, we observe two Laves phases, cubic C15 and hexagonal C14, in addition to the BCC majority phase. First-principles calculations predict the stable composition for each phase, which are consistent with experimental observations. We then rapidly synthesize Nb-Ti-V-Zr compositional libraries via laser deposition, and use these to map the crystal structures, microstructures and mechanical properties as a function of composition. Experimental results are compared with first-principles calculations. This work provides guidelines for predicting compositional effects on microstructure and properties, which will accelerate the design of CCAs for high-temperature applications.

High-throughput Calculations and Experimentation for the Discovery of Refractory Complex Concentrated Alloys: *Austin Hernandez*[1]; Sona Avetian[1]; Sharmila Karumuri[1]; Zachary McClure[1]; Logan Ware[1]; Alejandro Strachan[1]; Ilias Bilionis[1]; Kenneth Sandhage[1]; Michael Titus[1]; [1]Purdue University

Refractory complex concentrated alloys (RCCAs) are promising materials for replacing nickel-based superalloys in turbine engines, as RCCAs exhibit an attractive combination of properties, including high temperature strength, ductility, and phase stability. However, RCCAs are often prone to catastrophic oxidation at intermediate and high temperatures. To design high strength and oxidation resistant alloys, we begin with a design space of 9 refractory elements (Ti, Zr, Hf, V, Nb, Ta, Cr, Mo, W), along with aluminum, encompassing millions of possible compositions. We first evaluate these compositions using CALPHAD methods and utilize an active learning loop, coupled with machine learning models, to systematically interrogate the oxidation and hardness of alloys generated from down-selected CALPHAD calculations along a Pareto front. To allow for high-throughput experimentation, diffusion couples of Al-containing alloys along the pareto front with Al-free compositions have been examined, and the hardness and oxidation behavior along the resulting concentration gradients will be discussed.

High-throughput, High-temperature Heavy Ion Irradiation of Annealed CrFeMnNi Magnetron-sputtered Combinatorial Thin Film: *Calvin Parkin*[1]; Michael Moorehead[1]; Mohamed Elbakhshwan[1]; Kumar Sridharan[1]; Jason Hattrick-Simpers[2]; Alan Savan[3]; Alfred Ludwig[3]; Adrien Couet[1]; [1]University of Wisconsin-Madison; [2]National Institute of Standards and Technology; [3]Ruhr-Universität Bochum

In-core structural materials for advanced reactor designs are expected to demonstrate superior resistance to environmental degradation to currently-licensed stainless steels and ferritic-martensitic steels. High-entropy alloys (HEAs) present the opportunity to advance fundamental understanding of matrix composition as a design parameter for irradiation resistance, opening novel alloy design pathways for advanced reactor applications. Due to the vast range of the HEA compositional space, rapid screening of alloy compositions for nuclear reactors must adopt high-throughput experimental techniques to generate libraries of data linking trends in resistance to irradiation with composition. 4-inch diameter thin films, compositionally graded in CrFeMnNi, have been fabricated by magnetron co-sputtering, annealed at 500 \176C for 48 hours, and irradiated to 100 dpa at 500 \176C using an automated stage with laser heating. Libraries were characterized before and after irradiation using XRD, nano-indentation, profilometry, and for select compositions, TEM. Results are discussed alongside the limitations of irradiating thin films.

Break

Design of HEAs for Additive Manufacturing Using High-throughput Methods: *Dan Thoma*[1]; Alec Mangan[1]; Ankur Agrawal[1]; Behzad Rankouhi[1]; Zahabul Islam[1]; [1]University of Wisconsin-Madison

Designing process parameters for a high entropy alloy to be fabricated in laser powder bed fusion will be presented. First, a new dimensionless number with universal scaling capability has been developed and was used to evaluate the Cantor alloy. From the dimensionless number, a test matrix of process parameters was defined, and 200 hexagonal test coupons were fabricated within range of multiple processing parameters. Density and hardness measurements defined the process window, and the processing bounds were compared with theoretical models. The high-throughput method to design the process range takes 16 hours, offering a robust methodology to quickly predict process parameters. Within the defined processing window, microstructural characterizations and mechanical property assessments were used to develop property maps. The best compromise of microstructural, defect, and property control can be predicted from the property maps. The potential to further refine property response and design parameters for new alloys will be discussed.

High Throughput Design and Testing of Multi-principal Element Alloys (MPEAs) for Corrosion and Oxidation Resistance: Successes and Pitfalls: *Mitra Taheri*[1]; Emily Holcombe[1]; David Beaudry[1]; Elaf Anber[1]; Dan Foley[1]; Debashish Sur[2]; Nathan Smith[3]; Lauren Walters[3]; Michael Waters[3]; William Blades[4]; Christopher Pasco[1]; Charlotte Brandenburg[2]; John Scully[2]; Elizabeth Opila[2]; Tyrel McQueen[1]; Karl Sieradzki[4]; Chris Wolverton[3]; James Rondinelli[3]; Howie Joress[5]; Jason Hattrick-Simpers[5]; [1]Johns Hopkins University; [2]University of Virginia; [3]Northwestern University; [4]Arizona State University; [5]National Institute of Standards and Technology

Multi-Principal Element Alloys (MPEAs) are the subject of emerging interest due to their compositional profile, which holds the promise of superior mechanical properties, high thermal stability, and high strength at high temperature. It is critical to understand the atomic to mesoscale tuning parameters for MPEAs to harness critical properties, such as high yield strength, low mass density, and corrosion/oxidation resistance for materials in coatings, propulsion, energy absorption and hypersonic vehicles. With millions of permutations of MPEAs in existence, however, it's virtually impossible to nail down the "right" combination without both rapid assessment and innovation. Here we present a path forward for high throughput, physics informed alloy design, informatics, synthesis, and characterization. Our high throughput approach enables tracking, curation, and dissemination of thousands of possible MPEAs. We show that untapped compositional space, combined with precision processing, is a promising path toward realizing MPEA potential.

High-throughput and Machine Learning Accelerated Discovery of Corrosion-resistant Alloy for Molten Salt Applications: *Yafei Wang*[1]; Bonita Goh[1]; Phalgun Nelaturu[1]; Thien Duong[2]; Najlaa Hassan[1]; Raphaelle David[1]; Michael Moorehead[1]; Santanu Chaudhuri[2]; Adam Creuziger[3]; Jason Hattrick-Simpers[3]; Dan Thoma[1]; Kumar Sridharan[1]; Adrien Couet[1]; [1]University of Wisconsin, Madison; [2]Argonne National Laboratory; [3]National Institute of Standard and Technology

Insufficient availability of molten salt corrosion-resistant alloys severely limits the deployment of a variety of promising molten salt technologies that could otherwise have significant societal impacts. To accelerate the alloy development for molten salt applications, a set of high-throughput alloy synthesis, corrosion testing, characterization, and modelling techniques were developed to examine the corrosion resistances of a broad range of high entropy alloys (HEAs) in molten salt. By using these techniques, the corrosion resistance of 75 FeCrMnNi HEAs with different compositions was characterized and used as a performance metric for a random forest regressor algorithm to predict the most corrosion-resistant alloys in molten salt. The predicted corrosion-resistant alloys were further tested and their corrosion resistance were compared with the existing commercial alloys, such as Hastelloy-N and stainless steel. This study demonstrates the successful deployment of an integrated platform to accelerate corrosion-resistant alloy development by about three orders of magnitude.

High-throughput Characterization and Testing of MoNbTaW Multi-principal Element Alloy for Combinatorial Analysis: *Robert Quammen*[1]; Paul F. Rottmann[1]; [1]University of Kentucky

Multi-principal element alloy (MPEA) research initially focused on equiatomic compositions; however, non-equiatomic compositions have recently garnered interest with some exhibiting enhanced mechanical properties or phase stability. Computational approaches are being developed to efficiently explore this vast compositional space. Such studies require complementary experimental investigations to be done in parallel that are guided by and serve as a benchmark for computational results. This requires development of novel high-throughput approaches, as conventional fabrication, characterization, and testing techniques can be prohibitively time consuming and costly. In this work, multi-target co-sputtering was utilized to deposit MoNbTaW with variable compositions across a silicon wafer. Subsequently, thousands of freestanding micro-mechanical test specimens of varying composition were fabricated simultaneously through microfabrication techniques. Characterization was completed by employing methods such as SEM, TEM, and in-situ mechanical testing. These results were then used to determine compositions with unique or encouraging properties to be investigated further.

HEA/CCA Concept and High Throughput Screening in the Development of High-performance Al Alloys: *Patrick Conway*[1]; Ehsan Ghassemali[1]; [1]Jönköping University

The development of high entropy alloys (HEAs) and compositionally complex alloys (CCAs) have broadened the possibilities of alloy design by exploring wider regions of solid solubility. With an ever-increasing demand for high-performance lightweight alloys, the concepts developed within HEAs/CCAs is implemented into the design approach of new high performance Al alloys similar to the extensively used A357 cast alloy. Developing an alloy with an increase in the thermal stability or specific strength, will give the possibility to reduce emissions within the transportation sectors, particularly within the aerospace industry. A selection of alloys was designed via high throughput screening to maximise solid solubility in an Al-7Si alloy. Microstructural and mechanical characterisation via SEM, EBSD, DSC, hardness and high temperature tensile testing revealed an increase in both strength and ductility from room temperature to 200°C over the comparable A357 alloy, without forming additional phases.

Session III

Monday PM
December 6, 2021
Place

Room: University Ballroom CDE
Location: Hilton Charlotte University

Session Chair: To Be Announced

Introductory Comments

Invited

Entropy-driven Melting Point Depression in HEAs: *Raymundo Arroyave*[1]; Tanner Kirk[1]; [1]Texas A&M University

High Entropy Alloys (HEAs) are an increasingly dominant alloy design paradigm. The premise of entropic stabilization of single-phase alloys has motivated much of the research on HEAs. Chemical complexity may indeed help stabilize single alloy phases relative to other lower-entropy competing solid phases. Paradoxically, this complexity may de-stabilize these alloys against the liquid, potentially limiting the application space of HEAs at elevated temperatures. In this work, we carry out a comprehensive investigation of the phase stability in a number of HEA spaces using a state of the art CALPHAD database. By using modern visualization techniques and statistical analysis we examine the trade-off between chemical complexity and stability against the liquid state and identify a potentially difficult to overcome barrier for development of high temperature alloys.

Melting Temperature Prediction of High Entropy Alloys Asing Ab-initio Calculations: *Saswat Mishra*[1]; Alejandro Strachan[1]; [1]Purdue University

Many refractory complex concentrated alloys (RCCAs) have excellent high-temperature mechanical properties. Knowledge of the melting temperature of these alloys is critical from both applied and basic science points of view. Unfortunately, the experimental determination of the melting temperature of RCCAs is challenging. Thus, we use density functional theory-based molecular dynamics simulations to calculate the melting point of a representative RCCA alloy: equiatomic NbMoTaW. We obtain the free energy of the liquid and solid phases from their velocity power spectrum using the two-phase thermodynamic (2PT) framework to calculate the entropic contribution. We quantify various sources of uncertainties in this approach by comparing its predictions with large-scale simulations where the liquid and solid coexist in the same simulation cell. Our results indicate that the melting temperature of NbMoTaW is 3250±200 K and that the method can be extended to characterize the melting temperature of various RCCAs.

Thermodynamic and Mechanical Properties Prediction within the Cr-Fe-Mn-Ni Alloy System: *Tanguy Manescau*[1]; James Braun[1]; Olivier Dezellus[2]; [1]Université Paris-Saclay, CEA, Service de Recherches Métallurgiques Appliquées, 91191 Gif-sur-Yvette, France; [2]Univ. Claude Bernard Lyon 1, CNRS, LMI, 69100, Villeurbanne, France

Thermodynamic equilibrium calculations using Thermo-Calc and the TCHEA3 database were performed on the Cr-Fe-Mn-Ni system to determine the face centered cubic (fcc) single-phase solid solutions at given temperatures. Borders of the fcc composition zone were delimitated by acquiring zero phase fraction lines. For each calculation, temperature and chromium content were fixed to allow planar representation in the CrX-Fe-Mn-Ni system for a given temperature. Then, several solid-solution strengthening models from the literature were implemented in the Cr0.2(FexMnyNiz)0.8 pseudo-ternary system to identify elemental strengthening tendencies to optimize the composition. Free Gibbs energy differences between fcc and hexagonal close packed phases were also used as a tool to estimate stacking fault energy and thus, transformation induced plasticity likeliness. Lattice friction stress of 11 compositions of the alloy system were extrapolated from tensile tests at different grain sizes. The objective is to ease the solid-solutions selection for complex concentrated alloy development.

Computing Thermodynamic Properties for Reduced Activation High Entropy Alloys: Ying Zhou[1]; *Prashanth Srinivasan*[2]; Fritz Körmann[3]; Roger Smith[1]; Pooja Goddard[1]; Andrew Duff[4]; [1]Loughborough University; [2]University of Stuttgart; [3]Delft University of Technology; [4]STFC Daresbury Laboratory

A methodology is presented for computing the thermodynamic properties of multicomponent alloys. By calculating free energies using density functional theory (DFT), the thermodynamic properties can be computed up to the melting point. To achieve this a two-stage up-sampled thermodynamic integration using Langevin dynamics (TU-TILD) approach is applied to calculate the vibrational free energy. This method is a development of up-sampled thermodynamic integration using Langevin dynamics (UP-TILD). By including machine learning potentials (MTP) as intermediate reference states in the integration, the efficiency can be improved by orders of magnitude compared to a more conventional thermodynamic integration method. The TU-TILD method is applied to the low activation TaVCrW system as a first application of the approach in computing the full free energy-surface and thermodynamic properties of a compositionally-complex alloy. The thermal expansion, heat capacity and other properties will be reported at the meeting and compared with experiment.

Predicting Phase Stability of Refractory Complex Concentrated Alloys with Pairwise Mixing Enthalpy: *Zhaohan Zhang*[1]; Mu Li[1]; John Cavin[1]; Katharine Flores[1]; Rohan Mishra[1]; [1]Washington University in St.Louis

We present a first-principles-based method to predict refractory complex concentrated alloys (RCCAs) that are expected to form a single-phase solid solution as opposed to a mixture of solid solution and intermetallic phases. We find that the formation enthalpy of BCC solid solution in 20 RCCAs can be predicted with a mean absolute error of 0.015 eV/atom by using a regular solution model applied to pairwise mixing enthalpy obtained from density-functional-theory calculations. We then use this model to estimate the formation enthalpy of over 20,000 RCCAs. They are further combined with the formation enthalpy of binary and ternary intermetallics that are reported in databases, such as Materials Project, to identify the stable phases expected to form at any given RCCA composition and temperature. We will discuss the accuracy of the model with existing RCCAs, and also new alloy libraries involving NbVZrMx (M = Ti, Ta; x = 0 – 1).

Break

Strengthening in a Model Alloy: Theory and Experiment in AuNi: Binglun Yin[1]; Shankha Nag[2]; Jens Freudenberger[3]; *William Curtin*[4]; [1]Zhejiang University; [2]TU Darmstadt; [3]IFW-Dresden; [4]EPFL

Solute strengthening theory predicts AuNi alloy to be quite strong for Au alloys. The simplicity of solute-solute interactions and possible short-range order (SRO) make AuNi an attractive testbed for theory. AuNi alloys were thus fabricated, characterized, and tested. APT confirmed no segregation in samples annealed at 900 °C. We thus employed the theory, which was recently extended to include the effects of (i) solute-solute interactions in random alloys, and (ii) SRO caused by solute-solute interactions, to predict the strength. In random states, the strength prediction was in good agreement with experiments and suggested the strength is dominated by misfit volumes rather than solute-solute interactions. Then the SRO parameters were computed via Monte-Carlo and shown to be modest. The average strengthening due to SRO made some additional contribution to strength but the misfit contribution remained dominant. Overall, the general methodology and full theory validated here are broadly applicable to HEAs.

Data-driven Design of Refractory High-entropy Alloys: *Wei Chen*[1]; George Kim[1]; Chanho Lee[2]; Peter Liaw[3]; [1]Illinois Institute of Technology; [2]Los Alamos National Laboratory; [3]University of Tennessee

The material-design strategy of combining multiple elements in near-equimolar ratios has spearheaded the emergence of high-entropy alloys (HEAs), an exciting class of materials with exceptional engineering properties. While random mixing has been widely assumed in multi-principal element solid solutions, both experimental and computational evidence suggests short-range ordering (SRO) exists in many solid-solution HEAs. We employed an integrated first-principles and experimental approach to understand the thermodynamic effects of SRO in the refractory NbTaTiV and NbTaTiVZr HEA systems. The existence of SRO produces distinct lattice distortion features in these HEAs and affects their mechanical properties. The fundamental understanding of SRO and lattice distortion is coupled with high-throughput first-principles calculations and machine learning to design refractory high-entropy alloys.

