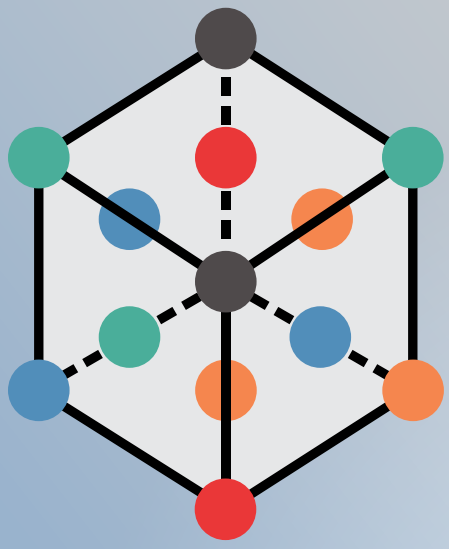

3rd WORLD CONGRESS ON

HIGH ENTROPY ALLOYS

HEA2023

November 12-15, 2023

Omni William Penn Hotel, Pittsburgh, Pennsylvania, USA

PRELIMINARY TECHNICAL PROGRAM

These sessions are current as of September 20, 2023. For an up-to-date technical presentation schedule, please refer to the online session sheets at www.tms.org/HEA2023.

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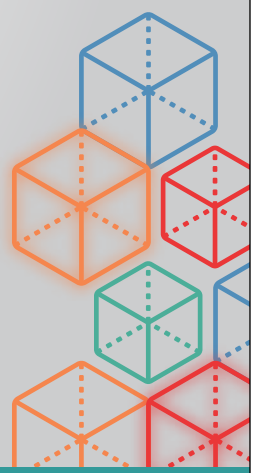

www.tms.org/HEA2023

SCHEDULE AT A GLANCE

Schedule subject to change. Current as of September 14, 2023.

Sunday, November 12	Time	Location
Registration	4:30 PM - 6:30 PM	William Penn Corridor
Welcome Reception	5:30 PM - 6:30 PM	Sternwheeler
Monday, November 13	**Time**	**Location**
Registration	7:00 AM - 6:30 PM	William Penn Corridor
Poster & Exhibit Installation	7:30 AM - 10:30 AM	Sternwheeler
Plenary Session	8:00 AM - 9:00 AM	William Penn Ballroom
Technical Sessions	9:00 AM - 12:15 PM	William Penn Ballroom, Three Rivers, Riverboat
Exhibition & Break	10:35 AM - 10:55 AM	Sternwheeler
Lunch	12:15 PM - 1:40 PM	*on your own*
Technical Sessions	1:40 PM - 5:15 PM	William Penn Ballroom, Three Rivers, Riverboat
Exhibition & Break	3:15 PM - 3:35 PM	Sternwheeler
Poster Session and Reception	5:30 PM - 6:30 PM	Sternwheeler
Tuesday, November 14	**Time**	**Location**
Registration	7:30 AM - 5:15 PM	William Penn Corridor
Plenary Session	8:00 AM - 9:00 AM	William Penn Ballroom
Technical Sessions	9:00 AM - 12:15 PM	William Penn Ballroom, Three Rivers, Riverboat
Exhibition & Break	10:35 AM - 10:55 AM	Sternwheeler
Lunch	12:15 PM - 1:40 PM	*on your own*
Technical Sessions	1:40 PM - 5:15 PM	William Penn Ballroom, Three Rivers, Riverboat
Exhibition & Break	3:15 PM - 3:35 PM	Sternwheeler
Congress Dinner	6:00 PM - 7:30 PM	Bob & Dolores Hope Room
Wednesday, November 15	**Time**	**Location**
Registration	7:30 AM - 4:30 PM	William Penn Corridor
Plenary Session	8:00 AM - 9:00 AM	William Penn Ballroom
Technical Sessions	9:00 AM - 12:15 PM	William Penn Ballroom, Three Rivers, Riverboat
Exhibition & Break	10:35 AM - 10:55 AM	Sternwheeler
Poster & Exhibit Tear-down	10:55 AM - 3:25 PM	Sternwheeler
Lunch	12:15 PM - 1:40 PM	*on your own*
Technical Sessions	1:40 PM - 3:25 PM	William Penn Ballroom, Three Rivers, Riverboat
Break	3:25 PM - 3:45 PM	Sternwheeler
Closing Plenary Session	3:45 PM - 4:35 PM	William Penn Ballroom

Monday Plenary

Monday AM **Room: William Penn Ballroom**
November 13, 2023 **Location: Omni William Penn**

Session Chair: To Be Announced

8:00 AM Introductory Comments

8:10 AM Plenary
High-entropy Alloys – A Twenty-year Perspective: *Daniel Miracle*[1]; [1]Air Force Research Laboratory

The high-entropy field is approaching its twenty-year milestone. This talk will recall the historical foundations of the field and will review the initial insights and themes as they formed and evolved over the past two decades. During the past ten years, major efforts have grown in new directions that broaden and enrich the high-entropy tapestry. These topics include refractory high-entropy alloys, high-entropy ceramic materials, chemical short-range ordering, the exploration of new high-entropy alloy families for a range of functional properties, and many others. Each of these new directions will be briefly introduced and added to the high-entropy palette. A fresh evaluation of high-entropy alloys as a distinct direction in materials science and engineering will be offered from this mid-term perspective, and a forward-looking glimpse will be suggested to inspire continued efforts and to anticipate important applications.

8:50 AM Break

Characterization of HEAs I

Monday AM **Room: William Penn Ballroom**
November 13, 2023 **Location: Omni William Penn**

Session Chair: To Be Announced

9:00 AM Introductory Comments

9:05 AM Invited
Short Range Order and the Evolution of Deformation Mechanisms in the CrCoNi Medium Entropy Alloy: *Andrew Minor*[1]; [1]University of California-Berkeley

This talk will describe our recent results utilizing electron microscopy and nanomechanical testing techniques to provide insight into multiscale deformation phenomena in the CrCoNi medium entropy alloy. In order to understand the effect of Short Range Order (SRO) in terms of the evolution of plasticity at different stages, the technique of 4D-STEM was used during in situ deformation and fracture experiments. 4D-STEM can provide both real-space imaging and diffraction analysis during in situ testing, making it possible to perform strain mapping via diffraction pattern analysis during in-situ deformation in a TEM. Our results from electron microscopy are then correlated with mechanical testing including nanoindentation to examine how SRO evolves with different processing conditions. Lastly, we will consider the role of both SRO and planar defects in the both the mechanical response as well as structural determination via electron diffraction as a function of heat treatment in the CrCoNi MEA.

9:35 AM
Multi-scale Characterization of 3D Printable CrCoNi-based ODS-MPEAs by Advanced Stereo-STEM Cross-correlated with EDS: *Milan Heczko*[1]; Timothy Smith[2]; Christopher Kantzos[2]; Veronika Mazanova[1]; Antonin Dlouhy[3]; Michael Mills[1]; [1]Ohio State University; [2]NASA Glenn Research Center; [3]Institute of Physics of Materials CAS

Our recent work (Nature, 2023) has demonstrated a new strategy to design alloys for high-temperature applications using additive manufacturing. Combining multi-principal element alloy (MPEA) and oxide-dispersion-strengthening (ODS) concepts opens up a vast unexplored compositional space to develop new 3D printable alloys. Here, we reveal the microstructural origins of the extraordinary performance of these new alloys using advanced multi-scale characterization approaches based on stereo-scanning transmission electron microscopy (STEM) cross-correlated with probe-corrected energy-dispersive X-ray spectroscopy (EDS). Stereo-STEM provides a direct and realistic 3D impression of the microstructure in a STEM foil. It enables precise measurement of local foil thickness, allowing quantitative assessment of the oxide dispersion including volume density and mean particle spacing. Combined with local defect density measurements, this approach provides detailed information about the microstructure of ODS-MPEAs. Critical aspects determining performance of 3D printable ODS-MPEAs are systematically identified and discussed.

9:55 AM
Understanding Processing Pathways for Chemical Short-range Order in Equiatomic CoCrNi Alloy: *Sakshi Bajpai*[1]; Yuan Tian[1]; Yutong Bi[1]; Xin Wang[1]; Calvin Belcher[1]; Vivek Verma[1]; Benjamin MacDonald[1]; Timothy Rupert[1]; Xiaoqing Pan[1]; Enrique Lavernia[1]; Diran Apelian[1]; [1]University Of California Irvine

The experimental detection of chemical short-range ordering (CSRO) in complex concentrated alloys (CCAs) has proven to be a difficult task. While predictions of CSRO have been well demonstrated by state-of-the-art modeling and simulation studies, there is a lack of conclusive experimental evidence regarding the evolution of CSRO in CCAs and its impact on mechanical behavior. This work systematically investigates the processing pathways that may induce CSRO in the ternary CoCrNi alloy by varying thermal treatment temperature, time, and cooling rates and characterizing the resulting microstructure. Appreciable variations in mechanical properties are established as a function of processing. Contributions to these properties are quantified with respect to various microstructural features measured through SEM EBSD as well as advanced TEM techniques. Critical considerations for the effective processing of CCAs are proposed and discussed.

10:15 AM
Towards More Robust EXAFS Analysis for Quantifying Short Range Order in Multicomponent Alloys: *Brian DeCost*[1]; Bruce Ravel[1]; Tyrel McQueen[2]; Mitra Taheri[2]; Howie Joress[1]; [1]National Institute of Standards and Technology; [2]Johns Hopkins University

Recent research has found that chemical short range order in high entropy alloys (HEAs) can play an important role on properties such as mechanical strength and corrosion resistance. EXAFS is a promising measurement technique for quantifying this aspect of local alloy structure and chemistry; however, the complexity of the models required for realistic analysis of multicomponent HEA systems poses a substantial barrier to obtaining meaningful insight. We present a principled Bayesian data analysis approach to EXAFS analysis to improve its reliability. We also show a novel approach to incorporate physical constraints into EXAFS models, with a focusing on the relationships between the short range order parameters for the different species in solid solutions. Our long term goal is automated online analysis that can drive adaptive measurement selection with the aim of enabling comprehensive understanding of the relationship between composition and short range order.