Spontaneous Grain Boundary Roughening in HEAs and Implications for Mobility: *Carolina Baruffi*[1]; William Curtin[1]; [1]EPFL

High Entropy Alloys (HEAs) possess intriguing combinations of properties including enhanced thermal stability against grain growth that is not understood. Here, we argue that natural compositional fluctuations in HEAs can enable a flat grain boundary to spontaneously roughen at zero temperature to a lower energy state. GB motion from this lower energy state is then naturally inhibited, providing an explanation for the resistance to grain coarsening observed in HEAs. This phenomenon is totally different from solute-drag/solute-segregation pinning and arises solely from the intrinsic randomness of HEAs. We present a parameter-free theoretical framework for this mechanism which predicts that, depending on GB structure and alloy composition, a GB will roughen to the smallest possible scales (structural unit scale) when solute/GB interactions are strong enough. The theory is applied to two high-angle GBs in fcc and validated by Molecular Statics simulations.

Atomistic Simulations of the Local Slip Resistances in Four Refractory Multi-principal Element Alloys: *Rebecca Romero*[1]; Shuozhi Xu[2]; Wurong Jian[2]; Irene Beyerlein[2]; Chintalapalle Ramana[1]; [1]University of Texas at El Paso; [2]University of California, Santa Barbara

Multi-principal element alloys (MPEAs) are alloys containing three or more principal elements on simple underlying lattices. They have intermediate structural and chemical complexities between single-element regular metals and multi-element disordered metallic glasses. The combination of refractory metals with oxidation resistance enhancing elements make them ideal candidates for high temperature applications. Due to their unique microstructures and chemical compositions, MPEAs exhibit excellent mechanical properties at elevated temperatures. Improving the mechanical properties of MPEAs requires knowledge of plastic deformation mechanisms, the core of which is dislocation slip. In metals, dislocation slip is intimately connected to the generalized stacking fault energies (GSFEs) and local slip resistances (LSRs). In this work, we conduct atomistic calculations to obtain GSFEs and LSRs on three slip planes – {110}, {112}, and {123} – in four refractory MPEAs. The four MPEAs have differing values of GSFE and LSR, and plastic anisotropy. The origin of these differences is discussed.

Cross-kinks Control Screw Dislocation Strength in Equiatomic bcc Refractory Alloys: *Xinran Zhou*[1]; Sicong He[1]; Jaime Marian[1]; [1]University of California, Los Angeles

Refractory multi-element alloys (RMEA) with bcc structure have been the object of much research over the last decade due to their high potential as candidate materials for high-temperature applications. It is known that the standard model of bcc plasticity based on thermally-activated screw dislocation motion cannot explain the observed temperature dependence of bcc RMEA strength. In this work, we quantify the contribution of screw dislocations to the strength of equiatomic Nb-Ta-V alloys using a kinetic Monte Carlo model fitted to solution energetics obtained from first principles. We find that chemical energy fluctuations along the dislocation line lead to measurable concentrations of cross kinks in equilibrium. Our simulations (i) confirm that the evolution of cross kinks and self-pinning are behind the so-called 'cocktail' effect in this alloy, and (ii) substantiate the notion that screw dislocations may not be responsible for the high temperature strength of bcc RMEA.

Session IV

Monday PM
December 6, 2021
Place

Room: University Ballroom AB
Location: Hilton Charlotte University

Session Chair: To Be Announced

Introductory Comments

Invited

A Materials Informatics Approach to High Entropy Alloy Design: *Andrew Detor*[1]; Scott Oppenheimer[2]; Emily Cheng[1]; James Ruud[1]; [1]GE Research; [2]Ge Research

The vast design space for high entropy alloys requires a modern approach for efficient discovery, development, and deployment. While high precision studies and deep fundamental understanding still play an important role, here we demonstrate a modern materials informatics framework that is well suited for rapid early discovery. Careful design of screening experiments coupled with machine learning and multi-objective optimization are applied to explore new refractory high entropy alloys for applications in extreme environments. Early tie-in with design requirements is discussed within the optimization framework and several examples are shown where different applications yield different optimal material solutions. Data management and visualization are also stressed as a critical part of the development process to identify candidate materials and trade-offs. The general approach presented here can be applied across many different applications and material systems and highlights the growing role of a materials informatics approach within the materials science discipline.

Preparation and Characterization of a HEA Thin Film Combinatorial Sample: *Peter Nagy*[1]; Nadia Rohbeck[2]; Zoltán Hegedüs[3]; Johann Michler[2]; László Pethö[2]; János Lábár[4]; Jeno Gubicza[1]; [1]Eötvös Loránd University; [2]EMPA Swiss Federal Laboratories for Materials Science and Technology, Laboratory for Mechanics of Materials and Nanostructures; [3]Deutsches Elektronen-Synchrotron (DESY); [4]Institute for Technical Physics and Materials Science, Centre for Energy Research

HEA thin films could be processed using a multiple beam sputtering system in PVD, which does not require preliminary manufacturing of HEA targets. Instead, it uses commercially pure metal targets. This method also demonstrates the capability of multiple beam sputtering techniques to produce compositional gradient samples with a wide range of elemental concentrations, enabling combinatorial analysis of multiple elements high-entropy alloy. The microstructure and the mechanical properties of the gradient sample were studied in detail. Synchrotron X-ray diffraction was used to create a diffraction map for the gradient sample. Therefore, we can examine the changes of the microstructure as a function of the chemical composition. The microstructure at the points of interest was further investigated by TEM. The chemical composition of the sample was mapped by XRF and EDS. The mechanical properties were characterized by nanoindentation.

Cluster Expansion Approach to Sigma Phase Site Occupancy and Stability in Compositionally Complex Stainless Steel Alloys: *Anna Soper*[1]; Savanah Diaz[1]; Holly Frank[1]; Jonas Kaufman[2]; Adam Shaw[3]; Kevin Laws[4]; Aurora Pribram-Jones[5]; Lori Bassman[1]; [1]Harvey Mudd College; [2]University of California, Santa Barbara; [3]California Institute of Technology; [4]University of New South Wales; [5]University of California, Merced

Stainless steels are used extensively in industry due to a combination of desirable material properties, such as corrosion resistance and strength. However, ferritic steels form a brittle sigma phase at moderately high temperatures which limits their utility. This first-principles work interrogates the validity of the cluster expansion method for modeling site occupancy and phase stability in the sigma crystal structure for a family of compositionally complex stainless steel substitutes. Finite temperature thermodynamic behavior is evaluated using Monte Carlo simulations and compared with experimental binary and ternary phase diagrams. Representative atomic configurations from the cluster expansion model are used with the Crystal Orbital Hamilton Population method to understand geometric and electronic factors that affect sigma phase stability at different compositions.

Computational Framework for Discovering High Entropy Alloy with Improved Properties: Stephen Giles[1]; *Debasis Sengupta*[1]; Scott Broderick[1]; Krishna Rajan[1]; Peter Liaw[1]; Hugh Short[1]; [1]CFD Research Corp

One of major challenges in improving the properties of HEAs is the exploration of the vast compositional space experimentally. To circumvent this challenge, material scientists often try to find answers to difficult questions, such as what are the most important parameters that dictate the properties of HEAs; what is the sensitivity of HEA properties with respect to changes in each elemental fraction; how can one systematically improve an HEA property starting from a base alloy; how can one rapidly down select a few HEAs for processing from a large pool of conceptual candidates. The present work addresses these challenges via developing a computational framework that intelligently and systematically improves the properties of HEA in a desired direction. We combine state-of-the art machine learning techniques with sensitivity analysis and optimization to develop a computational framework for discovering HEAs with target properties and phases.

Break

Poster Session

Monday PM
December 6, 2021
Place

Room: Glenwaters (Poster Area)
Location: Hilton Charlotte University

Session Chair: To Be Announced

A Low-density Non-equiatomic AlSiCrMnFeNiCu High Entropy Alloy Strengthened with In-situ Precipitation of Cr5Si3: *Yagnesh Shadangi*[1]; Joysurya Basu[1]; Kausik Chattopadhyay[1]; Nilay Mukhopadhyay[1]; [1]Indian Institute of Technology (BHU) Varanasi

In the present study efforts were made to study the structure, microstructure and mechanical properties of a low-density non-equiatomic AlSiCrMnFeNiCu high entropy alloy (HEA) prepared by vacuum induction melting. The structure, microstructure, chemical composition and thermal stability of HEA were investigated through X-ray diffraction (XRD), transmission electron microscopy (TEM), scanning electron microscopy equipped with energy dispersive spectroscopy, and differential scanning calorimetry (DSC). The as-cast alloy exhibited a major B2-type phase along with the uniform precipitation of a minor Cr5Si3 phase. The participation of a minor Cr5Si3 phase in B2-type HEA matrix was found to be responsible for good hardness (~8 GPa) and compressive strength of this HEA. The detailed indentation behaviour of these HEAs were established through instrumented indentation testing technique. Various thermodynamic parameters were evaluated to understand the phase evolution and stability of this HEA. The property diagrams generated by ThermoCalc software was used for understanding the phases evolved.

A Thermodynamic Model of Ductile Fracturing and Fatigue of High Entropy Alloys: *Alexander Umantsev*[1]; [1]Fayetteville State University

Novel paradigm of cradle-to-grave material design places significant emphasis on the fatigue properties of the materials in service. Researchers desire to simulate the microstructure and project its evolution over a large number of loading cycles, which simulates the real service conditions. However, it is not computationally efficient to maintain detailed microstructural information over hundreds of thousands of cycles, which is required by low/high-cycle fatigue testing. This calls for developing phenomenological models of fracturing and fatigue, which, on the one hand, would retain essential mechanical properties of the materials microstructure and, on the other hand, would allow for a long-time dynamical analysis of the specimen. Here we present a novel model of ductile fracturing and fatigue and apply it to the high entropy alloys. Simulation results of the model can be used in the process of material selection and product design.

Advanced Characterization of High-temperature Oxide Evolution in NbTiZr: *David Beaudry*[1]; Daniel Foley[1]; Elaf Anber[1]; Jean-Philippe Couzinié[2]; Loïc Perrière[2]; Michael Waters[3]; James Rondinelli[3]; Christopher Pasco[1]; Tyrel McQueen[1]; Keith Knipling[4]; Mitra Taheri[1]; [1]Johns Hopkins University; [2]University Paris-Est Créteil; [3]Northwestern University; [4]U.S. Naval Research Laboratory

Refractory High Entropy Alloys (RHEAs) offer a potential alternative to Ni-based superalloys in high-temperature turbine applications because of their specific strength at elevated temperatures. These alloys often undergo detrimental oxidation behavior due to their constituent refractory elements. Many RHEA compositions exhibit phase transformations that can both influence and be influenced by oxygen diffusion into the bulk. To better understand the fundamental oxide formation and evolution in these systems, a common derivative of studied RHEAs, NbTiZr, was selected for oxidation at 1050°C. A multi-layered surface microstructure formed with uniformity throughout each layer. High Resolution TEM and APT revealed that the oxygen influx stabilized a low-temperature phase transformation, resulting in two metallic phases with distinct oxygen content. The interplay of these oxygen-stabilized phases with oxide precipitation at their interface offers a novel "bottom-up" approach of high-throughput studies on altering bulk oxidation via doping to tune phase transformations at the bulk-oxide interface.

Atomic Simulations of FeCoCrMnSi High Entropy Alloys: *Riyadh Salloom*[1]; Michael Baskes[1]; Srivilliputhur Srinivasan[1]; [1]University of North Texas

High entropy alloys (HEAs) have many promising properties beneficial to advanced technologies. However, their underlying deformation mechanisms are largely unclear. We have developed a MEAM potential for the FeCoCrMnSi alloys to study such problems. Our Monte-Carlo and molecular dynamics simulations show both hexagonal close-packed (hcp) and face-centered cubic (fcc) phases have similar energies, which may explain the unique TRIP and TWIP effects of this alloy. Also, we calculated the free energy of the single phases and the interface free energy between them for understanding the interfacial mobility under stress and elemental segregation within interfaces. Insignificant elemental segregation or partitioning was observed in the fcc or hcp interfacial regions. The calculated short-range order (SRO) parameter values revealed no significant chemical ordering. The calculated free energy values for the fcc and hcp phases showed that fcc phase is more stable than hcp phase by 10 meV.

Building Data-driven Models with Noisy Input Features-

Application: Strength Prediction of High Entropy Alloys: *Sharmila Karumuri*[1]; Zachary McClure[1]; Ilias Bilionis[1]; Alejandro Strachan[1]; Michael Titus[1]; [1]Purdue University

Building models for predicting various properties of interest using descriptor information obtained from experiments is common practice. However, the issue is that some of the descriptor information coming from these experiments could be noisy leading to input uncertainty. Using these noisy inputs with traditional regression techniques, e.g., Gaussian process regression, is likely to lead to poor performance. To overcome this issue, we propose a hierarchical Bayesian approach which denoises the inputs prior to connecting them to the output quantity of interest. We demonstrate the problem and our proposed approach by carrying out a comparative study using noisy hardness information vs using denoised hardness information to predict the strength of high entropy alloys.

Combinatorial Thin Film Screening of Non-equiatomic Refractory High Entropy Alloy: *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 intrinsic mechanical properties of a single-phase solid solution depend on composition. The hardness of a refractory high entropy alloy (RHEA) is related to the lattice strain stemming from atomic mismatch, and ductility can be improved by reducing the valence electron concentration (VEC). In this work, the wide non-equiatomic configurational space of VNbMoTaW was studied with the combinatorial thin-film approach. 2D gradient thin film of this alloy system was prepared by magnetron sputtering. The alloy phase map was constructed using EDS and XRD. Nanoindentation was performed at three different strain rates to compare hardness, elastic modulus, and strain rate sensitivity. In-situ fragmentation testing was done on different compositions to investigate the VEC effect on the tensile properties. Configurations with enhanced ductility were suggested based on the crack onset strain and fracture morphology. Finally, bulk samples of screened alloys were prepared, and corresponding properties were compared with the thin-film counterparts.

Computing Properties of Multi-component Alloys: *Liangzhi Tan*[1]; Kawsar Ali[2]; Pooja Goddard[1]; Roger Smith[1]; Ashok Arya[2]; Partha Ghosh[2]; Ying Zhou[1]; [1]Loughborough University; [2]Bhabha Atomic Research Centre

High Entropy Alloys (HEAs) usually contain at least 5 elements arranged in different proportions so to determine the combinations required to produce optimal single phases is a formidable experimental or computational task. As a precursor to the study of low activation High Entropy Alloys (HEAs), binary and ternary metallic alloy combinations (Fe,Mn,V,W,Cr,Ti,Ta) are investigated theoretically using the Vienna Ab initio Simulation Package . By examining the formation energies of the alloys, clues can be given as to which combinations would form single phases when combined into systems with five or more individual components. Suitable measures to determine this include the formation energies, the distortion of the systems from a perfect body-centred cubic form and two other parameters involving the mixing enthalpy and configurational entropy. Besides these parameters the paper reports on the lattice and elastic constants and hints as to which systems would be best for combination into HEAs.

Demonstration of Latin Hyper Cube as a Tool for the Design of Experiment of Laser Additive Manufacturing for MPEAs: *Praveen Sreeramagiri*[1]; Hengrui Zhang[2]; Anton van Beek[2]; Wei Chen[2]; Ganesh Balasubramanian[1]; [1]Lehigh University; [2]Northwestern University

Processing parameters in laser additive manufacturing are have a profound impact on the structural properties of the deposited MPEA. Optimizing these is crucial and depend on design of experiments (DoE) with a window of three primary variables, viz., laser power, scan speed, and the powder flow rate in a parameter space. We present an approach using Latin hypercube sampling (LHS) as a tool for the DoE of processing parameters in laser additive manufacturing. The DoE using LHS spans a wide range of input parameters that bounds the lower and upper limits of the machine and can be tailored to span a range of energy densities. This technique can be used to systematically investigate the effect of varying processing parameters on the quality of the alloy and narrow the processing window to achieve optimized parameters. We demonstrate this method to fabricate samples of AlCoCrFeNi MPEA to produce dense deposits.

Design of Silicide Strengthening Refractory High-entropy Alloys: *Ziqi Xu*[1]; [1]Beijing Institute of Technology

Refractory high-entropy alloys have attracted much attentions owing to their excellent properties, especially under elevated temperatures. However, defects such as high density, poor oxidation resistance and limited ductility hinder their further applications. Microalloying could be a therapy for those problems. VNbTiTaMoSi and MoNbTiSi and VNbTiTaSix systems are prepared and investigated on the phase formation and mechanical properties. Silicides are proved to be effective in improving the strength of RHEAs. VNbTiTaMoSi exhibits high yield strength of about 900MPa at 1200°C, which are higher than that of NbMoTaW and VNbMoTaW. Compared with B2 and Laves phase strengthened alloys, silicide strengthened alloys exhibit excellent combinations of ductility and yield strength at elevated temperatures owing to the limited solubility of silicon in refractory elements. Under tensile test, VNbTiTaSix exhibit brittle fracture characteristics. Through hot rolling, the silicides are broken and distribute discontinuously in ductile matrix, and the tensile ductility are greatly enhanced.

Early Investigation of Hybrid Approaches to Joint Optimization for Accelerating the Design of Refractory High Entropy Alloys: Baldur Steingrimsson[1]; *Michael Gao*[2]; Graham Tewksbury[3]; Peter Liaw[4]; [1]Imagars LLC; [2]National Energy Technology Laboratory; [3]Portland State University; [4]University of Tennessee

We present a framework for joint optimization of the mechanical and physical properties of refractory high-entropy alloys (RHEAs), one accounting for material strength, temperature, creep, fatigue, fracture toughness, ductility, conductivity, and environmental (oxidation) resistance. The joint optimization scheme captures design objectives and requirements, as presented to alloy designers. The joint optimization involves extension to RHEAs of techniques originally developed by Rettig et al. and by Conduit et al., both for Ni-based superalloys. Whereas these techniques may work well for the Ni-based superalloys, for which plenty of data is available (after decades of study), and has already been collected, they may not be directly applicable to the much more recent HEAs, due to data limitations. We present hybrid approaches, where synthetic data points are computed using CALculations of PHAse Diagrams (CALPHAD) and density functional theory (DFT), to supplement those from CALPHAD only, and to make the most of the data available.

Effect of Cooling Rate on the Crystallization Temperatures and Lattice Distortion of AlCoCrFeNi MPEA: *Praveen Sreeramagiri*[1]; Ankit Roy[1]; Ganesh Balasubramanian[1]; [1]Lehigh University

Crystallographic features and phases formed during synthesis of a high entropy alloy, influence their structural properties significantly. We investigate the effect of cooling rates exerted during the synthesis of AlCoCrFeNi high entropy alloy on the crystallization (and glass formation) using molecular dynamics simulations. An increased cooling rate contributes to a severe under cooling during homogenous nucleation, reducing the crystallization temperatures, while promoting phase transformations. Our results predict the critical cooling rate of this alloy system to be 2.5 × 10^10 K/s, beyond which the melt will solidify into an amorphous solid. In addition, higher cooling rates contribute to an increased lattice distortion during solidification and enhance the structural properties by promoting the formation of deformation twins and increased dislocation densities.

Effect of Grain Refinement on the Mechanical Behavior of the $Cr_{40}Co_{40}Ni_{20}$ Medium-entropy Alloy: Gustavo Bertoli[1]; Lucas Otani[1]; *Diego Santana*[1]; Amy Clarke[2]; Claudio Kiminami[1]; Francisco Coury[1]; [1]Federal University of São Carlos; [2]Colorado School of Mines

The equiatomic CrCoNi medium-entropy alloy (MEA) stands out as one of the toughest materials ever made. The great combination of mechanical properties is partly due to the high work-hardening rate provided by the twinning-induced plasticity (TWIP) effect. While Cr additions improve solid solution strengthening, Co additions increase the tendency for transformation-induced plasticity (TRIP) effect to occur, which could provide even higher work-hardening rates than the TWIP effect. Thus, the Cr- and Co-rich $Cr_{40}Co_{40}Ni_{20}$ MEA was selected for the present study. This MEA was produced, hot and cold formed, and characterized in the annealed and deformed states, this alloy displayed promising mechanical properties and the TRIP effect is shown to occur extensively during deformation. Furthermore, this alloy displayed significant strengthening propensity by grain refinement as evidenced by a Hall-Petch curve. The impact of grain size on the TRIP/TWIP activation will be discussed.

Effect of Grain Size on the Low-cycle Fatigue Behavior of CoCrNiFeMn High Entropy Alloy: *Sezer Picak*[1]; Thomas Wegener[2]; S. Vahid Sajadifar[2]; Cesar Sobrero[2]; Julia Richter[2]; Hansoo Kim[1]; Thomas Niendorf[2]; Ibrahim Karaman[1]; [1]Texas A&M University; [2]University of Kassel

High Entropy Alloys (HEAs) such as CoCrFeMnNi are a new class of multi-component metallic materials. However, their relatively low yield strength level is a major drawback. In the present work, Equal Channel Angular Pressing (ECAP) was employed to improve the initial yield strength level of CoCrFeMnNi HEA. In light of envisaged fields in engineering, the HEA was also studied under cyclic loading as this might show different microstructural evolution as compared to quasi-static monotonic loading. To allow for meaningful comparison, both strain-controlled low cycle fatigue tests under fully reversed push-pull loading (R=-1) and quasi-static (tensile and compression) tests were conducted at room temperature. Very high tensile and compressive yield strength levels (1.1 GPa) and superior fatigue life were obtained after ECAP processing due to grain-refinement and high defect densities. Finally, the formation of cell structure in these kinds of alloys is, for the first time, rationalized by the Copley-Kear effect.

Electrical and Thermal Transport Properties of Medium-entropy SiyGeySnx Alloys: *Houlong Zhuang*[1]; Duo Wang[1]; Lei Liu[1]; [1]Arizona State University

Electrical and thermal transport properties of disordered materials have long been of both theoretical interest and engineering importance. As a new class of materials with an intrinsic compositional disorder, high/medium-entropy alloys (HEAs/MEAs) are being immensely studied mainly for their excellent mechanical properties. By contrast, electrical and thermal transport properties of HEAs/MEAs are less well studied. Here we investigate these two properties of silicon (Si)-germanium (Ge)-tin (Sn) MEAs. We find that increasing the compositional disorder in SiyGeySnx MEAs enhances their electrical conductivity while decreases the thermal conductivity. As a result, SiyGeySnx MEAs with high Sn content exhibit promising functional properties for thermoelectric applications. Our work demonstrates that HEAs/MEAs not only represent a new class of structural alloys but also a novel category of functional alloys with unique electrical and thermal transport properties.

Electron Diffraction-based Analysis of the Role of Chemical Short-range Order on the Dynamic Deformation Response of FCC and BCC Multi-principal Element Alloys: *Daniel Foley*[1]; David Beaudry[1]; Elaf Anber[1]; Yevgeny Rakita Shlafstein[1]; Partha Das[2]; Simon Billinge[3]; Andrew Matejunas[4]; Carolina Frey[5]; Leslie Lamberson[4]; Tresa Pollock[5]; Irene Beyerlein[5]; Garritt Tucker[4]; Chris Weinberger[6]; Mitra Taheri[1]; [1]Johns Hopkins University; [2]NanoMEGAS SPRL; [3]Columbia University; [4]Colorado School of Mines; [5]University of California, Santa Barbara; [6]Colorado State University

A chemically complex matrix with the potential for chemical ordering distinguishes multi-principal element alloys (MPEAs) from conventional alloys. As this pertains to mechanical behavior, a nominally disordered matrix presents a non-uniform energetic landscape for dislocation motion which can be modulated by varying degrees of ordering. Such energetics can lead to the development of microstructural features such as dislocation cells, twins, microbands, and martensite, the evolution of which are important in both in-service plastic response and the potential for tunable deformation processing. The present work investigates the effect of chemical short-range order (SRO) in FCC CoCrNi and BCC NbTiZr alloys on microstructural evolution due to high strain rate compression. Samples of each alloy were heat treated to induce different degrees of SRO and dynamically compressed via Kolsky (split-Hopkinson pressure) bar. Electron microscopy diffraction-based techniques are used to both measure the degree of chemical ordering as well as characterize the deformation substructure.

Enhanced Strength Ductility Synergy in AlCoCrFeNi HEA through Facile Post Processing Technique: *Mayank Garg*[1]; Harpreet Grewal[1]; Harpreet Arora[1]; [1]Shiv Nadar University

In this study, we demonstrate a facile technique to address the conflicting strength-ductility trade-off in AlCoCrFeNi high entropy alloy. The as-cast AlCoCrFeNi alloy showed a coarse-grained microstructure with BCC/B2 phase. The as-cast alloy was subjected to plastic deformation using a facile technique known as stationary friction processing (SFP). SFP resulted in significant reduction in the grain size along with BCC to FCC phase transformation. An outstanding combination of high strength and high ductility was achieved in AlCoCrFeNi high entropy alloy through SFP as compared to as-cast alloy. The processed sample demonstrated more than 2 times higher ultimate tensile strength (~650 MPa) compared to as-cast HEA (~310 MPa) with enhancement in ductility from 8 % to 15 %. The combination of fine grain structure along with BCC to FCC transition through SFP enable the HEA for exceptional properties. This approach can easily be extended for other alloy systems also.

Fabrication and Characterization of Nanoporous Multi Principal Element Alloy Thin Films by Vacuum Thermal Dealloying: *Tibra Das Gupta*[1]; Taohid Bin Nur Tuhser[1]; Maria Kosmidou[1]; Michael J Detisch[1]; Thomas Balk[1]; [1]University of Kentucky

Traditionally, nanoporous structures are made of single elements or binary alloys. Certain approaches for synthesizing these materials have been applied to multi principal element alloys (MPEAs), which are a combination of four or more elements that can impart enhanced phase stability. In this study, nanoporous MPEAs (np-MPEAs) were fabricated from magnesium-based refractory thin films (VMoNbTaMg and WVMoNbTaMg) that had been magnetron sputtered. A novel technique, vacuum thermal dealloying (VTD), which involves sublimation of higher vapor pressure element(s) from the precursor alloy, was employed for dealloying. When VMoNbTaMg and WVMoNbTaMg are heated under vacuum, the highest vapor pressure element (Mg) evaporates and creates a nanoporous structure. The np-MPEA exhibited an average ligament size of ~10 nm at 600°C, indicating stability against coarsening at high temperature. XPS depth-profiling indicates that the VTD results in less alloy oxidation compared to traditional dealloying techniques. The effect of precursor film thickness will also be discussed.

Fabrication, Testing and Characterization of a Non-equiatomic CrCoNi Alloy on a Semi-industrial Scale: *Vitor Pereira*[1]; Francisco Coury[1]; Guilherme Zepon[1]; [1]Universidade Federal de São Carlos

CrCoNi alloys are of wide interest due to the good inherent mechanical properties, the equiatomic composition for example is among the toughest materials ever produced. Up to date, most studies involve small production scales, with the final sample being some grams to a few kilograms. In the present study, the non-equiatomic Cr40Co30Ni30 alloy has been produced on a semi-industrial scale, with two different ingots being produced, with 50 and 25 kilograms. The ingots were hot forged and hot rolled following processing routes typically used for Ni superalloys. The material after hot forming was characterised and mechanically tested under tension and impact, the microstructure was again characterised after testing. The processing challenges in the melting and forming steps will be presented and discussed and the results will be compared to conventional alloys, the industrial prospects of the CrCoNi system will be discussed.

Feature Selection and Interpretation for Machine Learning Models: Reducing the Dimensionality of Complex Concentrated Alloys: *Zachary Mcclure*[1]; Alejandro Strachan[1]; [1]Purdue University

The inherent high dimensionality of complex concentrated alloy design prohibits full exploration of the material space via experimental means. Therefore, large efforts to model properties and phenomena of the design space coupled with validation is critical for efficient procedure. Since available datasets are limited, we often turn to machine learning models with carefully engineered features. With increased feature count is the reward of a more complex and accurate model. However, this is often at the cost of interpretability of individual features. In this study we develop random forest regression models with quantified uncertainties to predict the yield strength of CCAs, followed by an analysis of our selected features using game theory approximations. We use the methods of Shapely coefficients to score and evaluate the impact of our features, and offer explanations for individual feature impact on model predictions.

First-principles Investigation into Ductility of High Entropy B2-like Alloys

: *Emma Cuddy*[1]; Emily Hwang[1]; Jonas Kaufman[2]; Adam Shaw[3]; Kevin Laws[4]; Aurora Pribram-Jones[5]; Lori Bassman[1]; [1]Harvey Mudd College; [2]University of California, Santa Barbara ; [3]California Institute of Technology; [4]University of New South Wales; [5]University of California, Merced

Alloy compounds of the B2 crystal structure are known to exhibit minimal ductility due to their structural ordering and covalent bonding nature. However, some previously established B2 binary alloys and recently developed B2-structured precious metal-rare earth multicomponent alloys have demonstrated unusually high ductility. Previous work using density functional theory has successfully used the relative energies of stacking faults and antiphase boundaries on different slip planes to form a metric to indicate ductility in binary B2 and quaternary B2-like alloys. This study adapts the method for B2-like high entropy alloys with six elemental components. Due to the odd number of species on each sublattice, these also incorporate disorder for the first time. Disorder is approximated with special quasirandom structures, and particular attention is paid to alloys containing lanthanide elements due to their high prevalence in ductile B2-like alloys.

High Throughput Study of Hardening and Void Swelling in Ion Irradiated High Entropy Alloys: *Benoit Queylat*[1]; Michael Moorehead[1]; Phalgun Nelaturu[1]; Mohamed Elbakhshwan[1]; Dan Thoma[1]; Mukesh Bachhav[2]; Dane Morgan[1]; Adrien Couet[1]; [1]University of Wisconsin, Madison; [2]Idaho National Laboratory

Deployment of next-generation nuclear reactors, operating at high temperature and under extreme environments, requires the development of new alloys for claddings, internals, and structural materials. They are required to have excellent mechanical properties even after being irradiated to high fluences. HEAs have shown promising properties under extreme environments. However, considering the large compositional space of HEAs, manufacturing, characterizing and studying the effects of irradiation on their properties using conventional methods is not compatible with the deployment timeline of these reactors. In this study, we have combined innovative high-throughput HEAs processing method, using additive manufacturing, and high-throughput ion irradiation at high temperature, coupled with automated characterization methods to measure void swelling and hardening of a wide composition space of the Cr-Fe-Mn-Ni system as function of dpa. Preliminary results and importance ranking order based on Cr-Fe-Mn-Ni properties and void swelling/hardening performance metrics will be presented using a Random Forest Regressor algorithm.

Hydrogen Effects in Metastable High Entropy Alloys: *Haoxue Yan*[1]; Maria Ronchi[1]; C. Cem Tasan[1]; [1]Massachusetts Institute of Technology

Hydrogen embrittlement (HE) is one of the most significant challenges limiting the use of high strength alloys, understanding of which is complicated due to the various microstructural effects of hydrogen (H). In high entropy alloys (HEAs), various transformation pathways are available, which have the potential to provide enhanced damage-resistance. Here, with SEM based techniques, we investigate the impact of H on the microstructures of Fe-Mn based HEAs. With a unique integrated SEM-thermal desorption spectroscopy technique, we enabled coupling of microstructure evolution and H desorption to investigate the effects of H on austenite stability and the martensite formation process. Additionally, we utilize electron backscattering diffraction and electron channeling contrast imaging to examine the effects of H on surface dislocations in a bulk specimen. In this talk, we reveal the underlying mechanisms of H-induced transformations and dislocation activities and explore how these insights can be used in the search for HE-resistant alloys.

Investigating Oxidation of NiAl+ Hf Using Cellular Automata: *Indranil Roy*[1]; Pratik Ray[2]; Ganesh Balasubramanian[1]; [1]Lehigh University; [2]Indian Institute of Technology Ropar

Modeling oxidation of HEAs is a complex problem due to the dynamical nature of the oxidation process. Conventional techniques based on the first principle and thermodynamic analysis focuses on some of the particular aspects of the process but fail to model the overall phenomenon. We developed a stochastic cellular automata approach to model oxidation of NiAl and NiAl+Hf at high temperatures. The probability of reaction and diffusion is obtained from the relative reaction and diffusion rate of each component. We successfully analyzed oxide scale morphology, thickness, specific mass gain, and stress-strain field during the temporal evolution of the oxide scale. The majority of the oxide formed during oxidation of NiAl is composed of Alumina while the addition of "reactive element" Hf in the grain boundary slows the oxidation kinetics drastically. We have also prepared a simplified model to calculate stress-strain during transient oxidation based on Pilling-Bedworth ratios of the oxides.