10:35 AM Break

10:55 AM

Unraveling SRO in CrCoNi and FeCrCoNi Alloys: Insights from Indirect Methods: *Francisco Coury*[1]; Vinicius Bacurau[1]; Angelo Andreoli[1]; Eric Mazzer[1]; Robert Field[2]; Michael Kaufman[2]; [1]Universidade Federal de São Carlos; [2]Colorado School of Mines

This talk will discuss the challenges of characterizing short-range order (SRO) in Multi-Principal Element Alloys (MPEAs), especially in face-centered cubic (FCC) alloys. A series of results using direct and indirect methods for characterizing SRO in CrCoNi and FeCrCoNi will be presented and compared. The indirect methods include those that measure anomalies in functional properties. The direct methods involve the use of transmission electron microscopy methods including selected area diffraction pattern analysis to assess SRO. A framework will be proposed for establishing correlations between additional intensities and the presence of SRO in MPEAs. Our goal is to provide a better understanding of the ordering tendencies in multi-principal element alloys and highlight the potential of indirect techniques to these ordering tendencies.

11:15 AM

Diffuse Electron Scattering Reveals Kinetic Frustration as Origin of Order in CoCrNi Medium Entropy Alloy: *Annie Barnett*[1]; Dan Foley[1]; Mitra Taheri[1]; Michael Falk[1]; [1]Johns Hopkins University

Equimolar CoCrNi is driven towards a long-range structure with transformation characteristics similar to that of a strain glass alloy due to the specific stoichiometry and applied aging conditions. This work illustrates the frustrated and kinetically arrested state of this alloy, which develops nano-size, single-phase, isostructural ordered domains at temperatures above 1273K within a matrix of solid solution. Upon aging at lower temperatures, both atomistic simulation and TEM investigation demonstrate the chemical sensitivity of the matrix by localized symmetry changes which suppress any long-range transformation, mirroring the kinetics observed in strain-glass alloys. Careful quantification of experimental and simulated diffraction patterns from various aging conditions reveal the degree of order in CoCrNi to increase given longer aging times, with achievement of longer domain length scales only when subjected to temperatures below 873K. This evidence indicates a kinetically constrained, chemically sensitive transition from a disordered fcc to a partially ordered, lower symmetry structure given adequate aging time and temperature. Magnetic effects on the transformation are dictated on the specific alloy stoichiometry and aging temperature, which act to amplify any effects of the glassy kinetics.

11:35 AM

On the Strain Gradient Plasticity Phenomenon in CrCoNi Medium Entropy Alloys: Mobin Vandadi[1]; *Tabiri Asumadu*[1]; Desmond Klenam[1]; Nima Rahbar[1]; Winston Soboyejo[1]; [1]Worcester Polytechnic Institute

This paper presents results of experimental and theoretical/computational study of the strain gradient plasticity phenomenon in CrCoNi medium entropy alloy (MEA). The size dependence of the mechanical properties of the as-cast, hot-rolled and heat-treated alloys were studied using the mechanistic and phenomenological theories. Numerical simulations were validated based on the experimental data across the various microstructural length scale. The hardness of the material changed as the processing methods varied. The statistically stored and geometrically necessary dislocations densities were high in the heat-treated samples than for the as-rolled and as- received conditions. The impact of processing parameters on material length and dislocation microstructure evolution are further elucidated. The underlying strain gradient plasticity mechanisms are elucidated before exploring the implications of the current results for the design of robust of low-cost medium entropy alloys structural applications.

11:55 AM

Hard Zones and Superior Mechanical Properties Produced by Dense Nanoscale Recrystallization Twins in a Single-phase Heterostructured High-entropy Alloy: *Shu-Yi Tung*[1]; Ting-En Hsu[1]; Yuntian Zhu[2]; Ming-Hung Tsai[1]; [1]National Chung Hsing University; [2]City University of Hong Kong

Heterostructured high-entropy alloys (HSHEAs) integrate two innovative concepts in metallic materials that encompass alloy design and microstructural engineering. HSHEAs have demonstrated outstanding mechanical properties. However, the exploration of these materials remains challenging due to the intricate nature of their composition and microstructure. In this study, we introduced a heterostructure into a single-phase FCC HEA through cold rolling and partial recrystallization. This process resulted in an exceptionally high density of nanoscale recrystallization twins, leading to significant hardening and the formation of heterogeneous hard zones within the recrystallized regions. This tri-modal heterostructure induces secondary hetero-deformation-induced hardening, which sustains larger stable tensile plasticity, i.e. higher ductility. As a result, the alloy exhibits enhanced strength and ductility, yielding superior mechanical properties. The identification of the recrystallized hard zones is crucial for gaining a proper understanding of the hetero-zones in HEAs and provides valuable insights for the future design of HSHEAs.

Processing, Microstructure, and Properties of HEAs I

Monday AM **Room: Three Rivers**
November 13, 2023 **Location: Omni William Penn**

Session Chair: To Be Announced

9:00 AM Introductory Comments

9:05 AM Invited

Phase Stability and Tensile Properties of Refractory High-entropy Alloys: *Easo George*[1]; [1]University of Tennessee and Ruhr University Bochum

We investigated the phase stability of the VNbMoTaW and TiZrNbHfTa quinaries and their equiatomic quaternary, ternary, and binary subsets after long-term anneals at 1200-800 °C for 3-300 days. The propensity for forming single-phase solid solutions increased with increasing annealing temperature (vibrational entropy) but there was no correlation with increasing configurational entropy. There was good correlation between the number of BCC constituent elements and single BCC solid solutions, consistent with the Hume-Rothery crystal-structure criterion for extensive solid solubility. We also investigated the mechanical behavior of several pseudo-binary subsystems of the Ti-Zr-Hf-Nb-Ta alloy in which pairs of elements were varied while the concentrations of the remaining three constituent elements were kept constant. Only compositions resulting in singe-phase BCC solid solutions at room temperature were considered. The roles of shear modulus, melting point, and volume misfit on their room-temperature tensile properties (strength and ductility) will be discussed.

9:35 AM

Microstructure and Deformation Behavior of a MoReW Medium Entropy Alloy: *Oleg Senkov*[1]; Satish Rao[1]; Glenn Balbus[2]; Robert Wheeler[3]; [1]MRL Materials Resources LLC; [2]Air Force Research Laboratory; [3]UES, Inc.

Microstructure and mechanical properties of an equiatomic MoReW alloy, which has demanding combination of strength and ductility in the temperature range of 25˚C to 1200˚C, are reported. The alloy has a weak temperature dependence of yield stress resulting in remarkably good yield stress retention at high temperatures, and it shows strong strain hardening. Extensive deformation twinning occurred at the beginning of deformation and activation of other deformation modes at later deformation stages in this temperature range. To understand and explain the observed behaviors of the alloy, a detailed analysis of strengthening mechanisms associated with screw and edge dislocation glide, as well as with twin nucleation and propagation, has been conducted and reasonable qualitative models of yielding, strain hardening and ductility of the studied MoReW alloy have been proposed.

9:55 AM

Thermo-mechanical Processing of Refractory Multi Principal Element Alloys: *Nathan Peterson*[1]; Benjamin Ellyson[1]; Adira Balzac[1]; Nelson De Campos Neto[1]; Kester Clarke[1]; Amy Clarke[1]; [1]Colorado School of Mines

Refractory multi-principal element alloys (RMPEAs) have been identified as having potential for new alloy and microstructural designs for ultra-high temperature applications (≥1473 K, or 1200 °C), due to their high melting points compared to traditional Ni-base superalloys. Since large-scale production of RMPEAs will inevitably require the use of thermo-mechanical processing to control final microstructural conditions, it is important to ellucidate *processing-structure-property* relationships to identify potential manufacturing-relevant processing windows. Here we study two unique systems: an off-equiatomic NbTiZr-based RMPEA, $Nb_{26}Ti_{23}Zr_8V_{20}Mo_{23}$ and a ternary system, MoNbV. An evaluation of the strength and workability was performed up to 1300 °C using a Gleeble 3500 thermo-mechanical simulator at various strain rates (10^{-3} to 10 s^{-1}). In the off-equiatomic NbTiZrVMo alloy, discontinuous and continuous dynamic recrystallization was observed at 1000 °C and 1200 °C, respectively, under quasi-static strain rates. In MoNbV, only discontinuous dynamic recrystallization was observed at 1300 °C under quasi-static strain rates.

10:15 AM

ULTIMATE: Advanced Manufacturing of Refractory Complex Concentrated Alloy-based Composites: *Xingbo Liu*[1]; Xin Chen[2]; Fei Wang[2]; Bai Cui[2]; Michael Gao[3]; Shanshan Hu[1]; Dongsheng Li[4]; [1]West Virginia University; [2]University of Nebraska-Lincoln; [3]National Energy Technology Lab; [4]Advanced Manufacturing LLC

To develop new refractory alloys and composites that can be used as blade materials for turbine engine operated at 1300C, refractory complex concentrated alloys (RCCAs) were designed and experimentally fabricated and tested. A large number of new compositions of the single-phase RCCAs were designed based on the high throughput computational design. Experimental verification of these RCCAs was conducted by arc melting, spark plasma sintering, and laser power bed fusion. Mechanical properties, including yield strength, ductility, hardness, and creep properties, were measured at both room temperature and high temperatures. Optimized RCCA compositions with a combination of excellent mechanical properties were selected based on the experimental and simulation results. The mechanical properties of RCCAs were enhanced by the second phase of high entropy carbides.

10:35 AM Break

10:55 AM

Tensile Creep Behavior of a Nb45Ta25Ti15Hf15 Refractory High-entropy Alloy: Gianmarco Sahragard-Monfared[1]; Calvin Belcher[2]; *Mingwei Zhang*[3]; Cheng Zhang[2]; Andrew Minor[3]; Diran Apelian[2]; Enrique Lavernia[2]; Jeffery Gibeling[1]; [1]University of California, Davis; [2]University of California, Irvine; [3]Lawrence Berkeley National Laboratory

The tensile creep behavior of a plasma arc-melted and cold-rolled Nb45Ta25Ti15Hf15 refractory high entropy alloy was investigated at temperatures ranging from 1123-1223 K and constant true stresses ranging from 50-300 MPa. A stress exponent of 1.2 was observed at low applied stresses, while at high applied stresses, the exponent was 5.7. TEM analysis on creep samples interrupted at steady-state deformation revealed the control of long straight screw dislocation motion, contrary to the conventional power-law creep interpretation. The creep data was better described by an exponential equation, indicating thermally activated glide of screw dislocations. Samples that crept at lower applied stresses and longer time were affected by phase decomposition and Hf-oxide formation at grain boundaries, reducing creep ductility and life. Under higher applied stresses, Nb45Ta25Ti15Hf15 exhibited superior creep resistance and excellent creep ductility compared to TiNbHfZrTa (Senkov alloy) and FCC MPEAs.