Investigation of the Initial Stages of Oxidation in MoNbTaW and Comparison to Pure W: *Robert Quammen*[1]; Paul F. Rottmann[1]; [1]University of Kentucky

Refractory multi-principal element alloys (RMPEAs) are considered a promising class of materials for extreme environment applications due to their excellent high temperature properties. Refractory alloys, however, are widely known to be susceptible to environmental degradation at elevated temperatures. Thus, oxidation resistance is a key consideration when investigating RMPEAs. The vast majority of extant literature regarding the oxidation of RMPEAs has focused on high temperatures, typically 1000°C or higher, but these approaches do not directly provide information regarding the initial stages of oxidation and its progression. To this end, in air annealing at 200-400°C was conducted on MoNbTaW films. XRD, SEM, TEM, and XPS were used to quantify solute ingress and phases present. Comparison was then made to pure W thin films under the same conditions. Through understanding of the initial stages of oxidation, the alloy chemistry can be tailored to improve phase stability in extreme environments.

Machine Learning Based Intelligent Framework for Discovering High Entropy Alloy: *Debasis Sengupta*[1]; Stephen Giles[1]; Scott Broderick[1]; Krishna Rajan[1]; [1]CFD Research Corp

High-entropy alloys (HEA) are a promising class of materials that show elevated-temperature yield strengths, which are superior to superalloys. However, exploring the vast HEAs compositional space by traditional trial-and-error protocol is challenging. Consequently, only a small fraction of this space has been explored to date. The work presented here addresses this challenge and initiates the development of a framework by coupling the state-of-the-art machine learning (ML) and optimization method to intelligently explore the vast compositional space and drive the search in a direction that improves HEA mechanical properties at high-temperatures, thereby discovering new HEAs. We first develop a forward prediction model by coupling feature selection, boot strapping, and-k-fold validation. The forward model is the then used for discovering new HEAs with improved yield strengths. The computational framework developed is fully automatic and particularly useful for materials scientists to narrow the HEA design space.

Modelling of Equiatomic Mo-Nb-Ti-Zr and Mo-Nb-Ti Systems for Use in Irradiation Environments: *Anilas Karimpilakkal*[1]; Joseph Newkirk[1]; Frank Liou[1]; Jason Schulthess[2]; Sriram Praneeth Isanaka[1]; Julia Medvedeva[1]; [1]Missouri University of Science and Technology; [2]Idaho National Laboratory

Prediction of mechanical properties of materials for use in advanced nuclear reactors is critical as far as the complex radiation environment is concerned where a real time/in-situ performance evaluation may be impossible. A combined approach of Molecular Dynamics (MD) and ab-initio simulations on advanced materials like the High Entropy Alloys (HEAs), whose mechanical properties could be suitable for use in high irradiation environments, could serve to predict this response. For Equiatomic body centered cubic(bcc) Mo-Nb-Ti-Zr and Mo-Nb-Ti systems, supercell approximations to the true disordered state of a given number of atoms per supercell (Special Quasi-random Structure) were calculated. Energy and density optimization calculations for different supercell volumes were done using Vienna Ab initio Simulation Package (VASP) simulations and the atomic distance distribution and the nearest-neighbor environment were studied to define the defect energetics, especially the vacancy formation energies for the systems. Experimental results will be correlated and the comparisons discussed.

On the Phase Constituents of Ten CoCrFeNiX (X = Y, Ti, Zr, Hf, V, Nb, Ta, Cr, Mo, W) High-entropy Alloys after Prolonged Annealing: *An-Chen Fan*[1]; Jian-Hong Li[1]; Ming-Hung Tsai[1]; [1]National Chung Hsing University

Equilibrium/near-equilibrium phase data is critical for the development and application of high-entropy alloys (HEAs). However, the majority of reported data are based on as-cast or shortly-annealed alloys. Here, the phase constituents and microstructures in ten equimolar pseudobinary CoCrFeNiX HEAs after prolonged annealing at 1100, 900, 700, and 500°C were investigated. The data offers valuable insights into the phase formation behavior of HEA, which will be discussed. Existing phase formation theories were applied to predict the phase type in the alloys. However, the theories often fail to predict the formation of certain intermetallic phase types. This is owing to the physical characteristics of these phase types. Phase-specific theories were also applied to the alloys and are successful to certain extent. Finally, the experimental phase data was compared with CALPHAD predictions. The results are also not satisfactory, mainly due to the limited fraction of assessed ternary systems.

Ostwald Ripening in High Entropy Alloys: *Alexander Umantsev*[1]; [1]Fayetteville State University

High entropy alloys (HEA) experience aging same way as the conventional ones. However, theoretical description of aging of HEA is complicated by a large number of alloying components and a complicated structure of the mobility matrix. These two problems motivated the author on developing a general approach to the problem of Ostwald ripening in HEAs. In this presentation I will lay out the basic principles of the theory and provide the compact formulae for the rate of coarsening and distribution function of the second phase precipitates.

Phase Stability and Mechanical Properties of MgAlSiCr Containing Low-density High Entropy Alloys: Nandini Singh[1]; Priyatosh Pradhan[1]; Yagnesh Shadangi[1]; *Nilay Mukhopadhyay*[1]; [1]Indian Institute of Technology (BHU) Varanasi

In the present study we investigated the phase evolution and mechanical properties of MgAlSiCrFe, MgAlSiCrFeNi, MgAlSiCrFeCuZn low-density high entropy alloys (LDHEAs) processed through mechanical alloying (MA) and spark plasma sintering (SPS). The sequence of the phase evolution during MA and SPS was ascertained through X-ray diffraction (XRD) and transmission electron microscopy (TEM). The morphology, microstructure and chemical composition of these LDHEAs were investigated with the help of scanning electron microscope (SEM) equipped with EDS detector. These LDHEAs were found to be thermally stable upto ~400 as observed through the DSC thermogram and ex-situ XRD investigation of the annealed LDHEA powders. Further, efforts were made to investigate the indentation behaviour of these LDHEAs through instrumented microhardness tester. These LDHEAs exhibited high hardness and strength. The phases evolved during MA and SPS were understood with the help of various thermodynamic parameters and CALPHAD modelling using ThermoCalc software.

Stacking Fault Energy (SFE) of Multi-component Alloys Based in Fe80-X MnXCo10Cr10
(X= 20, 30, 40, 50 at%) Using a Computational Approach: *Katherine Paredes Gil*[1]; Jose Yesid Aguilar Hurtado[2]; [1]Universidad Tecnológica Metropolitana; [2]Universidad de Chile

Fe50-xMn30Co10Cr10Bx (x = 0, 3, 5 and 10 at.-%) alloys were recently manufactured showing a martensitic transformation from fcc to hcp as consequence of the stacking faults presence. This causes a reduction in the stacking faults energy (SFE) increasing the solid solution strengthening and activating several deformation mechanisms which are responsible of the increased mechanical properties. In this direccion, it is our interest to gain insight in the SFE of Fe80-xMnxCo10Cr10 (X=20, 30, 40, 50 at%) and Fe30Mn50Co10Cr10B5 using ab initio calculations. We employ the special quasi-random structures method (SQS) to predict the most probable positions the different atomic species in a supercell of 60 atoms, and after periodic DFT calculations using PBE functional, and a cutoff of 500 eV were carried out using VASP software. The SFE results based in the Stocks et.al model are agreement to experimental SFE and allow to rationalize the strain-hardening behavior since the structural characteristics.

Synchrotron X-ray Real-time Study of the Liquid and Solidification Structures of Al-based High Entropy Alloys: *Shi Huang*[1]; Jiawei Mi[1]; [1]University of Hull

In this paper, we report the design and characterization of two new Al-based low-density high entropy alloys based on the composition of Al65Si15Cu5M (M = Fe, Ti, Ni). The research has been focusing on studying the alloy atomic structure in the liquid and undercooled state as well as the multiphase 3D morphology in the solidified condition. We used synchrotron X-ray total scattering technique and the Empirical Potential Structure Refinement method to construct the 3D atomic structures of the alloys in the liquid state, tracking and the temperature dependent atomic structure evolution. We also used X-ray microtomography to characterize the complex multiphase 3D morphology of the solidified samples. The research revealed quantitatively the dynamic link between the atomic structures in the liquid state and the nucleation and growth of the complex multiphases formed in the solidification process, providing valuable information on designing and optimising high entropy alloys microstructures from atomic level.

The Cyclic Plastic Response and the Fatigue Induced Microstructural Changes of Equiatomic CrCoNi Medium-entropy Alloy: *Milan Heczko*[1]; Veronika Mazánová[1]; Connor Slone[2]; Ivo Kubena[3]; Mulaine Shih[1]; Tomáš Kruml[3]; Easo George[4]; Maryam Ghazisaeidi[1]; Jaroslav Polák[3]; Michael Mills[1]; [1]The Ohio State University; [2]Exponent; [3]Institute of Physics of Materials CAS; [4]Oak Ridge National Laboratory

Equiatomic CrCoNi alloy was subjected to strain-controlled low cycle fatigue tests at room temperature in a wide interval of strain amplitudes. Fatigue hardening/softening curves, cyclic stress-strain curves and fatigue life curves were evaluated. The evolution of the internal critical stresses and the effective saturated stress during cyclic loading was analyzed using a generalized statistical theory of the hysteresis loop. The deformation substructure was studied by atomic resolution electron microscopy and correlated with the cyclic response. Correlation of mechanical test data, modeling and characterization reveals details of the deformation mechanisms such as highly planar slip, deformation twinning and FCC-HCP transformation, which govern cyclic strength, cyclic plastic response and the fatigue life. Performance of the CrCoNi alloy, which is characterized by good cyclic strength combined with superior resistance to cyclic plastic deformation, is compared and discussed in relation to other structural alloys used in real service conditions.

Thermomechanical Processing of a CrMnFeCoNi by Cold Rolling and Annealing: *Caroline Gonçalves*[1]; Gustavo Sousa[1]; Eric Mazzer[1]; [1]Federal University of Minas Gerais

The study approachs the identification of suitable thermomechanical processing routes that allow an improvement of the mechanical properties in a CrMnFeCoNi HEA processed by spray forming. The alloy was submitted to cold rolling under differents reductions (30%, 50%, 90% and 140% of true strain) with and without subsequent annealing (temperatures ranging from 500 to 900 oC). Microstructural and mechanical characterizations were carried out in order to analyze the underlying deformation mechanisms such as dislocation mediated plasticity and twinning. It were observed difference between annealing and deformation twinning and their contributtion to deformation and hardening mechanisms.The results presented an alloy with excellent workability and exhibited a large work hardening capacity in cold rolling It is concluded that the main deformation and hardening mechanisms during cold work are associated with the nanotwinning deformation of this alloy, which is in agreement with the increase of 136% in the microhardness without subsequent annealing.

Session V

Tuesday AM
December 7, 2021
Place

Room: University Ballroom AB
Location: Hilton Charlotte University

Session Chair: To Be Announced

Introductory Comments

Theoretical Predictions of Short-range Order in High Entropy Alloys: You Rao[1]; *William Curtin*[1]; [1]EPFL

Chemical short-range order (SRO) has been suggested to have an impact on the mechanical properties of high entropy alloys (HEAs) but the experimental quantification of SRO is challenging and computational work is usually on specific alloys. Here we present a theoretical framework where a crystal is partitioned into assumed uncorrelated units as molecules in a gas, leading to an analytic solution for the equilibrium compositions of all possible molecule configurations, from which the Warren-Cowley SRO parameters can be determined. We apply the approach to various crystal structures/pair distances and demonstrate the accuracy by comparison to direct Monte Carlo simulations. It reduces to the quasichemical approximation for binary alloys with near-neighbor interactions and can be easily generalized to multicomponent systems. The method provides a fast estimate of SRO based on any approximate source of inputs and so can help guide the design of new alloys with desired levels of SRO.

Tuning Chemical Ordering in the Concentrated Solid Solution of High Entropy Alloys: *Sriswaroop Dasari*[1]; Abhishek Sharma[1]; Bharat Gwalani[1]; Rajarshi Banerjee[1]; [1]University of North Texas

While single-phase solid solution based high entropy alloys (HEAs) have attracted enormous attention in the last fifteen years, a controversy surrounds the fundamental question: How random are these complex concentrated solid solutions? Recent computational and experimental studies often have opposing viewpoints regarding the presence of local short-range order (SRO), or "clustered ordering" in these alloys. Using thermodynamic binary mixing enthalpies of constituent pairs, the present study demonstrates how the degree of chemical ordering can be systematically tuned within these concentrated solid solutions. Starting with a near ideal equiatomic CoFeNi solid solution, additions of Al and Ti promote local ordering, as evidenced by detailed electron diffraction coupled with atom probe tomography. Consequently, the tensile yield strength can be increased from 190 MPa (CoFeNi) to 280 MPa (Al0.25CoFeNi) to 450 MPa (Al0.3CoFeNi), finally to 800 MPa (Al0.3Ti0.2CoFeNi), more than a four-fold increase, with a progressive increase in the degree of local ordering.

Local and Near-boundary Environments in Multiple-principal Element Alloys: *Doruk Aksoy*[1]; Megan McCarthy[1]; Ian Geiger[1]; Timothy Rupert[1]; [1]University of California, Irvine

The continued advancement of multiple principal element alloys (MPEAs) depends on the ability to understand and manipulate the internal microstructures of these materials. In this talk, we investigate a number of important interfacial phenomena in MPEAs using atomistic modeling tools, including segregation-induced evolution of metastable boundary states, near-boundary segregation zones resulting from both structural and chemical patterning, and the influence of local atomic environments on segregation behavior in random polycrystalline networks. First, we use single element ground-state and metastable grain boundary configurations as reference states to investigate the energetic and structural effects of segregation in MPEAs. Next, spatial patterning in segregation at bicrystal and polycrystal models is studied, highlighting the diversity of structural and chemical motifs present. Finally, machine learning-based analysis is used to enable efficient prediction of segregation behavior in non-dilute and chemically complex environments. As a whole, our findings illuminate new paths to the interfacial design of MPEAs.

Break

Atomistic Simulations of Deformation Response in High Entropy Alloys: *Diana Farkas*[1]; [1]Virginia Polytechnic Institute

This talk reports atomistic simulation studies of mechanical behavior in a model quinary high entropy FCC alloy. The simulations are based on empirical interatomic potentials and use molecular dynamics atomistic techniques to study deformation. Virtual mechanical tests were performed using large-scale simulations and the material response analyzed using various techniques. The focus is on understanding the role that the local composition in the random alloy plays in the deformation mechanisms. It is found that it is most meaningful to compare the alloy deformation response with a corresponding "average atom" material that has the same average properties but no local randomness. The complex high entropy alloy presents a higher strength, and overall less plastic deformation for the same stress level. This is mostly driven by the fact that the dislocations do not glide as easily in the random alloy as they do in the average atom material.

Computational Design of a Lightweight and Ductile Refractory Alloy: Michael Gao[1]; David Alman[1]; *Michael Widom*[2]; [1]National Energy Technology Laboratory; [2]Carnegie Mellon University

There are urgent needs to develop next-generation alloys beyond Ni-based superalloys. The main obstacles lie in achieving balanced properties, such as optimizing room temperature (RT) ductility, RT fracture toughness, creep, fatigue, thermal stability, and oxidation resistance while remaining light weight and low cost. Here we present our ongoing research effort and progress on the development of high-performance refractory high entropy alloys supported by the ARPA-E ULTIMATE program. High throughput CALPHAD calculations are performed on the Nb-Mo-Ta-Ti-Zr-Hf-V-Cr-Al-C system to search for compositions that meet various thermophysical properties (such as density, cost, and solidus temperature) and promote precipitation of fine carbides We also perform first principles analysis of chemical order and both linear and nonlinear elasticity with a goal of using intrinsic ductility as a guide in our alloy design. Preliminary experimental results on microstructure and mechanical properties will be presented.

High-throughput Approach for Exploration of FCC High Entropy Alloys Based on Deformation Pathways: *K V Vamsi*[1]; Marie-Agathe Charpagne[1]; Tresa Pollock[1]; [1]University of California-Santa Barbara

Exploration of novel multicomponent systems has gained interest since the discovery of Cantor alloy and its subsets. It is known that unstable stacking/twin fault energies along with stable stacking faults in the generalized planar/stacking fault energy profiles control the deformation pathways in FCC structures. Estimation of these intrinsic energy barriers for arbitrary compositions is still a challenge experimentally and computationally and there is a need for high-throughput methodologies. In this work, we present a new approach for the exploration, using the FCC ternary Ni-Co-Ru system as a model, based on an operating deformation mechanism. Employing first-principles calculations, the stable stacking fault energies are estimated from a diffuse multi-layer fault model and the unstable fault energies are estimated by a recently found correlation with shear modulus in FCC structures. Deformation mode maps are developed, and regions are classified based on the deformation mode activated. Experimental results validating these predictions are discussed.

Modeling Dislocation Dynamics in Refractory Multi-principal Element Alloys: *Lauren Fey*[1]; Shuozhi Xu[1]; Yanqing Su[2]; Abigail Hunter[3]; Irene Beyerlein[1]; [1]University of California-Santa Barbara; [2]Utah State University; [3]Los Alamos National Laboratory

There is growing experimental and modelling evidence that dislocations in refractory multi-principal element alloys (MPEAs) behave in distinct ways from dislocations in conventional alloys. We develop a phase-field dislocation dynamics model for refractory MPEAs that incorporates variable glide resistances, differences between screw and edge dislocation behavior, and different crystallographic slip modes. The mesoscale model is informed by atomistic calculations and applied to study dislocation glide and multiplication in a model MPEA, MoNbTi. The inherent variability in dislocation glide resistance due to the disordered lattice causes the formation of athermal kink-pairs on screw dislocations, creating a wavy morphology during dislocation glide and probabilistic glide stresses. Our calculations show that the stresses required for screw dislocation glide are similar across several slip plane types, increasing the potential pathways for dislocations.

Disorder-driven Biasing of Deformation Tendencies in Concentrated FCC Solid Solutions: *Matthew Daly*[1]; Ritesh Jagatramka[1]; [1]University of Illinois-Chicago

The intrinsic competition between deformation mechanisms can be conveniently conceptualized by the fault energy landscape. In pure systems or dilute solutions, where a primary element occupies most atomic positions, the fault energy landscape can be considered as spatially homogenous. However, in concentrated solid solutions such as high entropy alloys, local fluctuations in the atomic distribution disrupt the periodicity of the fault energy landscape. These perturbations introduce new paths of least resistance within a topology, which give rise to localized tendencies for differing deformation behaviors. Here, we will discuss how randomized atomic distributions bias the operation of deformation mechanisms in concentrated FCC solid solutions. Our approach combines atomistic calculations with kinetic Monte Carlo-based models to connect the atomic-scale fluctuations in composition with changes in deformation tendencies. A physical model that incorporates stochastic effects into the description of deformation energy barriers will also be discussed.

Session VI

Tuesday AM
December 7, 2021
Place

Room: University Ballroom CDE
Location: Hilton Charlotte University

Session Chair: To Be Announced

Introductory Comments

Invited

Utilizing Nanoprecipitates to Modulate Phase Transformation, Strength, and Ductility of HEAs: *Ying Yang*[1]; Easo George[1]; [1]Oak Ridge National Laboratory

Solid solution high-entropy alloys (HEAs) with the face-centered cubic (fcc) structure can exhibit extensive tensile ductility and excellent toughness, but their room-temperature strength tends to be low. To increase strength, obstacles to dislocation motion such as grain boundaries, twin boundaries, solute atoms, and precipitates are typically added. However, with few exceptions, they tend to embrittle materials. Precipitates, in addition to spatially confining dislocations and increasing strength, can also retard phase transformation. In this presentation, we will demonstrate a strategy that utilizes nanoprecipitates to independently tune both phenomena. The precipitates, by synergistically modulating the strength and transformation of the HEA matrix, produce alloys with improved strength and ductility. We discuss how this strategy can be used to tailor variables such as precipitate size, spacing, volume fraction, and/or the chemical driving force of matrix phase transformation to activate deformation mechanisms precisely when they are needed during plasticity to optimize the strength-ductility combination.

Cold Spray of Medium and High Entropy VCoNi, CrCoNi and CrCoFeMnNi Coatings: Effects of Topical Oxides: Desmond Klenam[1]; Precious Etinosa[2]; Trevor Bond[2]; Arvand Navabi[2]; Ridwan Ahmed[2]; Mobin Vandadi[2]; Oluwaseun Oyewole[2]; John Obayemi[2]; *Nima Rahbar*[2]; Wole Soboyejo[2]; [1]Wits University; [2]Worcester Polytechnic Institute

This paper presents the results of experimental and theoretical/computational study of cold spray behavior of medium and high entropy VCoNi, CrCoNi and CrCoFeMnNi coatings on similar substrates. A combination of single powder spray and bulk cold spray techniques is used to study the cold spray behavior of these alloys. The effects of topical nano-scale oxide layer thickness are also studied using density functional theory and finite element models. These are used to compute the contact-induced bond deformation, splat deformation, stress/strain distributions, and the crack driving forces in powders that are cold sprayed onto similar substrates at different incident velocities. The mechanical properties of the cold sprayed layers and their interfaces are then studied using nanoindentation and interfacial fracture mechanics. The underlying crack/microstructure interactions and toughening mechanisms are elucidated before exploring the implications of the current results for the design of robust, cold sprayed, complex concentrated alloys and their coatings.

Production of Spherical, Refractory HEA Powders: *Karin Ratschbacher*[1]; [1]GfE Metals and Materials GmbH

Refractory metals based HEAs exhibit a relatively high melting point, as well as high strength. These circumstances promote the production of parts via additive manufacturing. This paper introduces two production routes that lead to spherical refractory metals HEA powders, mainly depending on the melting point of the alloy. First route: Elements are alloyed in an Electron Beam Furnace. The resulting ingot is remolten in an induction skull melter, poured to cylindrical rods and then EIGA atomized. Furnace specifications are introduced, features presented and examples for alloys, suitable for this production route are given. Second route involves mixing the element powders metallurgically, powders are compacted into cylindrical containers, which are HIPed and consequently atomized through an EIGA-process. This production route is suitable for alloys with very high melting points. Examples for process parameters and alloys are given. Resulting powders are characterized and results are being presented.

Break

Dissimilar Laser Welding of High Entropy Alloys: *Joao Oliveira*[1]; [1]FCT-UNL

Dissimilar laser welding of the CoCrFeMnNi to 316L stainless steel and Inconel 718 was successfully performed. Microstructure characterization by means of electron microscopy and high energy synchrotron X-ray diffraction were used to evaluate joint. Digital image correlation was used to evaluate how the different regions of the joints (base material, heat affected zones and fusion zone) deformed during tensile testing. High strength and ductility were obtained in the laser welded joints upon optimization of the process parameters. Thermodynamic calculations to analyze the microstructure evolution in the fusion zone of the welds was also performed and compared to the X-ray diffraction measurements. A correlation between process parameters, microstructure evolution and mechanical properties was established.The sound joints obtained in this work may open new potential applications for high entropy alloys in high demanding structural applications.

Development of Powder Metallurgy High-entropy Alloys by Using Superalloys Commercial Commodity Powders: S. Venkatesh Kumarán[1]; *Jose Torralba*[2]; [1]IMDEA Materials Institute; [2]Universidad Carlos III Madrid-IMDEA Materials Institute

High entropy alloys (HEAs) obtained by powder metallurgy (PM) can follow many processing routes. In this work, we propose the use of commercial commodity powders like superalloys as raw materials. There are no readily available pre-alloyed powders in the market for even the commonly studied HEAs because of which there is a need for atomizing/mechanical alloying the elemental powders before proceeding with the other PM steps. Moreover, the use of pure elemental powders has issues with health, storage and handling. But the commodity powders (those compositions most extended in most applications) are fully available in the market in gas atomized form, which can be blended in the right proportion to obtain a feedstock to make HEAs efficiently using most PM forming technologies. In this work, we will present an approach to this technological option, where we use field assisted techniques and selective laser melting to successfully obtain single phase HEAs.

Dense, Fine-grained Refractory Metal Alloys via a Low-temperature, Chemical-reaction-based Powder Metallurgical Process: Sona Avetian[1]; Sunghwan Hwang[1]; Austin Hernandez[1]; Mario Caccia[1]; Michael Titus[1]; *Kenneth Sandhage*[1]; [1]Purdue University

A significant increase in the temperature of operation of turbine engines could enable unprecedented enhancements in aircraft performance and in the efficiency of electricity production by power plants (with a corresponding reduction in greenhouse gas emissions). The temperature limitations of state-of-the-art, nickel-based superalloys have spurred interest in the development of higher-melting, refractory complex concentrated alloys (RCCAs) for use in next-generation engine components. Conventional liquid-based processing routes tend to yield refractory metal alloys with relatively coarse grains and residual microsegregation, whereas powder metallurgical approaches have the potential to produce homogeneous alloys with finer grain sizes. In this presentation, a low-temperature, chemical-reaction-based powder metallurgical process has been developed and examined for generating dense, fine-grained, ultra-high-melting W-Mo-based compositions. The microstructure, microchemistry, and preliminary mechanical properties of such alloys will be discussed.

Single Phase Formation in a CoCrFeNiAlCu High Entropy Alloy by an Ultrafast Sintering Technique: *PAULA OLMOS*[1]; Eduardo Reverte[1]; Juan Cornide[1]; Monica Campos[1]; Miguel Lagos[2]; [1]Universidad Carlos III de Madrid; [2]Tecnalia

The exceptionality of HEA lies in the formation of a single random solid solution which will determines their properties. The formation of this phase takes place thanks to a high configurational entropy derived from the high number of elements in its formulation. A study of the properties of the involved elements can predict the phase formation and, in fact, there are numerous works that propose the empirical rules to predict their behaviour. However, the kinetics of phase formation also play an important role in the formation of the final microstructure and must be studied for each HEA composition. In the present work, a new HEA composition has been designed and consolidated by two Powdermetallurgy techniques: conventional Pressing and Sintering and an ultrafast sintering technique: Electrical Resistance Sintering (ERS). Comparison of the microstructures obtained will allow to know how the physical characteristics of the processing influence phase formation and final properties.

Recent Progress in the CoCrNi Alloy and Derived Systems: *Sakshi Bajpai*[1]; Benjamin MacDonald[1]; Timothy Rupert[1]; Horst Hahn[2]; Diran Apelian[1]; [1]University of California Irvine; [2]Karlsruhe Institute of Technology, Germany

The equiatomic CoCrNi alloy has gained a lot of attention in recent years owing to its exceptional mechanical properties, particularly at cryogenic temperatures. Like the equiatomic CoCrFeNiMn Cantor alloy, from which it was derived, the CoCrNi ternary possesses low stacking fault energy that leads to complex deformation modes, in particular, the ease of twinning activation at ambient temperatures and increased strain. Furthermore, chemical short-range order and FCC-HCP transitions have recently been verified in this alloy and are key factors contributing to the alloy's properties. Efforts are being made to further enhance the performance of these alloys for demanding structural applications using two different approaches: thermomechanical processing and alloying additions. Through this presentation, the fundamental mechanisms of the CoCrNi alloy will be established. Recent studies on their process-driven microstructural evolutions, minor alloying additions to the base CoCrNi ternary, and the ongoing efforts at the University of California, Irvine will be discussed.

Tuesday Plenary

Tuesday AM
December 7, 2021
Place

Room: University Ballroom CDE
Location: Hilton Charlotte University

Session Chair: To Be Announced

Introductory Comments

Plenary

Applying Physical Metallurgy Principles to Multi-principal Element Alloys: *Amy Clarke*[1]; [1]Colorado School of Mines

Advances in physical metallurgy have resulted in societal advancements, such as the Bronze and Iron Ages. Much of modern physical metallurgy, i.e. processing-structure-property relationships in metals and alloys, has been developed based upon the outcomes of conventional processes like casting or wrought (thermomechanical) processing of alloys designed for these purposes. Multi-principal element alloys (MPEAs) have recently emerged onto the scene, given their potential for remarkable properties (e.g., exceptional strength/toughness combinations) unattainable by conventional alloys. For example, refractory multi-principal element alloys (RMPEAs) hold the promise to withstand continuous operation at ultrahigh temperatures above 1200 ˚C needed for advanced turbine engines and hypersonic flight. Opportunities exist to apply physical metallurgy principles established with conventional alloys (e.g., steels) and processes to MPEAs, but MPEAs are also challenging our current paradigm. Here we highlight the design of MPEAs for performance in extreme environments in the context of physical metallurgy principles.

Break

Session VII

Tuesday PM
December 7, 2021
Place

Room: University Ballroom AB
Location: Hilton Charlotte University

Session Chair: To Be Announced

Introductory Comments

Invited

Recent Advances, Hardening, Softening and Ductility in High Entropy Brasses and Bronzes: Kevin Laws[1]; *Patrick Conway*[1]; David Miskovic[1]; Lori Bassman[1]; Warren McKenzie[1]; [1]UNSW Sydney

The use of Brasses and Bronzes is subtly astounding, ranging from the keys in your pocket, zippers on your clothes, hinges, handle and lock mechanism of your front door, plumbing and electronic hardware, bearings, munitions and world coin currencies - arguably one of the most versatile alloy families on the planet. Using the design flexibility of the Cu-Mn-Ni-Zn-Al-Sn and extended alloy variants we demonstrate the vast range of applications/alloy solutions currently relevant to changing the Brass and Bronze industries as we know them, including the lead-free movement for free-machining and self-lubricating alloys. An integral part of this study are the effects of independent alloy additions within this system, how they effect strength/hardness through solid solution hardening and softening effects and the fine-tuning an extraordinary range of multi-phase microstructures. Here we report the most significant developments in this space over the last 5 years.

Exploring Phase Equilibria, Strength and Deformation Mechanisms of Non-equiatomic CrCoNi Compositions: Francisco Coury[1]; *Diego Santana*[1]; Gustavo Bertoli[1]; Claudio Kiminami[1]; Guilherme Zepon[1]; Vitor Pereira[1]; Amy Clarke[2]; [1]Universidade Federal de São Carlos; [2]Colorado School of Mines

The CrCoNi system has attracted a considerable amount of attention from the literature in recent years due to the attractive mechanical and anti-corrosion properties. While the equiatomic alloy has been studied in depth, several non-equiatomic compositions with very interesting properties are also being explored more recently. In this presentation it will be shown that this system is very versatile, the mechanical properties and deformation mechanisms are highly tunable by compositional modifications and processing routes. The experimental results from different compositions will be presented here and emphasis will be given on the effect of composition on the different strengthening and deformation mechanisms operating on these alloys. Furthermore, some corrosion and wear properties of such alloys will also be shown to highlight the versatility of these alloys. Ideas for future developments on this system will be discussed in light of our results and from others in the literature.

Precipitation and Strengthening in AlCoCrFeNi High Entropy Alloys: *Keith Knipling*[1]; Patrick Callahan[1]; David Beaudry[2]; [1]Naval Research Laboratory; [2]Johns Hopkins University

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. In this study we present the complex three-dimensional nanoscale microstructures formed 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). Atomic-scale clustering and ordering is assessed in three dimensions using atom-probe tomography and these experimental results are compared with the equilibrium phases predicted by thermodynamic modeling.

Effect of Dose Rate on the Irradiation Responses of CrFeNi-based Multi-principal Element Alloys (MPEAs): *Anshul Kamboj*[1]; Emmanuelle Marquis[1]; [1]University of Michigan

MPEAs are being considered for nuclear applications because of their potentially superior mechanical properties and irradiation resistance. Of particular interest are Ni-based MPEAs, specifically CrFeNiMn, CrFeNiCoMn, and CrFeNiCoPd with high swelling resistance and suppressed damage accumulation compared to stainless steels and dilute alloys. While these MPEAs appear stable against phase decomposition during high dose rate ion irradiation, electron irradiation and thermal annealing studies suggested that these alloys may be susceptible to phase decomposition. To clarify the role of dose rate during ion irradiation, alloys were irradiated using Fe ions at 5000C with an intermediate dose rate of 10-4 dpa/sec. Transmission electron microscopy and atom probe tomography observations revealed phase decomposition in the Mn and Pd containing alloys with a strong effect on dislocation loop structure. In addition, comparison among the irradiated responses of Cr18Fe39Ni38Mn5, Cr18Fe28Ni31Mn23, and Cr18Fe35Ni35Mn12 unveiled the effects of Mn concentration on phase decomposition and dislocation loop structure.