11:15 AM

Thermomechanical Processing Maps and Microstructure Characterization of Cr-containing Refractory Complex Concentrated Alloys: *Nelson Delfino De Campos Neto*[1]; John Rotella[2]; Todd Butler[2]; Samuel Kuhr[2]; Matthew Snyder[3]; Nathan Peterson[1]; Benjamin Ellyson[1]; Francisco Coury[4]; Kester Clarke[1]; Amy Clarke[1]; [1]Colorado School Of Mines; [2]Air Force Research Laboratory; [3]ARCTOS Technology Solutions; [4]Federal University of São Carlos

Refractory complex concentrated alloys (RCCAs) are a new class of metallic alloys under development for high-temperature performance. Cr-containing RCCAs can present a good combination of mechanical properties, suitable oxidation resistance, and perhaps even be compatible with coatings. Unlike single-phase, body centered cubic (BCC) RCCAs, these alloys tend to contain multiple phases, depending upon the constituent elements. For example, CrNb, CrNbTi, and CrNbTaTi RCCAs containing BCC + Laves (C15) phases have revealed promising mechanical properties and oxidation behaviors up to 1200 ˚C. But, the reduced ductility at room temperature and the sluggish diffusion leading to microstructural inhomogeneities still need to be overcome to produce consistent microstructures in bulk. Significant opportunity exists to tailor the microstructures and properties of multiphase Cr-containing RCCAs by thermomechanical processing. Here we report our recent progress in the development of thermomechanical processing maps and microstructural characterization of Cr-containing RCCAs for high-temperature applications.

11:35 AM

Quasi-static Mechanical Response and Microstructure Analysis of Tantalum-tungsten Alloys: *Charles Smith*[1]; Nathan Peterson[1]; Joseph McKeown[2]; Sharon Torres[2]; Kester Clarke[1]; Amy Clarke[1]; [1]Colorado School of Mines; [2]Lawrence Livermore National Laboratory

Ta-W alloys serve as structural alloys for high-temperature and corrosive environments. Renewed interest in refractory alloys for performance in extreme environments, including the development of refractory multi-principal element alloys (RMPEAs), is driving new investigations into the mechanical response of refractory alloys like Ta-W during quasi-static deformation to understand the microstructural response and inform alloy-microstructure-property design. Toward this aim, quasi-static tension testing has been performed at room and elevated temperatures on wrought Ta-10W (wt.%), along with microstructural characterization after deformation. Baselining the microstructure and mechanical response to quasi-static mechanical testing is needed to better understand the deformation mechanisms in Ta-W alloys, and to provide insights into the development of novel RMPEAs for aerospace, defense, and nuclear applications.

11:55 AM

Effect of Al and Ti Addition on the Strain Hardening Behavior of Non-equiatomic CoCrFeNi High Entropy Alloy: *Bushra Harun*[1]; E-Wen Huang[2]; An-Chou Yeh[2]; Suresh Neelakantan[1]; Jayant Jain[1]; [1]Indian Institute of Technology Delhi; [2]National Tsing Hua University

Near-equiatomic multicomponent systems have proven effective in achieving remarkable mechanical properties. This inspired researchers to comprehend the reason for their exceptional behavior and to analyze processes that would further enhance their properties. Precipitation strengthening is one such viable process. This study examined four precipitation hardenable high entropy alloy systems, AlxCo1.5CrFeNi1.5Tiy, where x = 0, 0.2, 0.3, 0.5, and x + y = 0.5 in molar ratios. Their strain hardening behavior, considering tensile testing, was analyzed in solutionized and peak-aged conditions using TEM, highlighting the microstructural influence of Al and Ti additions and precipitates formed in these systems. The results indicate increased Ti content and precipitation of different phases (B2 and L12) lead to enhanced strain hardening. However, Al addition provides improved ductility. The formation of complex dislocation substructures like Taylor lattices and stacking faults is observed in these systems.

Oxidation and Corrosion of HEAs I

Monday AM **Room: Riverboat**
November 13, 2023 **Location: Omni William Penn**

Session Chair: To Be Announced

9:00 AM Introductory Comments

9:05 AM Invited

Nb2TiO7 as a Protective Oxide for Refractory Alloys: *Elizabeth Opila*[1]; Charlie Brandenburg[1]; Brandol Galicia[1]; Hailey Boyd[1]; Mitra Taheri[2]; [1]University of Virginia; [2]Johns Hopkins University

Oxidation of NbTiZr refractory alloys are being studied as a model for refractory multiple principal element alloys (RMPEA). Oxidation of equimolar NbTiZr at temperatures between 900 and 1200C resulted in the formation of TiO2 and Nb2TiO7 surface oxides. In the 1960s, alloy B-1 (Nb-15Ti-10Ta-10W-3Al-2Hf, in wt%) was identified as a relatively oxidation resistant Nb-base alloy and it was hypothesized that the formation of Nb2TiO7 offered some protection. In this study oxidation kinetics of equimolar NbTiZr, C-103, and alloy B-1 are compared under the same conditions. In addition, the complex oxide Nb2TiO7 was synthesized from constituent oxides by spark plasma sintering to characterize properties important for protective thermally grown oxides including melting temperature and thermal expansion coefficient. The goal of this work is to contribute to our understanding of Nb- and Ti-containing RMPEA oxidation mechanisms.

9:35 AM

Electrochemical Technique to Characterize the High Temperature Oxidation Behavior of Materials: *Koen Verrijt*[1]; David Poerschke[1]; [1]University of Minnesota Twin Cities

Oxidation limits the lifetime of many materials in high temperature applications. Developing more durable materials requires detailed understanding of the oxidation reactions and rates. Some commonly used analytical techniques, such as thermogravimetric analysis, measure the net mass change of the specimen over time. Other techniques, such as cross-sectional analysis of oxidized specimens, provide insight into the oxide scale microstructure. However, the information obtained with these techniques is insufficient to understand complex oxidation phenomena. This work presents an analytical technique that utilizes solid-state electrochemical oxygen pumps to control the oxidation potential and measure the resulting oxygen consumption of a material. This approach, which provides specific advantages when studying multi-principal element alloys (MPEA) that form a mixture of condensed and gaseous oxides, was applied to study the effect of aluminum on the oxidation resistance of refractory MPEAs and better account for reactions resulting in simultaneous mass gain and loss for molybdenum-containing specimens.

9:55 AM

Oxidation Behaviors of Ta-Ti-Cr RMPEAs: *Noah Welch*[1]; Todd Butler[2]; Maria Quintana[1]; Samuel Kuhr[2]; Peter Collins[1]; [1]Iowa State University; [2]Air Force Research Laboratory, WPAFB

Refractory Multi-Principal Element Alloys (RMPEAs) have been shown to exhibit favorable oxidation resistance at high temperatures (>1000˚C) due to the formation of complex oxides and suppression of simple, deleterious oxides such as Ta2O5. The TaTiCr alloy family shows promise in this space with relatively low density, high melting temperature and enhanced oxidation resistance when compared to traditional, dilute refractory alloys. An in-depth characterization of the role of microstructure, alloy chemistry and temperature on the resulting oxidation behaviors will be discussed. The resulting oxides, kinetics and associated thermodynamics will be addressed with respect to related alloys systems. Future challenges with respect to the understanding of RMPEA oxidation will also be described.

10:15 AM

Tuning Scale Formation in Al-containing Refractory High Entropy Alloys via Reactive Elements Addition: *Elaf Anber*[1]; David Beaudry[1]; Charlie Brandenburg[2]; Sebastian Lech[1]; Michael Waters[3]; Nathan Smith[3]; James Rondinelli[3]; Chris Wolverton[3]; Elizabeth Opila[2]; Jean Phillippe Couzinie[4]; Mitra Taheri[1]; [1]Johns Hopkins University; [2]University of Virginia; [3]Northwestern University; [4]University Paris-Est Créteil (UPEC) - IUT

Refractory high entropy alloys (RHEAs) hold the promise of superior mechanical properties at high temperatures, however, their oxidation resistance is still a major drawback because of the formation of non-protective scales. The classical concept (i.e. addition of Cr/Al) of providing oxidation resistance to high temperature alloys has been unsuccessful due to the inability to form a continuous scale. Using a combination of multiscale microscopy and thermodynamic calculations, we examined the role of Al and reactive elements (REs) addition on scale formation in RHEAs, and the alloys tend to passivate, forming continuous Al2O3, with decreasing REs/Al additions. We also observed the formation of complex oxides such as Nb2O5 and Nb2Zr6O17 with increasing Al/REs concentration. The structure, composition and density of these oxides will be discussed in terms of concentration of oxygen/metal vacancy. These results provide a one step closer towards designing new RHEAs that are better suited for high temperature environments.

10:35 AM Break

10:55 AM
High Temperature Oxidation Mechanisms of NbTiZr using 18O Tracer Technique: *Charlie Brandenburg*[1]; David Beaudry[2]; Mitra Taheri[2]; Elizabeth Opila[1]; [1]University of Virginia; [2]Johns Hopkins University

Refractory multi-principal element alloys (RMPEAs) are of interest for their mechanical strength at high temperature, however, rapid oxidation rates limit their use in these environments. Equimolar NbTiZr was studied as a model alloy for high temperature oxidation of RMPEAs. Double oxidation experiments using 1%O2 (balance argon) and 18O2 tracer gas were performed at 1050°C and 1250°C using a resistive heating system. Time-of-Flight Secondary Ion Mass Spectrometry (ToF-SIMS) was used to map the distribution of 18O in sample cross-sections. 18O exposure for 1 minute and 30 seconds after oxidation at 1050 and 1250°C, respectively, resulted in an 18O reaction depth of approximately 40m. ToF-SIMS maps of the sample oxidized at 1250°C show high concentrations of 18O in ZrO2 grains, suggesting rapid transport of oxygen within ZrO2.

11:15 AM
Multi-scale Characterization of $Al_{0.3}CrFeNiTi_{0.3}$ High-entropy Alloy Coatings Produced by High-velocity Oxygen-fuel (HVOF) Spraying: *Rasim Eris*[1]; Ashok Meghwal[2]; Surinder Singh[2]; Christopher C. Berndt[2]; Andrew Siao Ming Ang[2]; Paul Munroe[1]; [1]UNSW Sydney; [2]Swinburne University of Technology

Incorporating lighter elements, such as Al and Ti, into $Al_xCrFeNiTi_y$ high-entropy alloys (HEAs) produced by bulk processing methods significantly enhances both strength and ductility, compared to many CrFeNi-based HEAs. Nevertheless, high entropy alloy coatings (HEACs) allow these alloys to be exploited as protective films. In this current work, a high-performance $Al_{0.3}CrFeNiTi_{0.3}$ HEAC was produced by the high-velocity oxygen-fuel (HVOF) thermal spraying technique and characterized by scanning and transmission electron microscopy. Micro-hardness and nano-indentation tests were used to establish a correlation between specific microstructural features and local mechanical properties. Accordingly, strengthening was seen to be enhanced by the presence of dispersed oxides formed by in-flight oxidation "IFO" during deposition. Moreover, this coating exhibits a highly complex multiphase microstructure including ordered structures with distinctive grain morphologies and local chemical heterogeneities that contributed to the attractive mechanical properties.

11:35 AM
Effect of Surface Deformation on the High-temperature Oxidation Response of Equimolar CrMnFeCoNi: *Thomas Valenza*[1]; Kate Moo[1]; Emmanuelle Marquis[1]; [1]University of Michigan

Because of its role in the high-temperature oxidation of many alloys, surface deformation has the potential to influence the oxidation response of HEAs. To demonstrate its importance for HEAs, we compared the oxidation response of an equimolar CrMnFeCoNi alloy subjected to different surface finishes. Specimens were either polished to a mirror finish, to minimize surface deformation, or ground with coarse SiC paper, to maximize surface deformation. Prepared specimens were oxidized in air at 800 ˚C, and the resulting oxide scales and sub-surface microstructures were characterized. The oxidation response differed dramatically as a function of the surface finish. Differences were noted in the oxide scale thicknesses, oxidation products, and internal oxidation. Furthermore, diffusion-induced grain-boundary migration appears to play a key role in the oxidation process of deformed surfaces. The present results point to possible variations in the oxidation response of commercial components due to varying processing conditions and surface finish.

11:55 AM
A High Throughput CALPHAD Method of Designing Low Density, Compositionally-complex Alloys Toward Understanding Lightweighting Elements' Effects on Passivity: *Peter Connors*[1]; John Scully[1]; [1]University of Virginia

The emergence of compositionally-complex alloys (CCAs) as a new frontier of corrosion-resistant alloys has opened doors for advanced optimization of the usage of corrosion-resistant elements for promoting passivation of each phase and self-healing. However, researchers must contend with a design space unfathomable in compositional and microstructural possibilities. In this work, a methodology for the rapid (~1 alloy/second) testing of alloy compositions for desired phase stability using the CALPHAD approach is presented. This approach utilizes equilibrium information of a composition at its solidus temperature to maximize the probability of discovering an alloy with a disordered matrix-(or single-)phase microstructure. Additionally, for multi-phase alloy design, this approach engineers the distribution of passivating elements throughout the predicted microstructure and interfacial area between phases of interest. Alloys with constant phase compositions and variable area fractions are evaluated. A system discovered using this technique is explored toward understanding lightweight, passivating elements' effects on overall passivation.

Fundamental Theory and Modeling I

Monday PM **Room: William Penn Ballroom**
November 13, 2023 **Location: Omni William Penn**

Session Chair: To Be Announced

1:40 PM Introductory Comments

1:45 PM Invited
Quantifying Short-range Order and its Domain Size in High-entropy Alloys: *Rodrigo Freitas*[1]; [1]Massachusetts Institute of Technology

Complete characterization of short-range order is challenging to realize because of the sheer number of local chemical configurations that must be accounted for. Moreover, the chemical complexity of concentrated solid-solution phases is often described as the tendency for some of these configurations to be more common than others (i.e., "slightly less random than completely random"), which does not translate easily into a physically intuitive and quantifiable picture. In this talk I will introduce an approach that combines statistical mechanics and information theory with machine learning techniques to quantify the space of local chemical configurations available for high-entropy alloys. I will show that this approach leads to a predictive framework for evaluation of short-range order domain sizes.

2:15 PM
Bond-stiffness Based ML Approach to Predict Atomic Level Properties in MPEAs: Nathan Linton[1]; Dharmendra Pant[1]; *Dilpuneet Aidhy*[1]; [1]Clemson University

On the one hand, the presence of multiple elements in large proportions in multi-principal element alloys (MPEAs) present opportunities to unravel novel properties, whereas on the other, they pose a large computational challenge due to the large phase space, especially for density functional theory (DFT) calculations, that are inherently very expensive. We present PREDICT (PRedict properties from Existing Database In Complex alloys Territory), a machine learning framework coupled with DFT whereby properties in MPEAs could be predicted simply by learning from the binary alloys database. The physics is included via bond stiffness derived from DFT to predict elastic constants, vibrational entropy and other related properties in FCC based MPEAs leading to accurate predictions. This approach enables probing any MPEA composition by just including DFT information of constituting binary alloys, thereby altogether bypassing DFT calculations in MPEAs.

2:35 PM

Local Order Average-atom Approach for Simulating Refractory High Entropy Alloys: *Chloe Zeller*[1]; Ellad Tadmor[1]; [1]University of Minnesota - Twin Cities

Refractory high-entropy alloys (RHEAs) are characterized by their high service temperature and superior strength and are thus promising materials for harsh-environment aerospace applications, such as exhaust nozzles and thermal protection materials on hypersonic vehicles. High-fidelity molecular dynamics (MD) simulations are a promising approach for predicting the thermomechanical response of RHEAs, however large simulations are required to obtain good statistics to account for local chemical fluctuations that can have a large effect on properties. To reduce system size, Average-Atom (AA) interatomic potentials, where interactions between species are weighted according to their occurrence probability in a random alloy, have been used to predict phase averages of properties of interest. We extend this approach by accounting for local ordering in multicomponent alloys, i.e. preferential short-range arrangements of atomic species. Using this new Local Order Average-Atom (LOAA) approach, we study the effect of local ordering on the mechanical properties of prototypical multicomponent systems.

2:55 PM

Quantitative Assessment of Local Chemical Ordering in Atomistic Simulations of High-entropy Alloys: *Killian Sheriff*[1]; Yifan Cao[1]; Rodrigo Freitas[1]; [1]Massachusetts Institute of Technology

High-entropy alloys (HEAs) exhibit exceptionally good combinations of properties recently reported to correlate with chemical short-range ordering (cSRO). However, in atomistic simulations, their state of cSRO has only been so far characterized using the Warren-Cowley parameters. Yet, this approach is incomplete as distinct local atomic configurations sharing the same chemical concentration are indistinguishable. Here, we propose a generalized framework, based on graph-convolution neural networks equivariant to E(3) symmetry operations, statistical mechanics, and information theory, capable of completely identifying the set of distinct local atomic bonding environments and their associated population densities in HEAs. This approach leads to a quantitative characterization of the cSRO state and provides a predictive framework for evaluation of cSRO domain sizes, thus offering novel avenues to explore the relationships between processing, structure, and properties in HEAs.

3:15 PM Break

3:35 PM

Atomic Representations of Local and Global Chemical Effects of Mechanical Strength: *Mitchell Wood*[1]; Megan McCarthy[1]; Mary Alice Cusentino[1]; [1]Sandia National Laboratories

The exceptional properties observed in complex concentrated alloys (CCAs) arise from the interplay between crystalline order and chemical disorder at the atomic scale, complicating the determination of properties. The base metallurgical argument for CCAs' observed strength is the maximization of solid solution strengthening effects, but is difficult to quantitatively address from experiments alone. Herein we present a quantum-accurate interatomic potential(IAP) for use in molecular dynamics simulations of MoNbTaTi that efficiently scales to systems that are converged with respect to size, time and chemical complexity. Furthermore, we use this IAP to quantify the relationship between inhomogeneous lattice strains and novel definitions of local chemical environment. We will highlight the improvement of this reduced order model over historical arguments of local atomic volume and element-wise attribution of strengthening in these complex alloys.

3:55 PM

Capturing Short-range Order in High-entropy Alloys with Machine-learning Potentials: *Yifan Cao*[1]; Killian Sheriff[1]; Rodrigo Freitas[1]; [1]Massachusetts Institute of Technology

Chemical short-range order (cSRO) is recently reported to strongly influence the mechanical properties of various high-entropy alloys (HEA). However, the intricate nature of cSRO has made it challenging for current machine-learning potentials (MLP) to capture this feature, and many proposed approaches lack quantitative analysis of MLP performance on this task. In this work, we propose a generalized strategy to construct first-principles training databases and effectively train MLPs capable of characterizing cSRO in HEAs. We demonstrate this strategy by quantitatively analyzing the MLP performances in reproducing cSRO effects in various properties of CrCoNi HEA, including defect properties and phase stability.

4:15 PM

Accelerating the Discovery of Low-Energy Structure Configurations: A Computational Approach that Integrates First-principles Calculations, Monte Carlo Sampling, and Machine Learning: *Md Rajib Khan Musa*[1]; Yichen Qian[1]; Dr. David Cereceda[1]; [1]Villanova University

In this work, we developed a novel and highly efficient computational approach that combines MC sampling, DFT calculations, and Machine Learning (ML) techniques to accelerate the discovery of low-energy structure configurations of alloys. Our method is inspired by the well-established cluster expansion technique, leveraging its strengths while addressing its limitations. Specifically, we enhanced the reliability of the cluster expansion by avoiding out-of-sample prediction using machine learning. We performed first-principle Density Functional Theory (DFT) calculations for those samples. We applied our novel approach to several tungsten-based alloys. Our results show a noteworthy reduction in root mean square error (RMSE) compared to cluster expansion, suggesting its superior accuracy and reliability.

4:35 PM

Computational Discovery of B2 Phases in the Refractory High Entropy Alloys: *Junxin Wang*[1]; Maryam Ghazisaeidi[1]; [1]Ohio State University

The Multi-Cell Monte Carlo method for phase prediction for multicomponent alloys has demonstrated great potential in simulating coexisting phases in many-component crystalline systems. To find potential B2 structures in high entropy alloys, this method is applied to composition space, spanning through the refractory element range in the periodic table. First, we explore the refractory elements with BCC ground state structures (MoNbTaW/V) and then the ones with HCP ground state structures (TiZrHfOsReRu). Ordered structures are found in both systems and their thermal stability are analyzed. We further look into the combination of all the refractory elements (both HCP and BCC elements) and try to identify the most possible groups to form a B2 structure.