Microstructural and Mechanical Characterization of a Concentrated FCC CrCoNi Matrix Containing Dispersed L12 Precipitates: *Diego de Araujo*[1]; Fransciso Coury[1]; Claudio Kiminami[1]; [1]Universidade Federal de Sao Carlos

The ternary CrCoNi alloy presents a good combination of strength, toughness, and corrosion resistance, as showed by different studies in the last years. In this work, we report the microstructural and mechanical behavior of $Cr_{29.7}Co_{29.7}Ni_{35.4}Al_{4.0}Ti_{1.2}$ (at. %) alloy, which was designed to present dispersed nanometric $L1_2$ precipitates in a Cr-Co-Ni matrix. The aimed microstructure was successfully achieved, experimentally determined precipitates volume fraction and the solvus temperature showed a good agreement with CALPHAD calculations. Aging treatments were performed at 850 °C for different amounts of time up to 166 h. The uniformly distributed spherical precipitates had a coarsening rate constant lower than those of different /' alloys reported in the literature. The $s_{0.2\%}$ yield strength gain upon aging was analyzed based on conventional precipitation hardening models. The values are compared to those obtained in some traditional wrought superalloys.

Break

Session VIII

Tuesday PM
December 7, 2021
Place

Room: University Ballroom CDE
Location: Hilton Charlotte University

Session Chair: To Be Announced

Introductory Comments

Invited

Guidelines for Beneficial Short-range Ordering: Composition-dependent Plasticity Effects: *Hyunseok Oh*[1]; Michael Xu[1]; Shaolou Wei[1]; James LeBeau[1]; Cemal Cem Tasan[1]; [1]Massachusetts Institute of Technology

Short-range order (SRO) has been proposed in modern alloys including high entropy alloys (HEAs), arising from various origins such as magnetic frustrations, strong electronic interactions, or the formation of complexes with interstitial elements. However, beneficial utilization of SROs in the design of new alloys has been difficult, due to the lack of understanding about SRO-dislocation interactions. The classical understanding of SRO, i.e., detrimental planar slip induced by SROs, does not do full justice to the complexity of this problem, as can be seen in recently developed HEAs with unexpected improvements in mechanical properties while having planar slip mechanisms. In efforts to find simple guiding principles for customizing beneficial SROs, we here present a classification of SROs in various face-centered cubic alloys based on their composition-dependent effects on dislocations explored through stress-relaxation tests, in-situ deformation studies, and direct observations via revSTEM techniques.

Effect of Short-range Ordering on the Plastic Deformation of NiCoCr Medium Entropy Alloy: *Sezer Picak*[1]; Prashant Singh[2]; Daniel M. Salas[1]; Yury Chumlyakov[3]; Duane Johnson[2]; Raymundo Arroyave[1]; Ibrahim Karaman[1]; [1]Texas A&M University; [2]Ames Laboratory; [3]Tomsk State University

Medium- and high-entropy alloys (M/HEAs) exhibit an outstanding combination of high strength and ductility, which has been linked to the activation of various deformation modes triggered by low-energy stacking faults. However, the question remains: is the plasticity of M/HEAs governed only by SFE, or does short-range ordering (SRO) play a role? To answer this question, we investigated the effect of SRO on the plastic deformation in single crystalline NiCoCr MEA. We demonstrated that SRO promotes twinning- and transformation-induced plasticity, depending on the crystallographic orientation of the crystals. We also discovered a new hierarchical strain induced phase transformation sequence (fcchcpD019) at room temperature, which was attributed to a weaker degree of SRO in the hcp phase based on novel density-functional theory methods. By controlling the degree of SRO through aging at high temperatures, the level of twinning and strain-induced phase transformation has been increased, further enhancing the ductility levels in NiCoCr.

Solute-strengthening in Alloys with Short-range Order: Shankha Nag[1]; *William. A. Curtin*[2]; [1]TU Darmstadt; [2]École Polytechnique Fédérale de Lausanne

Recent surging interest in strengthening of High Entropy Alloys (HEAs) with possible chemical ordering motivates the development of new theory. An existing theory for random alloys accounts for solute-dislocation and solute-solute interactions across the slip plane. Here, this theory has been extended to include strengthening due to short-range order (SRO) as characterized by the well-known Warren-Cowley SRO parameters. Closed form expressions are presented for the yield strength and energy barrier of dislocation motion in alloys with SRO based on inputs of atomic misfit volumes, average lattice and elastic constants, effective pair interactions and the SRO parameters. The predictive expression includes the average strengthening effect unique to SRO. The theory is applied to several HEAs with good success. This generalized solute-strengthening theory is the most comprehensive to date that is applicable to any alloys that are macroscopically homogeneous single-phase alloys and has inputs that can be measured or computed.

Role of Local Chemical Order on Orientation Relationship Determination in High Entropy Alloys: *Elaf Anber*[1]; Daniel Foley[1]; Diana Farkas[2]; Anatoly Frenkel[3]; Mitra Taheri[1]; [1]Johns Hopkins University; [2]Virginia Tech; [3]Stony Brook University

High entropy alloys (HEAs) have attracted the major interest due to their novel mechanical and structural properties. Local chemical ordering (LCO) plays an important role in determining thermal and electrical conductivity of solid solutions, diffusion, and passivity of alloys containing elements that are electrochemically active. Here, we examined the role of LCO on the OR of BCC precipitates in annealed Al0.3CoCrFeNi via using in-situ and ex-situ TEM heating techniques, where we report a new BCC-ORs due to local chemical fluctuations. These studies were coupled with Extended Electron Energy Loss Fine Structure (EXELFS) and Energy-dispersive X-ray spectroscopy (EDS). Additional insight is obtained from molecular dynamics atomistic simulations that examine the various possible orientation relationships and interface dislocations for the B2 precipitates in these Al containing HEA'S. Overall, the LCO associated with ORs offers new opportunities to tune properties, enabling a more predictive view of designing remarkable age-hardening alloys.

Cores of 1/2<110>-type Dislocations in the CrMnFeCoNi High-entropy Alloy Investigated by STEM, the Center of Symmetry and the Nye Tensor Mapping Techniques: *Milan Heczko*[1]; Veronika Mazánová[1]; Roman Gröger[2]; Tomáš Záležák[2]; Mohammad Hooshmand[3]; Easo George[4]; Michael Mills[1]; Antonín Dlouhý[2]; [1]The Ohio State University; [2]Institute of Physics of Materials CAS; [3]University of California; [4]Oak Ridge National Laboratory

The influence of small pre-strains on the elevated-temperature stability and microstructure of the equiatomic CrMnFeCoNi high-entropy alloy is investigated. Attention is given to whether any of the alloy elements segregate to individual dislocations. Samples were deformed in tension at room temperature to plastic strains of 0.2 and 2.3%, and subsequently annealed at 973 K for 800 hours. The pre-strains activated planar slip of 1/2<110>-type dislocations on {111}-type glide planes. Interactions of this planar slip with special S3 grain boundaries formed a number of dislocation segments with a <110>-type crystallographic orientation suitable for a credible end-on analysis. Results of atomic resolution STEM and Super-X EDS experiments combined with the center of symmetry and the Nye-tensor mapping suggest that the indicated thermomechanical treatments did not cause any chemical changes to dislocation cores. Important implications of presented results on the mechanisms of high-temperature creep in this class of materials are discussed.

3:40 PM Break

Session IX

Wednesday AM
December 8, 2021
Place

Room: University Ballroom AB
Location: Hilton Charlotte University

Session Chair: To Be Announced

Introductory Comments

Invited

. . . So You Want to Make a Refractory Alloy? A Primer on R-MPEA Processing Challenges: *Noah Philips*[1]; Matthew Carl[1]; [1]Allegheny Technologies

Understanding that successful alloy development depends on a process, a composition and economic constraints, this talk aims to guide the recent explosion of interest in refractory multi-principal element alloys (R-MPEAs) with some context on the processing of these materials. We review the paths used for manufacturing of refractory alloys with an eye toward the lessons from the last 70 years. In addition to the technical challenges associated with high melting temperatures, contamination control and thermomechanical processing we will present some of the more practical concerns that have prevented alloy adoption in the past that concern modern alloy designers. Looking forward to the exciting potential of R-MPEAs we will explore some of the challenges of emerging technologies (e.g. powder and Additive Manufacturing, computational tools) informed by past research and experience.

Microstructure and Deformation Processes of a Refractory Complex Concentrated Alloy Exhibiting B2-type Order: Jean-Philippe Couzinie[1]; *Milan Heczko*[2]; Veronika Mazanova[2]; Oleg Senkov[3]; Rajarshi Banerjee[4]; Maryam Ghazisaeidi[2]; Michael Mills[2]; [1]The Ohio State University & Université Paris Est ICMPE; [2]The Ohio State University; [3]Air Force Research Laboratory; [4]University of North Texas

Refractory complex concentrated alloys (RCCAs) are currently among the most promising structural materials in the high-entropy field as they retain high mechanical properties up to 1000˚C. The ordered B2 phase plays a key role in some of RCCAs behavior, and promising compositions are found in systems for which it is present, whether the B2 phase is continuous or forms coherent precipitates in the matrix. They are currently seen as interesting candidates for future structural applications, but some basic challenges have still to be addressed. The understanding of the deformation mechanisms and of the influence of order on those mechanisms is a crucial one. Thus, the present talk aims at giving some insights into the deformation processes of the Al0.5NbTa0.8Ti1.5V0.2Zr material after compressive testing at room temperature and 600˚C. Detailed analysis of the defects governing the plastic deformation will be reported and discussed in light of the transmission electron microscopy observations.

Microstructural Inversion Accompanied by B2 to hP18 Phase Transformation in a BCC based Refractory Complex Concentrated Alloy: *Abhishek Sharma*[1]; Sriswaroop Dasari[1]; Vishal Soni[1]; Oleg Senkov[2]; Daniel Miracle[3]; Rajarshi Banerjee[1]; [1]University of North Texas; [2]UES Inc.; [3]Air Force Research Laboratory

A continuous ordered B2 matrix with discrete cuboidal BCC pockets, like a superalloy microstructure, is often observed in RCCAs or RHEAs. Such a microstructure has been attributed to concomitant spinodal decomposition coupled with chemical ordering within the BCC matrix. The $Al_{0.5}Mo_{0.5}NbTa_{0.5}TiZr$ RCCA exhibits this microstructure at the initial stages when annealed at 800\176C. Longer term annealing at 800\176C results in a phase inversion into a continuous BCC matrix with discrete B2 precipitates. However, these B2 precipitates appear to be a metastable transition phase which eventually transform to an hP18 ordered phase which is a derivative of the ordered omega type structure. This transformation occurs via collapse of the {111} type planes of the parent B2 structure, a phenomenon well reported in other BCC-based alloy systems such as Zr-Al-Nb and Ti-Al-Nb. Here, the compositional and structural changes associated with this transformation, have been characterized using detailed TEM and APT based techniques.

Break

Designing High-entropy Intermetallic Alloys: Refractory B2 Phases: *Jie Qi*[1]; Xuesong Fan[2]; Rui Feng[3]; Peter Liaw[2]; S. Poon[1]; [1]University of Virginia; [2]The University of Tennessee; [3]Oak Ridge National Laboratory

Data-driven methods, such as supervised machine learning (ML), have shown success in predicting the compositions of solid-solution high-entropy alloys (HEAs). However, this method is rarely applied to predicting intermetallic phases due to limited data and the low effectiveness of ML features. Ordered high-entropy body-centered-cubic (BCC) phases with the B2 structure, particularly those formed with refractory elements and aluminum (refractory-B2), are of interest due to their high strength, and corrosion and oxidation resistance. The design of refractory-B2 using ML and characterization of structural and mechanical properties will be presented. Several B2 refractory HEAs developed with the use of physics-based features and optimized by feature engineering and active learning have shown great compression plasticity and high strength.

Ab Initio Study of the Phase Stability and Transition-induced Plasticity of Body-centered Cubic Refractory High-entropy Alloys: Yuji Ikeda[1]; *Prashanth Srinivasan*[1]; Konstantin Hubaev[1]; Fritz Körmann[2]; Blazej Grabowski[1]; [1]University of Stuttgart; [2]Delft University of Technology

Recent experiments revealed for several body-centered cubic (bcc) refractory high-entropy alloys (HEAs) the ability to improve their ductility by enabling transition-induced plasticity (TRIP), transforming bcc to hexagonal close-packed (hcp) structure. However, the instability of the bcc phase is also often related to the phase, whose precipitates are also found in bcc HEAs and can cause embrittlement. To design alloys with improved mechanical properties, the knowledge of the detailed phase stability of such HEAs is essential. We present a thermodynamic and dynamic stability analysis of bcc refractory HEAs from ab initio. We demonstrate that it is essential to first analyze whether alloys relax to a bcc or phase. Based on the proposed structure descriptor, ab initio predicted bcc–hcp phase stability threshold compositions are found close to the experimentally observed TRIP compositions in Ti–Zr–Nb–Hf–Ta-based HEAs, opening an avenue for high-throughput alloy design strategies.

Characteristics of Slip Localization in the HfNbTaTiZr Refractory High Entropy Alloy: *Jean-Charles Stinville*[1]; M.A. Charpagne[1]; F. Wang[1]; L.H. Mills[1]; D.S. Gianola[1]; T.M. Pollock[1]; [1]University of California-Santa Barbara

Refractory high entropy alloys are promising for high temperature structural applications. However, the plastic deformation processes that occur at roomtemperature have important consequences for the ductility of these alloys. A better understanding of these processes may provide opportunities to improve room temperature properties. The micro-scale plasticity, including the onset of slip and early plastic localization, has been examined in tension in wrought processed polycrystalline bcc HfNbTaTiZr using high-resolution digital image correlation (HR-DIC) analysis coupled to electron back-scattered diffraction measurements. Slip activity is studied in a statistical manner over large representative regions containing hundreds of grains. Two different behaviors are identified with regard to the tendency for strain localization. These behaviors are discussed in relation to dislocation glide and avalanche processes and their consequences for mechanical properties at room temperature.

Atomistic Modeling of High Temperature, Low Strain Rate Plasticity in BCC Refractory-based HEAs: *Joel Berry*[1]; Kate Elder[2]; Aurelien Perron[1]; [1]Lawrence Livermore National Laboratory; [2]Northwestern University / LLNL

The origins of the excellent high temperature mechanical properties of refractory-based BCC HEAs are not well understood. At sufficiently high temperatures, plasticity in these alloys should be mediated by a mix of conservative and nonconservative defect motion, e.g. dislocation glide and climb and vacancy diffusion through the bulk and/or grain boundaries. Further, in HEAs these processes may be significantly modulated by the complex, co-evolving compositional environment. The above effects can span multiple scales and are difficult to simultaneously incorporate into computational models. This has been one factor keeping the microstructural origins of refractory HEA mechanical performance shrouded. We explore a way to address this issue through phenomenologically time-averaged atomistic simulation approaches that incorporate all of the above effects. Simulations span from atomistic to microstructural lengths and cover experimentally relevant, diffusive times. Model development and parameterization issues will be addressed and analysis of preliminary results from simulated deformation experiments presented.

One Order of Magnitude Improvement of the Magnetocaloric Effect of Rare-earth-free High-entropy Alloys: *Jia Yan Law*[1]; Álvaro Díaz-Garcia[1]; Luis Moreno-Ramírez[1]; Victorino Franco[1]; [1]Sevilla University

One of the most reported functional properties of high-entropy alloys (HEAs), the magnetocaloric effect (MCE), only shows large values among those compositions that include rare-earth (RE) elements. However, they have yet to become competitive when compared to conventional magnetocaloric materials. Here we present that the MCE of RE-free HEAs can be improved by more than one order of magnitude upon introducing a magneto-structural phase transition: from 1.7 to 13.1 J kg1K1 (for a moderate magnetic field change of 2.5 T). Instead of sampling the vast HEA compositional space by brute force, we have adopted a directed search procedure to develop FeMnNiGexSi1-x HEAs that enabled us to put the functionality of HEAs comparable to some of the high-performance traditional materials.

Session X

Wednesday AM
December 8, 2021
Place

Room: University Ballroom CDE
Location: Hilton Charlotte University

Session Chair: To Be Announced

Introductory Comments

Invited

Dislocation Pathways in Refractory Multi-principal Element Alloys: *Daniel Gianola*[1]; [1]University of California, Santa Barbara

Refractory multi-principal element alloys (MPEAs) are promising candidates for structural applications demanding mechanical robustness at temperatures exceeding the capacity of state-of-the-art superalloys. While excellent high temperature strength has been demonstrated in many refractory MPEAs, a fundamental understanding of the nature of dislocation pathways in the BCC versions of these chemically complex alloys and their ability to enable macroscopic ductility is still in its infancy. We present a study of a ternary MPEA, MoNbTi, through a combination of in situ dislocation observations, microstructural investigations, and atomistic calculations. Our results highlight multi-planar, multi-character dislocation slip in MoNbTi at low homologous temperature, encouraged by the substantial dispersion in the glide resistance for dislocation due to the atomic-scale chemical fluctuations. The ability of dislocations to choose the easy gliding direction and plane enables an excellent combination of strength and homogeneous plasticity in this alloy, traits that are not simultaneously observed in conventional metallic alloys.

Twinning Engineering of High-entropy Alloys: *Hyoung Seop Kim*[1]; [1]Pohang University of Science and Technology

To improve the mechanical properties of high entropy alloys, especially strain hardening performance, a long-proven concept of 'twinning engineering' developed in relation to TWIP steels has been applied to this group of materials. The strategy chosen included a two-stage thermodynamic treatment consisting of low-temperature pre-transformation and subsequent annealing. This approach has been tested with an exemplary high entropy alloy in CoCrFeMnNi. The selected annealing conditions ensured that the strain pairs created in the low-temperature strain were maintained while the dislocation density was restored. The viability of this strategy has been convincingly confirmed for the room temperature deformation of the alloy. A constituent model has been proposed to account for the influence of the transforming twins before transformation. It has been shown to provide a reliable explanation for the low and room temperature variants of CoCrFeMnNi.

Deformable Plastic Strain-induced Epsilon-martensite in Medium-entropy Alloys: A Pathway towards Multi-stage Metastability Engineering: *Shaolou Wei*[1]; Cem Tasan[1]; [1]Massachusetts Institute of Technology

In contrast to pseudo-elastic martensitic phases, typical BCT-martensite formed through plastic straining often exhibits brittle-like features, largely ascribed to the extensive defect density and the pronounced plastic accommodation in the vicinal parent phase. A somewhat intermediate situation occurs when epsilon-martensite is nucleated during plastic deformation: the similar atomic stacking sequence between HCP and FCC lattices enables more moderate interfacial mismatch, alleviating plastic accommodation. In light of this, we will show that through appropriate compositional design, highly deformable strain-induced epsilon-martensite can be achieved in medium- or high-entropy alloys. We will detail in this presentation: (1) the exploration of a sequential FCC-HCP-FCC martensitic transformation chain by plastic straining; (2) the understanding of an atomic shuffle-involved "twinning" in strain-induced epsilon-martensite; and (3) the atomistic procedures that accomplish "twinned" epsilon-martensite to final FCC transformation. Finally, a discussion towards the feasibility of multi-stage TRIP/TWIP metastability engineering will also be included.

Break

The Cyclic Plastic Strain Localization and the Fatigue Crack Initiation in Equiatomic CrCoNi Medium-entropy Alloy: *Veronika Mazanova*[1]; Milan Heczko[1]; Connor Slone[2]; Mulaine Shih[1]; Easo George[3]; Maryam Ghazisaeidi[1]; Jaroslav Polak; Jaroslav Polak; Jaroslav Polák[4]; Michael J. Mills[1]; [1]The Ohio State University; [2]Exponent; [3]Oak Ridge National Laboratory; [4]Institute of Physics of Materials CAS

Multi-principal-element alloys became a topic of significant interest thanks to their outstanding mechanical properties at room and low temperatures. However, there is still lack of the information about their fatigue properties. In current work, the attention is focused on model system, equiatomic CrCoNi alloy in fully recrystallized microstructural state which combines good cyclic strength with superior resistance to cyclic plastic deformation. The cyclic plastic localization and its role in the fatigue crack initiation during low cycle fatigue loading were studied. A sophisticated experimental workflow was designed to extract information from the surface and the bulk of tested material using a combination of SEM, EBSD, ECCI, FIB and HR-STEM. High fraction of annealing twin and the fatigue induced deformation twin boundaries were preferential sites for localized cyclic plastic strain. Moreover, stress concentrations near deformation twins led to activation of TWIP and TRIP plasticity and early, well-development of surface relief.

Mechanism and Prediction of Hydrogen Embrittlement in fcc Stainless Steels and High Entropy Alloys: Xiao Zhou[1]; Ali Tehranchi[2]; *William A Curtin*[1]; [1]EPFL; [2]Max-Planck-Institut für Eisenforschung GmbH

Recent experiments on new fcc high entropy alloys (HEAs) seem to exhibit unique response to Hydrogen Embrittlement (HE): some HEAs absorb more hydrogen than pure Ni and conventional stainless steels but are less susceptible to HE. The possible uniqueness of HEAs with respect to HE, if true, poses a huge opportunity. Here we present a new mechanism of embrittlement based on an intrinsic ductile to brittle transition caused by H. Using first principles inputs plus statistical and applied mechanics, we predict critical H concentrations for HE across stainless steels and HEAs in very good agreement with experiments. In particular, the HE resistance ranked as CoNiV>SS316L>NiCoCr>CoCrFeNi>CoCrFeMnNi>SS304>Ni is understood in terms of the effects of H on different alloy properties. While HEAs are not unique, complex alloys can be beneficial for HE and the theory opens an avenue toward design of HEA with good resistance to HE.

Low Cycle Fatigue Behavior of the Equiatomic CrMnFeCoNi High Entropy Alloy: *Dayane Oliveira*[1]; Easo George[2]; Jeffery Gibeling[1]; [1]University of California, Davis; [2]Oak Ridge National Laboratory

The new concept of material design introduced by high entropy alloys (HEAs) combined with their promising mechanical performance has attracted significant recent research interest. However, there is still a limited number of studies focused on the fatigue behavior, particularly the mechanisms of cyclic deformation in these materials. In this work, we aim to understand the fundamental processes that induce fatigue damage in the equiatomic CrMnFeCoNi HEA using true plastic strain-controlled fully reversed low cycle fatigue (LCF) tests. The LCF results describe the evolution of the flow stress and the microstructural changes that accommodate plastic deformation during cyclic straining. After failure, observations of the polished gage sections and fracture surfaces reveal the slip characteristics, the crack path and the localized processes responsible for failure in this material. Additionally, comparisons with the LCF behavior of an austenitic stainless steel highlight the main differences in performance and cyclic deformation mechanisms.

Tensile Creep Behavior of NiCoCr and ODS-NiCoCr Multi-principal Element Alloys: *Gianmarco Sahragard-Monfared*[1]; Timothy Smith[2]; Jeffery Gibeling[1]; [1]University of California, Davis; [2]NASA Glenn Research Center

Multi-principal element alloys (MPEA) have been proven to exhibit excellent room temperature and cryogenic strength and ductility. However, MPEAs with an FCC crystal processed by arc melting generally exhibit low strengths at elevated temperatures. Alternative manufacturing processes provide an opportunity to introduce dispersoids into the matrix to improve high temperature properties. In this study the influence of oxide dispersion strengthening (ODS) on the creep behavior of an MPEA produced by additive manufacturing (AM) is investigated. AM-NiCoCr and an oxide dispersion strengthened variant containing one weight percent yttria (ODS-NiCoCr) were creep tested at 973-1173K. Stress exponents and activation energies determined from these tests highlight the differences in deformation mechanisms of these MPEAs. Transmission electron microscopy of specimens crept to steady state was used to characterize the morphology of dislocations and their interactions with other dislocations and dispersoids. These results were compared to recent creep results for a CrMnFeCoNi MPEA.

CALPHAD Database Development and Optimization of Refractory-HEAs: *Aurelien Perron*[1]; Vincenzo Lordi[1]; Joel Berry[1]; Brandon Bocklund[2]; Richard Otis[3]; Alexander Landa[1]; Charles Tong[1]; Amit Samanta[1]; Hunter Henderson[1]; Zachary Sims[1]; Thomas Voisin[1]; Scott McCall[1]; Joseph McKeown[1]; [1]Lawrence Livermore National Laboratory; [2]Pennsylvania State University; [3]Jet Propulsion Laboratory, California Institute of Technology

Refractory high-entropy alloys (RHEAs)–encompassing refractory multi-principal element and complex concentrated alloys–are gaining attention as structural materials due to their promising high-temperature properties. However, the fundamental understanding of the complex behavior of RHEAs remains unclear, leading to inefficient design of new high-performance RHEAs. One criterion to be considered during alloy optimization is the phase stability (solid solutions, long/short-range order, miscibility gap, Laves phases, etc.), since properties stem from microstructure and thus phase composition of the alloy. We will present CALPHAD assessments with uncertainty quantification of binary systems from groups 5-6 elements {V, Nb, Ta, Mo, W} based on literature review and new experimental and ab initio data. Extrapolations to multicomponent systems for RHEAs will be discussed with a focus on bcc miscibility gaps and ordering. Finally, TAOS (The Alloy Optimization Software) will be presented, with RHEA optimization used as a case study. Prepared by LLNL under Contract DE-AC52-07NA27344.

Wednesday Plenary

Wednesday AM
December 8, 2021
Place

Room: University Ballroom CDE
Location: Hilton Charlotte University

Session Chair: To Be Announced

Introductory Comments

Plenary

Materials Systems Consideration in Design of High Entropy Alloys: *Elsa Olivetti*[1]; [1]Massachusetts Institute of Technology

We suggest applying a lens of practicality to high entropy alloy design related to alloy economics and resource usage issues. A framework for HEA materials selection could assist the metallurgical community in screening for HEAs with feasible implementation possibilities by identifying unsuitable alloying elements based on price or metrics of supply availability. For some metrics, such as price volatility, the elemental diversification in HEAs could prove beneficial, while for others, such as recyclability, elemental breadth introduces significant challenges.

Break

Session XI

Wednesday PM
December 8, 2021
Place

Room: University Ballroom AB
Location: Hilton Charlotte University

Session Chair: To Be Announced

Introductory Comments

Invited

Defining Pathways for Realizing the Revolutionary Potential of High Entropy Alloys: A Science & Technology Accelerator Study: *Dan Miracle*[1]; George Spanos[2]; [1]Air Force Research Laboratory, Wright-Patterson Air Force Base; [2]The Minerals, Metals, and Materials Society

Since their discovery less than twenty years ago, High Entropy Alloys (HEAs) have demonstrated exciting new property combinations. However, due to the vast array of possible combinations of elements, processing conditions, and microstructures, HEAs are still in the infant stages of identifying specific pathways toward direct implementation/application. Thus, on behalf of the Defense Advanced Research Projects Agency (DARPA) and the Air Force Research Laboratory (AFRL), The Minerals, Metals & Materials Society (TMS) has led a science and technology (S&T) accelerator study on HEAs. This study (1) prioritizes application and alloy domains of most promise, particularly for defense-related applications, (2) identifies key needs, barriers, and enablers of the next stage of HEA research and development, and (3) defines critical pathways and provides recommendations and detailed action plans to realize the revolutionary potential of HEAs. This presentation will provide key highlights from this recently completed HEA S&T accelerator study.

Probing the Property Design Space of Ti-V-Nb-Hf Refractory High-entropy Alloys via Al-alloying: *Shaolou Wei*[1]; Cem Tasan[1]; [1]Massachusetts Institute of Technology

Owing to their excellent yield strength preservation at elevated temperatures, refractory high-entropy alloys (RHEAs) have drawn increasing attention in seeking optimal mechanical performances and exploring the underlying physical foundations. However, the apparent brittleness at ambient temperature, the necessity of extensive thermo-mechanical processing, and the presence of catastrophic oxidation, still remain as serious challenges. Following the natural mixing tendency amongst all refractory elements, our previous study has detailed the exploration of a Ti-V-Nb-Hf RHEA family that exhibits promising tensile ductility at room temperature. In this presentation, we will expand the property design space of this RHEA system via Al alloying, aiming to address the following three topics: (1) how much intrinsic strengthening (or softening) is associated with Al alloying? (2) how will dislocation plasticity micro-mechanisms vary in response to Al alloying? and (3) how does Al modulate the phase stability and thereby precipitation pathways at intermediate temperatures?

Processing Pathways and Tensile Ductility of Polycrystalline Refractory Multi-principal Element Alloys: *Leah Mills*[1]; Jean-Charles Stinville[1]; Marie-Agathe Charpagne[1]; Carolina Frey[1]; Noah Philips[2]; Valéry Valle[3]; Daniel Gianola[1]; Tresa Pollock[1]; [1]University of California-Santa Barbara; [2]ATI Specialty Alloys and Components; [3]Institut PPRIME Université de Poitiers

The high temperature strength of Refractory Multi-Principal Element Alloys (RMPEAs) is promising for extreme structural applications but presents challenges for thermomechanical processing of this class of materials. This motivates novel methods of generating thin film and bulk specimens for evaluation of ambient temperature tensile ductility, including splat quenching and hot compressing arcmelted specimens using a spark plasma sintering system. Microstructure development along these processing paths and the mechanical performance of the RMPEAs HfNbTaTiZr and MoNbTi are investigated. Characterization of plastic deformation in these polycrystalline materials by High-Resolution Digital Image Correlation (HR-DIC) is employed to investigate the heterogeneity of dislocation slip on a grain-to-grain basis and locally at the scale of individual slip traces as well as its relationship to macroscopic tensile properties.

Accelerated Development of Refractory Multi-principal Element Alloys via Machine Learning: *Carolina Frey*[1]; Christopher Borg[2]; James Saal[3]; Bryce Meredig[3]; Noah Philips[4]; Tresa Pollock[1]; [1]University of California Santa Barbara; [2]Citrine Informatics ; [3]Citrine Informatics; [4]ATI Specialty Alloys and Components

Refractory Multi-principal Element Alloys (RMPEAs) present an opportunity for new high temperature alloys that can operate at temperatures above 1200˚C, but they remain relatively underexplored compared to other MPEA categories due to processing challenges. Machine learning methods have the potential to reduce the number of needed experiments and more efficiently discover interesting materials demonstrating both high temperature strength and room temperature ductility. This presentation will discuss the use of random forest machine learning algorithms in concert with CALPHAD and rapid processing techniques to guide sequential alloy design. Predictive models for room temperature, 1000˚C and 1200˚C yield strengths are presented. Hf-Mo-Nb-Ta-Ti was identified as a potentially high performing system. Compressive mechanical properties of as-cast alloys at room and high temperature in this system are reported, and the effect of iteration on model fidelity is discussed. Splat quenched foils were utilized to reduce segregation and grain size to probe potential tensile ductility.

Microstructural and Mechanical Evolutions of a Ti-V-Nb-Ta Refractory High-entropy Alloy during Thermal Aging: *Junliang Liu*[1]; Bo-Shiuan Li[1]; Hazel Gardner[1]; Guanze He[1]; David Armstrong[1]; Angus Wilkinson[1]; [1]University of Oxford

The equiatomic Ti-V-Nb-Ta is one of the few single-phase BCC refractory high-entropy alloys (RHEA) which exhibits considerable potentials for applications in fast reactor environments. In this study, we have used a combination of state-of-the-art microscopes (Transmission Electron Microscopy, Transmission Kikuchi Diffraction, Electron Energy Loss Spectroscopy and Atom Probe Tomography) and nano-indentation technique to characterise the microstructural and mechanical evolutions of a Ti-V-Nb-Ta RHEA during diffusion annealing and thermal aging. Microstructural analysis shows the homogenisation of the as-cast alloy can be achieved when it underwent diffusion annealing at 1500˚C for 72 hrs, with an increase of the hardness from 4.1 GPa to 5.1 GPa. However, the hardness of the homogenised alloy was observed to decrease with increasing aging time at 700˚C. Based on the microstructural and microchemical analysis, a mechanism describing the age softening phenomenon via oxygen-assisted phase segregation in the Ti-V-Nb-Ta RHEA was proposed.