4:55 PM

Deciphering the Strength-vs-ductility Trade-off for High-entropy Alloys with AI-driven Fully ab Initio-based Material Modeling: *Max Hodapp*[1]; Ivan Novikov[2]; Olga Kovalyova[2]; Alexander Shapeev[2]; Franco Moitzi[1]; Oleg Peil[1]; [1]Materials Center Leoben; [2]Skoltech

In this talk, we present a novel Bayesian multi-objective optimization framework that fully automatically predicts multicomponent refractory alloys with Pareto-optimal strength-vs-ductility ratios. Our framework involves predictive material models as objective functions that are fed with ab initio-based data exclusively, coming from efficient CPA calculations or atomistic simulations using machine-learned interatomic potentials, allowing for a screening over the whole alloy space at an acceptable cost. More broadly, our framework is neither limited to two objectives nor to specific mechanical properties, and, therefore, we anticipate that it also enables us to accelerate the discovery of new materials with exotic properties for various other applications. Further, we outline how magnetism can be brought into the game so that our methodology would allow for screening over a much larger space of (magnetic and non-magnetic) alloys than the space that can currently be approached with state-of-the-art methods.

Characterization of HEAs II

Monday PM **Room: Riverboat**
November 13, 2023 **Location: Omni William Penn**

Session Chair: To Be Announced

1:40 PM Introductory Comments

1:45 PM Invited

Achieving Exceptional Mechanical Properties in High Entropy Alloys via Thermodynamically Guided Local Chemical Ordering: Sriswaroop Dasari[1]; Abhishek Sharma[1]; Chao Jiang[2]; Bharat Gwalani[3]; Stephane Gorsse[4]; An-Chou Yeh[5]; Srinivasan Srivilliputhur[1]; *Rajarshi Banerjee*[1]; [1]University of North Texas; [2]Idaho National Laboratory; [3]North Carolina State University; [4]University of Bordeaux; [5]National Tsing Hua University

Understanding the local chemical ordering propensity in random solid solutions, and tailoring its strength, can guide the design and discovery of complex, paradigm-shifting multi-component alloys. A simple thermodynamic framework was employed, based solely on binary enthalpies of mixing, to select optimal alloying elements to control the nature and extent of chemical ordering in high entropy alloys (HEAs). Subsequently, high resolution electron microscopy, atom probe tomography, and computational modeling have been coupled to demonstrate how controlled additions of Al and Ti and subsequent annealing drive chemical ordering (from short-range ordered domains to long-range ordered precipitates) in nearly random equiatomic FCC CoFeNi solid solution, boosting its tensile yield strength by a factor of four while also substantially improving ductility, which breaks the so-called strength-ductility paradox. The generality of this approach was demonstrated via addition of Al for introducing chemical ordering and enhancing mechanical properties in another nearly random BCC refractory NbTaTi HEA.

2:15 PM

Development of Refractory Metal-based CCAs with Improved Mechanical Properties: Stephan Laube[1]; Steven Schellert[2]; *Alexander Kauffmann*[1]; Bronislava Gorr[1]; Yolita Eggeler[1]; Hans-Juergen Christ[2]; Martin Heilmaier[1]; [1]KIT Karlsruhe; [2]University of Siegen

Refractory compositionally complex alloys (RCCA) are promising candidates for high-temperature structural applications. To achieve good mechanical performance at elevated temperatures, the proper formation of a strengthening phase is crucial. In order to mimic the microstructures of precipitation-strengthened Ni-based superalloys, we developed an A2 matrix alloy, 82(TaMoTi)-8Cr-10Al (at.%) with B2 particles that are formed by a precipitation reaction, namely by diffusion-controlled nucleation and growth. The Al content is crucial to obtain the proper reaction sequence. By adjusting Al concentration, the ordering temperature can be tailored to be congruent with the maximum temperature of the two-phase field as a first prerequisite. In order to reveal the distinct nature of phase separation sequence, i.e. nucleation and growth, atom probe tomography and electron microscopy techniques were utilized on samples that were annealed over orders of magnitude in time at temperatures beyond 800°C and the impact of coherent particle strengthening on mechanical properties is discussed.

2:35 PM

Microstructures and Properties of AlCrFeMnV, AlCrFeTiV, and AlCrMnTiV High-entropy Alloys: *Keith Knipling*[1]; Patrick Callahan[1]; David Beaudry[2]; [1]Naval Research Laboratory; [2]Johns Hopkins University

A series of high-entropy alloys (HEAs) containing AlCrFeMnV, AlCrFeTiV, and AlCrMnTiV have been designed using a combination of thermodynamic prediction by Thermo-Calc and by experimental observation of the microstructure and phases present in arc-melted alloys. These alloys are predominantly BCC, with some alloys forming additional minor phases. A particularly intriguing microstructure is observed in the AlCrMnTiV alloy, which contains a high number density of 50 nm ordered B2 cuboids that are coherent with the BCC matrix, resembling the well-known -' microstructures in Ni-based superalloys but in a BCC system. We will correlate the alloy microstructures, observed using a combination of X-ray diffraction (XRD), scanning and transmission electron microscopy (SEM/TEM), and atom-probe tomography (APT), to the alloys' mechanical properties measured by Vickers microhardness and nanoindentation.

2:55 PM

Accelerating EXAFS Analysis of SRO in HEAs: Challenges and Opportunities: *Howard Joress*[1]; Elaf Anber[2]; Bruce Ravel[1]; Jonathan Hollenbach[2]; Mitra Taheri[2]; Brian DeCost[1]; [1]NIST; [2]Johns Hopkins

It has become clear that most HEAs are not completely disordered, with certain elements having a proclivity for bonding. Further, this short-range order can have a large effect on properties. Extended x-ray absorption fine structure (EXAFS) is a powerful tool for characterizing this disorder, however challenges exist in analysis of the data. In this talk we will describe in detail the difficulties inherent to applying EXAFS to HEAs, including low Z contrast, secondary phases, long-range order, and the large number of variables involved in the fits. We will also describe our efforts to accelerate EXAFS mapping and quantitative data analysis. To speed the acquisition of EXAFS data we demonstrate the use of on-the-fly unsupervised learning to select subsequent samples for measurement. We then demonstrate the use of modern statistical methods, including bayesian inference to quantify the short-range order.

3:15 PM Break

3:35 PM

Development of Coherent Ru-based BCC + B2 Alloys with High Thermal Stability: *Carolina Frey*[1]; Anthony Botros[1]; Sebastian Kube[1]; Haojun You[1]; Tresa Pollock[1]; [1]University of California Santa Barbara

Refractory Multi-Principal Element Alloys (RMPEAs) are a new class of structural alloys for extreme environments with the potential to push operating temperatures above 1200 ˚C. However, the development of alloys that can operate at desired temperatures of 1300-1400 ˚C has been limited by a lack of coherent strengthening precipitates that can persist at the target temperatures. For this investigation, solution and ageable BCC + B2 alloys have been developed with Ru-based B2 phases that are coherent and stable to 1300-1900 ˚C. Relationships between the different elemental additions, B2 solvus temperatures, B2 volume fractions, and B2 compositions were determined via annealing studies and subsequent SEM investigations. The effect of aging on alloy hardness and precipitate morphology are also presented. Consistent with precipitate evolution in nickel superalloys, the morphologies of the coherent Ru-B2 precipitates evolved from spherical to cuboidal to cuboidal arrays with increasing aging time.

3:55 PM

Direct Determination of Short-range Order in Materials Using Spatial Statistics: *Michael Xu*[1]; Shaolou Wei[1]; Cemal Tasan[1]; James LeBeau[1]; [1]Massachusetts Institute of Technology

While short-range order (SRO) in chemistry and structure can have significant impact on material properties, capturing their distribution at the nanoscale can be inherently difficult. Scanning transmission electron microscopy (STEM) offers a local probe of material chemistry and structure, yet projection of the three-dimensional structure being imaged presents its own challenges in distinguishing SRO from local random fluctuations. Using a combination of STEM and Geographic Information Systems (GIS), we demonstrate first how incorporating spatial statistics tools can enable quantification of SRO at the atomic scale. We will consider a case study oxide material to validate the approach and extend it to measure non-random SRO in the refractory high entropy alloy TiVNbHf. Comparing experiment with null-hypothesis random and ordered structures shows that chemical order exists at extremely local length scales (<1 nm). Finally, the addition of Al is demonstrated to enhance the degree of SRO as well.

4:15 PM

Characterization of Microstructure and Deformation Behavior of Several AlNbTaTiVZr Refractory Complex Concentrated Alloys (RCCAs): *Bryan Crossman*[1]; Oleg Senkov[2]; Jean-Philippe Couzinie[3]; Rajarshi Banerjee[4]; Maryam Ghazisaeidi[1]; Michael Mills[1]; [1]Ohio State University; [2]Air Force Research Labs; [3]Institute of Chemistry and Materials Science (ICMPE); [4]University of North Texas

Refractory complex concentrated alloys (RCCAs) can offer attractive high temperatures properties and provide a potential solution to the increasing need for higher operating temperatures in transportation and energy applications. Many RCCAs are limited by their poor ductility at room temperature and phase instability at high temperature. Using SEM-based techniques, as well as atomic resolution STEM and high resolution EDS, this work investigates the microstructure and deformation behavior of an $Al_{10}Nb_{20}Ta_{15}Ti_{30}V_5Zr_{20}$ BCC+B2 RCCA, as well as alloys having the composition of the individual phases. The primarily single phase BCC and B2 alloys showed surprising plasticity at room and elevated temperatures in a previous study [1]. Of special interest is the deformation twinning observed in the B2 alloy, which is generally unfavorable in B2, contributing to the plasticity.[1] Senkov O., et al. "Mechanical Properties of an $Al_{10}Nb_{20}Ta_{15}Ti_{30}V_5Zr_{20}$ A2/B2 Refractory Superalloy and Its Constituent Phases." Acta Materialia (2023): 119017.

4:35 PM

Phase Stability in Refractory High Entropy Alloys: *Vishal Soni*[1]; SriSwaroop Dasari[1]; Abhishek Sharma[1]; Advika Chesetti[1]; Oleg Senkov[2]; Daniel Miracle[3]; Rajarshi Banerjee[1]; [1]University of North Texas; [2]MRL Materials Resources LLC; [3]Air Force Research Laboratory

Al-containing refractory high entropy alloys or complex concentrated alloys (RHEAs or RCCAs) often exhibit a patterned BCC+B2 microstructure, resembling the FCC+L12 microstructure typically observed in Ni/Co base superalloys. There is a rapidly growing interest in these BCC+B2 microstructures, especially due to their promising balance of elevated temperature mechanical properties. Unfortunately, such BCC+B2 microstructures are often reported to be unstable and upon long term annealing, results in transformation of the B2 phase to ordered omega phase which is detrimental to mechanical properties. The current study focuses on investigating the stability of BCC+B2 microstructure and the detrimental ordered omega phase in several Al-containing RHEAs at elevated temperatures (600C-1400C). The results are compared with CALPHAD based predictions to understand the stability of such phases and thus tune the alloy compositions to get elevated temperature stability of the BCC+B2 and at the same time, avoid the formation of undesired phases.