Break

High-pressure Induced Phase Transitions of a Metastable Complex Concentrated Alloy System with Varying Stacking Fault Energies: *Christopher Reynolds*[1]; Alden Watts[1]; Marcus Young[1]; Rajiv Mishra[1]; Dean Smith[2]; Dmitry Popov[2]; Jeffrey Lloyd[3]; [1]University of North Texas; [2]Advanced Photon source, Argonne National Laboratory; [3]US Army Research Laboratory

The ability to decrease the stacking fault energy (SFE) in metastable complex concentrated alloys (CCAs) has led to the development of twinning induced plasticity (TWIP) and/or transformation induced plasticity (TRIP) CCAs. One such TRIP-CCA system of interest is the $Fe_{(40-x)}Mn_{20}Cr_{15}Co_{20}Si_5Cu_x$, where x varies from 0.0 to 3.0 at. %. The purpose of our study is to investigate of the high-pressure phase transformation of the γ-f.c.c. to the ε-h.c.p. as function of the SFE and to explore the phase compatibility at the interfaces. In this study, the high-pressure mechanical response of the base alloy, $Fe_{40}Mn_{20}Cr_{15}Co_{20}Si_5$, is compared to the response of alloys with a Cu content of 1.5 and 3.0 at.% using a diamond anvil cell experiment coupled with synchrotron radiation X-ray diffraction. In addition to identifying the critical pressure for phase transformation, the stability of the ε-h.c.p. phase upon decompression is investigated. Results are compared with microstructural observations.

Boron Addition in a Non-equiatomic Fe50Mn30Co10Cr10 Alloy Manufactured by Laser Cladding: Microstructure and Wear Abrasive Resistance: *Jose Yesid Aguilar Hurtado*[1]; Alejandro Vargas-Uscategui[2]; Katherine Paredes-Gil[3]; Maria Jose Tobar[4]; Jose Manuel Amado[4]; [1]University of Chile; [2]CSIRO-Manufacturing ; [3]Metropolitan Technological University; [4]University of A Coruña

Fe50Mn30Co10Cr10 High-Entropy Alloy was prepared by laser cladding on a stainless steel 316L. The effects of boron addition on the microstructure, hardness and abrasive wear-resistance were investigated. The coatings were exposed to abrasive wear conditions using the dry sand/rubber wheel test. The microstructure of the laser claddings exhibited columnar dendrites formed by a dual phase (FCC+HCP) with the same chemical composition. The HCP structure was the result of the partial martensitic transformation of the FCC structure. Boron addition led to the segregation of a eutectic phase into interdendritic regions containing lath M2B borides. When boron content was increased from 0 at% to 5.40 at% the microhardness of the material was from 291 HV to 445 HV. Similarly, the boron content improved the behavior against abrasive wear by more than 30% when is compared with the alloy without boron content due to the increased volume fraction of borides in the microstructure.

In-situ X-ray and Thermal Imaging of Refractory High Entropy Alloying during Laser Directed Deposition: Hui Wang[1]; Benjamin Gould[2]; Michael Moorehead[3]; Marwan Haddad[1]; Adrien Couet[3]; *Sarah Wolff*[3]; [1]Texas A&M University; [2]Argonne National Laboratory; [3]University of Wisconsin–Madison

MoNbTiV high-entropy alloy was in-situ alloyed by laser power-blown directed energy deposition additive manufacturing from a mixture of four elemental powders of Mo, Nb, Ti, and V. This study aimed at providing a fundamental understanding of the alloying process through the in-situ high-speed synchrotron X-ray imaging and infrared camera. High-speed X-ray imaging was applied for investigating the in-situ alloying process through direct observation. The particle delivery velocities of four different elemental powders under the same processing conditions were studied to reveal the performance of different elemental powders during the in-situ alloying process. The velocities of the melt pool flow showed the melt flow dynamics in such a process. The residence time of each elemental powder could be also obtained. With the assistance of an infrared camera, we reported the thermal gradient and cooling rates on the melt pool surface, the change of thermal properties, and melt pool morphology during alloying.

High-throughput First-principles Design and Screening of Additively Manufactured Corrosion-resistant HEA: *Santanu Chaudhuri*[1]; Dan Thoma[2]; Xiaoli Yan[3]; Phalgun Nelaturu[2]; Thien Duong[1]; [1]Argonne National Laboratory; [2]University of Wisconsin; [3]University of Illinois at Chicago

The composition space of high-entropy alloys is increasing in complexity. It is hard to mine for meaningful correlations in corrosion vulnerability. We made progress in first principles estimation of phase stability in high temperatures, the free-energy of corrosion reactions, and work-function based analysis of corrosion vulnerability. Additively manufactured HEAs provide an exciting experimental high-throughput screening route when coupled to CALPHAD modeling to reduce the size of possible compositions. We will discuss our closed-loop approach between our model and printing for the design of experiments. Our inputs from calculated data are surface energy, work-function, mobility, and stability of the phases. A combined Bayesian uncertainty quantification for predicting a single-phase alloy, corrosion vulnerability, and printing conditions can provide valuable insight for alloy design. In addition, we will discuss work-function and hardness correlations for Fe-Ni-Mn-Cr HEAs.

Session XII

Wednesday PM
December 8, 2021
Place

Room: University Ballroom CDE
Location: Hilton Charlotte University

Session Chair: To Be Announced

Introductory Comments

Corrosion and Passivation of Multi-principal Element Alloys in Aqueous Solutions: *John Scully*[1]; Angela Gerard[1]; Samuel Inman[1]; Debashish Sur[1]; [1]University of Virginia

Multi-principal element alloys (MPEAs) offer the possibility of considerable degrees of freedom in the choice of alloying elements to produce either single or multi-phase solid solution alloys. A wide range of material properties, sometimes unique, have been observed based on the alloying elements selected and microstructures developed. However, a structure, composition, and processing paradigm governing the corrosion properties of MPEAs have not yet emerged. The quest for superior corrosion properties requires an understanding of the fate of each element during corrosion and its subsequent functions. Gaps in knowledge exist regarding the (a) specific functions of each element, (b) effects of elements in unusual combinations, and (c) possible formation of complex protective oxides which regulate corrosion and breakdown. These issues are discussed with the goal of accelerating the understanding of the corrosion behavior in this class of materials.

High-throughput Oxidation of Additively Manufactured Refractory High Entropy Alloys: *Michael Niezgoda*[1]; Michael Moorehead[1]; Chuan Zhang[2]; Adrien Couet[1]; Dan Thoma[1]; [1]University of Wisconsin-Madison; [2]Computherm LLC.

The Optomec LENS MR7 was used for a high throughput (HT) fabrication of twenty-five sample array with varying compositions of six elements: Tantalum, Niobium, Molybdenum, Titanium, Chromium, and Aluminum. With a unified set of build parameters, all twenty-five samples were built up to approximately one centimeter cubed to provide sufficient surface area for meaningful oxidation testing. After printing, samples were ground to a common level and given a homogenization treatment of 1500C for 24 hours in an ultra-high vacuum furnace. Prior to oxidation, EDS mapping and XRD analysis was performed, and the samples showed uniform compositions of mostly BCC character. High-Throughput oxidation was carried out at 1000 degrees Celsius for three hours in a continuously refreshed dry air atmosphere. Samples displayed a wide range of protective capabilities on a single plate, permitting rapid interrogation methodology of many alloys for oxidation resistance of designed refractory HEA's influenced by thermodynamic simulation.

Suppression of Disorder in High Entropy Oxides: *Abhishek Sarkar*[1]; Benedikt Eggert[2]; Ralf Witte[3]; Johanna Lill[2]; Leonardo Velasco[3]; Qingsong Wang[3]; Janhavika Sonar[3]; Katharina Ollefs[2]; Subramshu Bhattacharya[4]; Frank de Groot[5]; Richard Brand[2]; Heiko Wende[2]; Oliver Clemens[6]; Horst Hahn[3]; Robert Kruk[3]; [1]Technical University Darmstadt; [2]University of Duisburg-Essen; [3]Karlsruhe Institute of Technology; [4]Indian Institute of Technology Madras; [5]Utrecht University; [6]University of Stuttgart

Utilization of configurational entropy for designing novel functional oxides started with the discovery of high entropy oxides (HEOs). HEOs have already received enormous attention owing to the wide variety of compositions, crystallographic structures and distinctive properties. Hitherto reports have always considered random and non-preferential ionic arrangements in HEOs. However, recent case studies on high entropy alloys have shown that the deviation from complete disorder can substantially improve their properties. However, this aspect of fundamental importance remains unexplored in HEOs. This work provides a direct experimental evidence for extremely preferential cationic arrangement in a model spinel-HEO (S-HEO), in contrast to the previous reports that always assumed random occupation. To unambiguously unravel the cationic occupation in chemically-complex S-HEO a combined and cross-referenced spectroscopy, diffraction and magnetometery approach is followed here. The study highlights the importance of enthalpy parameters in HEOs as the occupation model indicates the state with the least configurational disorder.

Multi-component Rare Earth Silicates for Dual Purpose Thermal/Environmental Barrier Coatings: Mackenzie Ridley[1]; Cameron Miller[1]; David Olson[1]; Kathleen Tomko[1]; Alejandro Salanova[1]; Patrick Hopkins[1]; Jon Ihlefeld[1]; Cormac Toher[2]; *Elizabeth Opila*[1]; [1]University of Virginia; [2]Duke University

SiC ceramic matrix composites (CMCs) for application in turbine engine hot sections require environmental barrier coatings (EBCs) to prevent thermochemical reactions with the combustion environment. Dual-purpose thermal/environmental barrier coatings (T/EBCs) are proposed materials to decrease operating temperatures and oxidation rates of the underlying CMC and the required silicon bond coat. Multi-component rare earth silicates represent T/EBC candidates through their low thermal conductivities compared to single rare earth cation silicate materials. The phase stability, thermal expansion coefficient (CTE), and high-velocity steam reactivity of multi-component rare earth silicates were analyzed. Phase stabilization of low-CTE polymorphs desired for EBCs and tailoring of steam reaction products will be addressed.

Synthesis and Evaluation of High Entropy Perovskite Oxides as Solid Oxide Fuel Cell Cathodes: Zhongqiu Li[1]; Wenyuan Li[1]; Bo Guan[1]; Wei Li[1]; Liang Ma[1]; *Xingbo Liu*[1]; [1]West Virginia University

Perovskites have been the predominant materials for solid oxide fuel cells (SOFCs)cathodes. In this study, a wide range of equimolar A (La, Sr, Ba, Pr, Gd, Y, Sm, Nd) and/or B (Cr, Mn, Fe, Co, Ni) site elements have been screened in the ABO3 formula to synthesize perovskite-structured high-entropy oxides for the application as SOFCs cathode. XRD, TEM, XPS, and ICP-MS have been applied to investigate the phase structure and chemical composition of samples prepared by different routes. 6 out of 13 formulas are formed with high-entropy perovskite structure. The electrochemical evaluation shows that some of these specimens display improved performance, stability and/or tolerance toward CO2 under typical SOFCs operation conditions when compared to the benchmark LSCF cathode. These findings suggest a great promise to use high entropy perovskites to tackle the stability and performance issues of current cathode candidates, and encourage further refinement on the current equimolar composition design.

Break

Nanoscale Origins of Passivation in a Refractory High Entropy Alloys: *Elaf Anber*[1]; David Beaudry[1]; Daniel Foley[1]; Lavina Backman[2]; Keith Knipling[3]; Elizabeth Opila[2]; Jean Philippe Couzinié[4]; Mitra Taheri[1]; [1]Johns Hopkins University; [2]University of Virginia; [3]Naval Research Laboratory; [4]University Paris-Est Créteil (UPEC) - IUT

Refractory high entropy alloys (RHEAs) are being targeted for high-temperature applications, such as aerospace industries, due to their high melting temperature, and promising combination of high strength and low ductility. A key challenge in the advancement of RHEAs is maintaining high temperature stability and oxidation resistance. Here we describe the recent progress of oxide evolution studies of an AlxHfNbTiTaZr (x=0.0,0.25, and 0.75) RHEA in high temperature environments. In this study, the role of Al addition on oxide structure, evolution, and complexity was studied using theoretical calculations coupled with phase and orientation analysis using precession electron diffraction techniques. Overall, the work described provides a foundation for understanding the oxide stability window for candidate RHEAs in extreme environments. These results are discussed in the context of the growing literature comparing the ideal methods for passivation mechanisms in complex alloys for use in high temperature, corrosive environments.

Investigating the Internal Oxidation of a Refractory High Entropy Alloy: *Indranil Roy*[1]; Eric Osei-Agyemang[1]; Ganesh Balasubramanian[1]; [1]Lehigh University

High entropy alloys (HEAs) are primarily used as structural materials and are exposed to oxidizing environments in such applications. This may result in catastrophic failure for the intended purposes. Detailed knowledge in understanding the mechanism of internal oxidation is needed to fine-tune the materials for better performance. We examine the reaction and diffusion process during internal oxidation of a refractory HEA using first principle ab initio methods in combination with atomistic thermodynamic modeling. In addition, we examined the effect of varying metal compositions on the different oxides formed from the alloy at different temperatures.

Elevated-temperature Creep Properties and Deformation Mechanisms in a CrMnFeCoNi High-entropy Alloy: *Mingwei Zhang*[1]; Easo George[2]; Jeffery Gibeling[1]; [1]University of California, Davis; [2]Oak Ridge National Laboratory

Despite the abundance of cryogenic and room temperature studies of FCC high-entropy alloys (HEAs), their elevated-temperature deformation mechanisms have not been explored in detail. In the present study, we report on the results from steady state and stress reduction creep experiments under various initial and reduced stresses. A stress exponent of 3.7 was obtained for steady state creep. The activation area for deformation of CrMnFeCoNi was measured to be approximately 100 b^2 and to decrease with increasing applied stress, indicating the presence of both concentrated solid solution and forest dislocation control. Quantitative separation of the two mechanisms was carried out using a Haasen plot, which shows that creep in CrMnFeCoNi relies heavily on thermal activation and the majority of creep strength comes from solid solution hardening. The analysis reveals that steady-state creep deformation of CrMnFeCoNi can be adequately described by existing concentrated solid solution hardening and forest dislocation hardening models.

Design of Low Cost Compositionally Complex Alloys (CCAs) with Excellent Corrosion Resistance: *Samuel Inman*[1]; Jie Qi[1]; Mark Wischhusen[1]; Carol Glover[1]; Junsoo Han[2]; Sean Agnew[1]; Joseph Poon[1]; John Scully[1]; [1]University of Virginia; [2]Chimie ParisTech

This project seeks to design lightweight, low cost, compositionally complex alloys with combinations of strength, ductility, and corrosion resistance in marine environments. Corrosion resistance depends on balancing phase composition to enable natural passivation and minimize solute depletion near phase interfaces. High throughput, machine learning-based methods were used to select alloying elements favorable for synthesis based on cost, density, passivation ability, and phase stability. Alloys were synthesized, characterized, and experimentally examined for nanostructure, phase stability, and mechanical properties. Selected alloys were experimentally verified to have an FCC matrix and B2 secondary phase regions with XRD. Potentiodynamic polarization experiments were performed in dilute NaCl solutions of varying concentrations and pH. Passive film compositions were investigated with ex-situ XPS. Corrosion resistance surpassing stainless steel may be attributable to Al, Cr, and Ti enriched oxide formation. Single-element composition adjustments suggested trade-offs between improving corrosion resistance and promoting microstructural stability, establishing foundations for compositional optimization.

A High Throughput Closed Loop for the Study of High Entropy Oxides: *Leonardo Velasco estrada*[1]; Juan Castillo[2]; Kante Veerraju[1]; Jhon Olaya[2]; Pascal Friederich[1]; Horst Hahn[1]; [1]Karlsruhe Institute of technology; [2]Universidad Nacional de Colombia

The chemical deviations of high entropy materials (deviations from the equiatomic amounts) offer a vast compositional-structural space. However, exploring such compositional space using traditional approaches, one experiment at a time, is prohibitively costly and time consuming. Here, we present a high throughput synthesis and characterization, coupled with machine learning techniques of high entropy oxides. The results are presented in a multicomponent phase-property diagram (material library), integrating the compositional space with the crystallographic structures and the landscape of a given property. The high throughput loop is closed by selecting specific chemical variations to optimize materials properties, leading to iterative suggestions for the synthesis and characterization steps. The establishment of materials libraries of high entropy materials and multicomponent systems correlated with their properties, together with machine learning based data analysis opens a pathway towards virtual development of novel materials.

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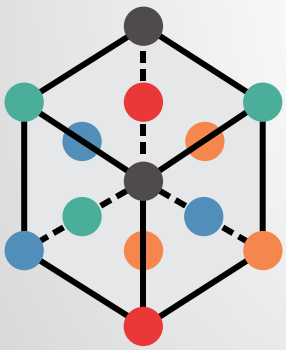

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