4:55 PM

Defect Mediated Microstructural Evolution and Phase Transformations in a BCC Based $Al_{0.5}NbTa_{0.8}Ti_{1.5}V_{0.2}Zr$ Refractory High Entropy Alloy: *Abhishek Sharma*[1]; Advika Chesetti[1]; Tirthesh Ingale[1]; Vishal Soni[1]; Hamish Fraser[2]; Stéphane Gorsse[3]; Rajarshi Banerjee[1]; [1]University of North Texas; [2]The Ohio State University; [3]Université de Bordeaux

This study focuses on how prior deformation influences the phase transformation pathway and the resultant microstructural evolution in the BCC-based $Al_{0.5}NbTa_{0.8}Ti_{1.5}V_{0.2}Zr$ refractory high entropy alloy (RHEA). The solutionized alloy was cold-rolled prior to annealing, which resulted in an extremely refined HCP-based ordered omega phase dispersed within a disordered BCC matrix. This microstructure is in contrast to the B2+BCC microstructure that forms when this alloy is annealed at the same temperature, a transformation pathway which has been previously reported. Presence of deformation substructure consisting of dislocations, twins, etc. provides a high number density of heterogenous nucleation sites distributed within the matrix resulting in a lower nucleation barrier for crystallographically mismatched phases such as the hexagonal ordered omega phase. The compositional and structural changes associated with the ordered omega precipitation, were characterized in detail by TEM and APT, and provide insights for microstructural design of RHEAs.

Fundamental Theory and Modeling II

Monday PM **Room: Three Rivers**
November 13, 2023 **Location: Omni William Penn**

Session Chair: To Be Announced

1:40 PM Introductory Comments

1:45 PM Invited
Multi-scale Modelling of Multiple-principal Element Alloys: From Electrons to Atoms to Continuum using Machine Learning: *Shyue Ping Ong*[1]; Hui Zheng[1]; Lauren Fey[2]; Irene Beyerlein[2]; [1]University of California-San Diego; [2]University of California, Santa Barbara

Refractory multi-principal element alloys (RMPEAs) are promising for high-temperature structural applications. In this talk, I will discuss how multi-scale modeling of RMPEAs from electrons to atoms to continuum can be achieved with recent advances in machine learning (ML). Using the MoNbTi and TaNbTi RMPEAs as examples, we investigate the role of short-range ordering (SRO) on dislocation glide. An accurate ML interatomic potential (MLIP) was developed using DFT calculations. Monte Carlo/molecular dynamics simulations with the MLIP show that MoNbTi exhibits a much greater degree of SRO than TaNbTi, and the local composition directly affects the unstable stacking fault energies (USFEs). These atomistic simulations were then used to parameterize a phase-field dislocation dynamics (PFDD) model. From PFDD simulations, we find that the gliding dislocations experience significant hardening due to pinning and depinning caused by random compositional fluctuations, with higher SRO decreasing the degree of USFE dispersion and hence, the amount of hardening.

2:15 PM
Simulations and Modelling of the High Temperature Yield Behavior of BCC Refractory Complex Concentrated Alloys (RCCA's): *Satish Rao*[1]; Brahim Akdim[2]; Oleg Senkov[1]; Daniel Miracle[3]; Todd Butler[3]; [1]Mrl Materials Resources Llc; [2]UES Inc; [3]AFRL

Atomistic simulations, using Johnson-Zhou and/or Machine learning potentials, of the core structure and mobility of ½[111] screw, edge and mixed dislocations in complex concentrated BCC alloys are presented. The core structure and its variations obtained for screw dislocations in NbTiZr using atomistic simulations are compared with first-principles calculation results and good agreement is found. Average solute-dislocation core interaction energies are used to determine the critical stress for the motion of screw dislocations as a function of temperature using Rao- Suzuki model In addition, diffusional effects at very high temperatures on the predicted yield behavior are modelled. Edge dislocation mobilities in these alloys are modelled using the Maresca-Curtin model. Experimental and molecular dynamics yield data for MoNbTaW are analyzed using Rao-Suzuki model as well as Maresca-Curtin model. The model results on yield behavior are shown to be in good agreement with experimental data in selected BCC complex concentrated alloys.

2:35 PM
Dislocations in Complex Alloys: Insights from PeierlsNabarro Modeling: Terrence Moran[1]; Bastien Aymon[1]; *William Curtin*[1]; [1]Swiss Federal Institute Of Technology

Dislocations in alloys with random solute distributions, short-range order, or clustering have a range of competing length and energy scales that overall establish energy barriers to dislocation motion. The flow behavior then depends on many different underlying material parameters and it becomes difficult to formulate theories that include all these factors. Here, to guide development of theories, we show how a Peierls-Nabarro/Phase-Field (PN/PF) model can enable efficient and accurate parametric exploration of dislocation behavior as a function of controllable material parameters. Key often-overlooked elements of the PN/PF model are discussed. First applications of the PN//PF model to (i) understanding dislocation line tension in both fcc and bcc metals and (ii) the emergence of characteristic dislocation length scales in random alloys, are then presented and discussed in the context of current theories.

2:55 PM
Investigating Alloying Element Effects on Screw Dislocation Trajectories in Multicomponent bcc Alloys: *Amir Hassan Zahiri*[1]; Liang Qi[1]; [1]University of Michigan

This research explores the impact of alloying elements, particularly Hf and/or Ti, on the slip behavior of Nb and Ta-based multicomponent solid solution alloys with a body-centered cubic (bcc) crystal structure using molecular dynamics (MD) simulations. The study compares different binary and multicomponent bcc alloys under shear deformation. Without alloying elements, the a/2<111> screw dislocation's slip plane changes from the {110} plane to the {112} twinning slip plane in both pure Nb and Ta. However, with the addition of Hf and Ti, the slip plane transitions from the {112} twinning slip plane to the {110} slip plane at intermediate concentrations of alloying elements. At high concentrations, the slip plane shifts to the {112} anti-twinning slip plane. These transitions depend on strain rates, temperatures, and the stability of metastable phases. Understanding these slip plane transitions can improve the mechanical properties of bcc multicomponent alloys by reducing strain localization and enhancing ductility.

3:15 PM Break

3:35 PM
Screw and Edge Dislocation Strengthening in BCC High Entropy Alloys, and Efficient Yield Strength Prediction: *Francesco Maresca*[1]; William Curtin[2]; [1]University of Groningen; [2]Brown University

We introduce and validate a holistic, parameter-free strengthening theory of screw and edge dislocations in BCC high entropy alloys. In contrast with screw-controlled pure BCC metals, in non-dilute BCC alloys both edge and screw dislocations are pinned due to strong local energy fluctuations. Thus, three strengthening regimes are found in screws: (1) low-temperature, Peierls-barrier controlled strength; (2) intermediate-temperature strength, due to kink migration over barriers scaling with solute/dislocation interaction; (3) high-temperature strength, scaling with energy of vacancy and self-interstitials forming after unpinning of cross-kinks. Edge dislocation strengthening scales with misfit volumes and elastic moduli. The edge theory is cast in an analytical form that is parameter-free and depends on physical quantities that can be determined ab-initio or experimentally. The reduced edge theory enables screening over 10 million compositions in the whole Al-Cr-Mo-Nb-Ta-W-V-Ti-Zr-Hf alloy family to find the strongest BCC HEAs.

3:55 PM

Strength Reductions of Metal Alloys with Short-range Order as Revealed by Atomistic Simulations: *Xin Liu*[1]; William Curtin[1]; [1]EPFL

A theory for strengthening for multicomponent non-dilute alloys possessing short-range order (SRO) has recently been developed. The theory predicts that, in addition to athermal strengthening, there is a notable effect of SRO on the solute-dislocation interactions that can change the strength relative to a random alloy. Atomistic simulations in a model binary NbW alloy are used to demonstrate that alloy strength due to solute-dislocation interactions can be increased or decreased depending on the SRO. Specifically, SRO is introduced using fictitious solute-solute interactions and the Nudged Elastic Band method is used to compute the energy barriers for edge dislocation motion. Energy barriers can be decreased when the SRO parameters are negative. The theoretical predictions for the same system are in reasonable quantitative agreement with the simulation results. These findings demonstrate the unexpected possibility of reduced strength due to SRO and validate the analytical theory as a tool to guide alloy design.

4:15 PM

Investigating the Stability of a Al0.5NbTa0.8Ti1.5V0.2Zr BCC/B2 RCCA: *Julian Brodie*[1]; Junxin Wang[1]; Jean-Philippe Couzinie[2]; Milan Heczko[1]; Veronika Mazanova[1]; Michael Mills[1]; Maryam Ghazisaeidi[1]; [1]Ohio State University; [2]University Paris-Est Créteil (UPEC) - IUT

Recently, the AlNbTaVTiZr class of BCC/B2 Refractory Complex Concentrated Alloys (RCCAs) have drawn increased interest as the bcc analogue to the well-known Ni-based super alloys with gamma/gamma' microstructure. Previous experimental results on the microstructure of these alloys have been varied where some have found the formation of brittle phases within the BCC matrix along with the B2 precipitates. Since the mechanical properties of these alloys are highly dependent on their microstructure, it's crucial to understand why these phases form. We use Density Functional Theory to study the phase stability of the B2 phase in a BCC/B2 Al0.5NbTa0.8Ti1.5V0.2Zr RCCA. We calculate the formation energy using DFT and study the effects of non-equilibrium conditions, such as temperature and strain, on the competing phases. We also explain how the microstructure is unstable and is prone to transform into an Omega, tetragonal, or hexagonal phase.

4:35 PM

Testing the Origin of the High Strength of Complex Concentrated Alloys using Large-scale Molecular Dynamics Simulations: Vasily Bulatov[1]; *Xinran Zhou*[2]; Jaime Marian[2]; [1]Lawrence Livermore National Laboratory; [2]University of California Los Angeles

We report results of large-scale Molecular Dynamics simulations of plastic flow in single crystalline complex alloys subjected to high-rate compression and tension over a wide range of compositions, temperatures and straining rates. Utilizing several sets of interatomic potentials previously developed for multi-component metal alloys, our simulations are defined to test applicability of popular analytical models of strengthening in complex multi-component alloys and, at the same time, to reveal full details of dislocation motion mechanisms contributing to strengthening.

4:55 PM

Predicting Yield Strength of High Entropy Alloys from Density Functional Theory: Siming Zhang[1]; *Guofeng Wang*[1]; [1]University of Pittsburgh

To enable rational design of high entropy alloys (HEAs), we have developed a first principles density functional theory based computational approach to predict the yield strength of single phase HEAs. Specifically, we applied the developed method to calculate the yield strength of some select HEAs with face-centered cubic (fcc) or body-centered lattice (bcc) structure and with varying chemical composition. We have examined our computational approach for four fcc alloy systems, i.e., NiCoFe, CoCrFeNi, CoCrFeCuNi, and RdIrPdPtNiCu, and four bcc alloys systems, i.e., MoNbTaW, MoNbTaV, AlCoCrFeNi, and AlCoCrFeNiZr0.3. For these HEAs with dramatically different chemical composition, our predicted yield strengths are found to agree well with experimental values. Consequently, we have demonstrated that the developed first principles based computational approach is a reliable computational tool for understanding the composition-structure-property relation of HEAs and, particularly, exploring novel HEAs with superior mechanical properties over vast composition space.

Tuesday Plenary

Tuesday AM
November 14, 2023

Room: William Penn Ballroom
Location: Omni William Penn

Session Chair: To Be Announced

8:00 AM Introductory Comments

8:10 AM Plenary

Through the Looking Glass: Recent Progress in the Characterization of High Entropy and Compositionally Complex Alloys: *Mitra Taheri*[1]; [1]Johns Hopkins University

High entropy alloys possess various superior functional and structural properties based on the complexity of their compositional landscape. Much research has been dedicated to the fingerprinting of specific aspects of this landscape, from short range order phenomena to unique phase evolution and stability. While marked advancements in both theory and experiment have been made toward these property-determining factors, characterization of these alloys has been fraught with challenges. In this talk, the motivating factors for understanding atomic-scale "fingerprints" in the quest for new alloys, the critical nature of multiscale characterization, and the progress toward these efforts across the HEA community will be discussed. An outlook on how characterization tools can be linked to theory and the role of machine learning will be reviewed in the context of future opportunities for tackling this exciting area of metallurgy and materials innovation..

8:50 AM Break

Oxygen Effects and Atomic-scale Processes

Tuesday AM **Room: Three Rivers**
November 14, 2023 **Location: Omni William Penn**

Session Chair: To Be Announced

9:00 AM Introductory Comments

9:05 AM Invited
Metastability, Coarsening, and Strengthening Induced by Oxygen Interstitials in BCC Ti-Nb Alloys: *Ravit Silverstein*[1]; Florent Mignerot[1]; Nicoló Maria della Ventura[1]; Carlos G. Levi[1]; Tresa M. Pollock[1]; Daniel S. Gianola[1]; [1]University of California, Santa Barbara

The design of refractory BCC alloys with interstitial elements, particularly those based on group number IV, reveals a unique combination of mechanical properties. Interstitial incorporation leads to phase instabilities in the BCC parent structure, resulting in a rich variety of new structures and microstructures. Compositional variance, coarsening behavior, and their corresponding effects on mechanical properties are actively being studied, but key mechanisms are not fully understood. The presence of Ti and Nb in most refractory multi-principal element alloys (RMPEs) makes their binary system attractive for establishing a fundamental understanding of the more complex RMPEs. This work elucidates the role of oxygen, in dilute concentration (~1 at%), in mediating phase evolution and transformation pathways in Ti-Nb alloys. Small-scale mechanical testing that can target specific O-mediated microstructures reveals exceptional properties with hardnesses and tensile yield strengths as high as 7 GPa and 3 GPa, respectively. Potential deformation mechanisms will be discussed.

9:35 AM
Oxygen-induced Hierarchical Heterogeneities and Enhanced Hardness in RMPEAs: *David Beaudry*[1]; Michael Waters[2]; Gianna Valentino[3]; Daniel Foley[1]; Nathan Smith[2]; Elaf Anber[1]; Yevgeny Rakita[4]; Charlie Brandenburg[5]; Jean-Philippe Couzinie[6]; Loic Perriere[6]; Toshihiro Aoki[7]; Keith Knipling[8]; Patrick Callahan[8]; Benjamin Redemann[1]; Tyrel McQueen[1]; Elizabeth Opila[5]; Christopher Wolverton[2]; James Rondinelli[2]; Mitra Taheri[1]; [1]Johns Hopkins University; [2]Northwestern University; [3]University of Maryland; [4]Ben Gurion University of the Negev; [5]University of Virginia; [6]University Paris Est Creteil; [7]University of California, Irvine; [8]U.S. Naval Research Laboratory

Refractory multiprincipal element alloys (RMPEAs) offer superiority to incumbent high-temperature structural alloys due to high melting points and retained strength at elevated temperatures. Of this class of alloys, those containing Group IV and V elements possess adequate ductility, low density, and the necessary formability. However, these elements have dramatically different interactions with oxygen, which creates uncertainty in predicting oxide evolution and in alloy design for oxidation resistance. We used high fidelity characterization and Monte Carlo simulations to decipher the complex sub-surface phase evolution during high-temperature oxidation of Group IV-V RMPEAs. We found that a refined hierarchical microstructure of phase-separated oxides form, which leads to a hardness increase of over 600% while preserving the ductility of the base metal. High-throughput computational screening identified doping elements that would capitalize on our fundamental phase evolution findings to improve oxidation resistance and mechanical properties in these alloys.

9:55 AM
Cracking the Code: Demystifying Early-stage Oxidation in High Entropy Alloys: *Bharat Gwalani*[1]; Andrew Martin[1]; Elizabeth Kautz[1]; Sten Lambeets[2]; Thevuthasan Suntharampillai[2]; Anil Battu[2]; Martin Thuo[1]; Matthew Olszta[2]; Sten Lambeets; Arun Devaraj[2]; [1]North Carolina State Universtiy; [2]Pacific Northwest National Laboratory

Oxide film formation on material surfaces, upon oxygen contact, is critical. While it can protect from further corrosion in some instances, it can also degrade the material over time. Therefore, it's vital to understand early oxide film formation stages for designing corrosion-resistant materials. This study utilized correlative and in situ techniques, specifically transmission electron microscopy (TEM) and atom probe tomography (APT), to examine oxide film's initial formation stages on a high entropy alloy (HEA). By observing the chemical changes and phase transformation from a single to a multi-layer oxide film over time, we garnered valuable insights into the process. This research underscores these techniques' potential in facilitating a deeper comprehension of oxide film formation, aiding in designing durable, corrosion-resistant materials.

10:15 AM
Combinatorial Exploration of Passivating Elements on Refractory High Entropy Alloys: *Sebastian Lech*[1]; Elaf Anber[1]; David Beaudry[1]; Howie Joress[2]; Charlie Brandenburg[3]; Brian DeCost[2]; Elizabeth Opila[3]; Mitra Taheri[1]; [1]Johns Hopkins University; [2]National Institute of Standards and Technology; [3]University of Virginia

Refractory high entropy alloys (RHEAs) are candidate materials for next-generation high-temperature materials surpassing superalloys. However, despite high melting temperatures and promising mechanical properties, their oxidation resistance remains a challenge, limiting their applicability in extreme environments. Systematic exploration of passivating elements role is the key to unlocking the full potential of RHEAs. Current work explores experimental design strategies to enhance the oxidation resistance of RHEAs. The focus is on the addition of passivating elements and the development of compositional gradients using additive manufacturing via the directed energy deposition technique. The role of passivating elements on oxide scale formation was investigated by high-resolution scanning- and transmission electron microscopy along with phase analysis and thermodynamic modeling. Obtained results can be used as a guideline towards sufficient oxidation resistance of RHEAs for applications in aerospace and energy.

10:35 AM Break

10:55 AM
Microstructural Engineering in HEAs Undergoing Spinodal Assisted Phase Transformations: *Shalini Roy Koneru*[1]; Kamal Kadirvel[2]; Zachary Kloenne[1]; Hamish Fraser[1]; Yunzhi Wang[1]; [1]Ohio State University; [2]Computherm LLC

Researchers attributed the recently observed nano-scale periodic multi-phase microstructures in HEAs such as $AlMo_{0.5}NbTa_{0.5}TiZr$, $Al_{0.5}NbTa_{0.8}Ti_{1.5}V_{0.2}Zr$, TiZrNbTa and $Fe_{15}Co_{15}Ni_{20}Mn_{20}Cu_{30}$ to spinodal assisted phase transformation pathways (PTPs). Microstructures in such HEAs could be further engineered by studying the underlying PTPs in detail and identifying the critical alloy and processing parameters affecting the microstructural evolution. Thus, through phase-field simulations, we investigated the effect of interplay between different alloy parameters such as volume fraction of, lattice misfit and modulus mismatch between coexisting phases on microstructure topology in HEAs undergoing spinodal assisted PTPs. We further systematically investigated the effect of different heat treatments such as isothermal aging vs continuous cooling vs two-step heat treatments on microstructural evolution. It is demonstrated that the microstructural topology could be inverted by appropriate selection of alloy composition and heat treatment design. Further, we illustrate that a range of hierarchical microstructures could be designed in HEAs undergoing spinodal assisted PTPs.

11:15 AM

B2 Phase in Refractory High Entropy Alloys: Macroscopic B2 Ordering Signal May Not Really Represent B2 Stability: *An-Chen Fan*[1]; Yun-Syuan Chen[1]; Chong-Chi Chi[2]; Chih-Hao Hsu[1]; Kai-Cheng Yang[1]; Daniel Miracle[3]; Ming-Yen Lu[2]; Ming-Hung Tsai[1]; [1]National Chung Hsing University; [2]National Tsing Hua University; [3]AF Research Laboratory

Refractory high entropy alloys (RHEAs) with superalloy-like BCC+B2 microstructure, namely refractory high-entropy superalloys (RHESAs), have demonstrated superior resistance to thermal softening compared to single-phased BCC RHEAs, resulting in enhanced strength at elevated temperatures. However, the understanding of the equilibrium condition of the B2 phase in RHEAs remains unclear. In this study, three alloys from the Al-Nb-Ta-Ti-Zr system were selected to investigate the phase constituents, phase composition, and microstructure at different temperatures, as they potentially contain the B2 phase. Surprisingly, nanoscale interconnected structures consisting of BCC+B2 phases were observed in all the macroscopic "B2" phases in these alloys. Detailed analysis of these structures suggests that the B2 phases within the interconnected structure are formed through spinodal decomposition during the quenching process, indicating the absence of an equilibrium B2 phase above 700°C in the three alloys. The challenges associated with accurately identifying the equilibrium B2 phase in these materials are also discussed.

11:35 AM

Multi-principal Element Nanostructures via Nanosecond Laser-induced Dewetting: *Ritesh Sachan*[1]; Soumya Mandal[1]; Ashish Gupta[1]; Jordan Hachtel[2]; Andrea Konečná[3]; [1]Oklahoma State University; [2]Oak Ridge National Laboratory; [3]Brno University of Technology

Multi-principal element alloy (MPEA) nanostructures have recently gained a great deal of attention due to their promising properties relevant to energy-relevant applications. However, the development of processing techniques that could fabricate MPEA nanoparticles with spatial order and tunable physical characteristics, such as size and microstructure, has been challenging owing to achieving a homogeneous mixing of constituent elements. Here we discuss how pulsed laser melting of ultrathin alloy films can be a powerful but simple and cost-effective technique to fabricate MPEA nanostructures. Ultrathin metal films (1-30 nm) on inert substrates such as SiO2 are generally unstable, with their free energy resembling that of a spinodal system. Such films can spontaneously evolve into predictable nanomorphologies with well-defined length scales. Here we review this laser-based experimental technique and provide examples of resulting robust nanostructures that can have applications in catalysis and optics.

11:55 AM

Synthesis & Characterization of Bulk Materials Towards the Development of Spinodally-hardened, Superhard High Entropy Ceramics: *Christopher Desalle*[1]; Caillin Ryan[1]; Ryan Crealese[1]; Simon Divilov[2]; Hagen Eckert[2]; Stefano Curtarolo[2]; Douglas Wolfe[1]; [1]Penn State Applied Research Lab; [2]Duke University

The increasing demand for materials that exhibit superior thermomechanical and thermochemical properties during extreme environment operation is driven by applications such as aerospace/hypersonic vehicles, friction stir welding, and machining. High entropy ceramic alloys have garnered significant interest due to a combination of solid-solution strengthening, phase stability control, and precipitation hardening effects via coherent spinodal decomposition. With a focus on the synthesis, analytical characterization, and performance evaluation of bulk materials, experimental advances have been achieved in relation to the development of spinodally-hardened, superhard high entropy ceramics. Attrition milling studies of various constituent ceramic nanoparticles for subsequent consolidation via field-assisted sintering technology (FAST) with in-situ heat treatments have enabled the synthesis of high entropy carbonitrides. This study highlights and deconvolutes the phase dependence of elasto-plasticity while introducing in-situ sintering heat treatments to realize the effects of spinodal nucleation and decomposition on phase evolution and mechanical properties.

Oxidation and Corrosion of HEAs II

Tuesday AM
November 14, 2023

Room: Riverboat
Location: Omni William Penn

Session Chair: To Be Announced

9:00 AM Introductory Comments

9:05 AM Invited

Understanding Oxidation in High Entropy Alloys: *Todd Butler*[1]; Byron McArthur[1]; Samuel Kuhr[1]; Oleg Senkov[1]; Satish Rao[1]; Daniel Miracle[1]; [1]Air Force Research Laboratory

High entropy alloys are innovative materials that show great promise for future use in high temperature applications. Their compositional complexity offers extended ability to promote enhanced capability across mechanical, thermal and environmental domains, while reducing the barrier to balancing multiple performance factors. Oxidation resistance is of particular interest, especially in the refractory domain, due to the formation of more favorable complex oxides that do not readily form in dilute alloys. This talk will highlight the oxidation behaviors of both 3d-transition metal-based and refractory high entropy alloys. Each domain will be discussed relative to classical oxidation mechanisms and associated models. Key technical gaps and future opportunities will be addressed.

9:35 AM

Tuning Composition via Computational Thermodynamics to Improve Corrosion Resistance of CoCrFeMnNi Multi-principal Element Alloys: *David Silva*[1]; Guilherme Koga[2]; Valmor Mastelaro[3]; Michael Kaufman[1]; Amy Clarke[1]; Francisco Coury[2]; Claudemiro Bolfarini[2]; [1]Colorado School of Mines; [2]Federal University of Sao Carlos; [3]University of São Paulo

A computational thermodynamic approach has been employed to design non-equimolar CoCrFeMnNi multi-principal element alloys (MPEAs) with systematically varied compositions (Co((80-X)/2) Cr((80-X)/2)FeXMn10Ni10 with x = 30, 40 and 50) and enhanced corrosion behavior. MPEAs were successfully designed, synthesized and confirmed to possess a single-phase FCC structure. This work focuses on detailed analysis of the passivation film characteristics of these newly developed, non-equimolar MPEAs in two different electrolytes, i.e., 0.6 M NaCl and 0.5 M H2SO4 solutions, referred to as salt and acid solution environments, respectively. The characteristics of the passivation films were assessed using a potentiodynamic polarization test, immersion tests, electrochemical impedance spectroscopy (EIS), and X-ray photoelectron spectroscopy (XPS). In both electrolytes, the corrosion resistance of the three non-equimolar MPEAs was improved over that of the equimolar alloy. The present work reveals a way to increase corrosion resistance by tuning the composition via computational thermodynamics.

9:55 AM

A High Throughput to High Fidelity Study of Aqueous Passivation in [FeCoNi]CrxAly Alloys Across Classical Cr Threshold Concentration: *Debashish Sur*[1]; Emily Holcombe[2]; William Blades[3]; Howie Joress[4]; Jason Hattrick-Simpers[5]; Ben Redeman[2]; Tyrell McQueen[2]; Karl Sieradzki[3]; Mitra Taheri[2]; John Scully[1]; [1]University of Virginia; [2]Johns Hopkins University; [3]Arizona State Univeristy; [4]National Institute of Standards and Technology; [5]University of Toronto

FeCoNiCrxAly alloys with x+y < 0.25 (at.%) were studied with the goal of delineating the role of Al in long term passivation performance. A combinatorial thin film library with 177 different compositions was deposited and characterized through x-ray fluorescence and synchrotron x-ray diffraction to obtain compositions and phases present in each individual alloy. Their aqueous passivation behavior was examined using a scanning droplet cell in sulfuric acid by DC and AC electrochemical methods to identify the best-performing alloys. Bulk alloys containing Al and near the classical threshold of 12 at% Cr were prepared based on the thin-film screened compositions for further analysis. Passive film formation and growth behaviors were characterized using electrochemical techniques and x-ray photoelectron spectroscopy. An Al-Cr synergy was found to significantly improve corrosion performance. The passivation and corrosion protection behavior of Al-Cr alloys was investigated in chloride-free and chloride-containing environments.

10:15 AM

Development of Innovative Structural Materials from High Entropy Alloys Obtained by a Hybrid Powder/Wire Additive Manufacturing Process: *Ayse Uyanik*[1]; Caroline Toffolon[2]; Laure Martinelli[2]; Wilfried Pacquentin[3]; Hicham Maskrot[1]; [1]Université Paris-Saclay, CEA, Service de Recherche en Matériaux et procédés Avancés (SRMA); [2]Université Paris-Saclay, CEA, Service de Recherche en Corrosion et Comportement de Matériaux (S2CM); [3]Université Paris-Saclay, CEA, Service de Physico-Chimie (SPC)

Owing to the vast compositional space, high entropy alloys (HEAs) open a new path in the development of new materials for molten salt reactors. In this work, high-throughput screening route are used to target compositions with the desired microstructural characteristics via numerical design tools using Thermo-calc and the TCHEA5 thermodynamic database in order, to produce alloys using laser additive manufacturing technologies (Direct Energy Deposition process and a hybrid powder/wire laser innovative process). Once fabricated, the corrosion resistance of these alloys has been tested in a salt molten environment.The microstructural characterisations by scanning electron microscopy (SEM), energy dispersive spectroscopy (EDS) and X-ray diffraction (XRD) has allowed to suggest interesting alloy compositions for the targeted application.

10:35 AM Break

10:55 AM

High-temperature Oxidation Behavior of Refractory Complex Concentrated Alloys in Ta-Nb-Cr-Ti-Al system: *Willian Pasini*[1]; Filip Baciak[1]; Aleksandra Bętkowska[1]; Filip Kateusz[1]; Dorota Wilk-Kołodziejczyk[1]; Wojciech Polkowski[1]; [1]Krakow Institute of Technololgy

Refractory Complex Concentrated Alloys (RCCAs) are promising structural candidates to surpass Ni superalloys in high-temperature environments. However, the oxidation resistance of refractory metal-based alloys represents one of their major drawbacks. Recently, a novel approach to providing inherent protection for RCCA was proposed based on the alloying of Ta and Cr to produce CrTaO4 on a Ta-Mo-Cr-Ti-Al system. Nevertheless, substantial Cr and Ta additions cause the precipitation of the brittle intermetallic Laves phase. Through the calculation of semi-empirical parameters and Calphad calculations, this work explores and designs new compositions of RCCAs with varied ratios of Ta and Cr, attempting to control the Laves phase formation. Prediction and validation of oxidation behavior were performed by artificial neural network models and 24 h long TGA tests at 1300°C in synthetic air (80/20 N2/O2 by volume) to reveal initial oxidation kinetics and short-term high-temperature degradation performance of news RCCA alloys.

11:15 AM

Lateral Variation in Multi-phase HEA Passive Films: Implications for Corrosion Resistant Alloy Design: *Samuel Inman*[1]; Peter Connors[1]; Mark Wischhusen[1]; Diego Ibarra Hoyos[1]; Joseph Poon[1]; Sean Agnew[1]; John Scully[1]; [1]University of Virginia

HEAs allow for new strategies to target passivity and resistance to aqueous corrosion. The improved the compositional homogeneity can promote the formation long-range ordered or disordered solid solution oxides between multiple passivating elements. However, formation of such species can be hindered by elemental partitioning from second phase. While previous work has shown depletion of passivating elements can promote localized corrosion, little work has been done to evaluate the effects of microstructural partitioning on local and global passive film chemistry. This work evaluates corrosion behavior and lateral variation the dual-phase Al0.3Cr0.5Fe2Mn0.25Mo0.15Ni1.5Ti0.3 passive film. Two distinct compositions are formed with defined lateral bounds matching the bulk microstructure. Thus, controlling microstructural partitioning and interface engineering may be effectively utilized as a tool to alter passive film chemistry, and by extension corrosion performance. The findings are discussed with respect to the lightweight low-cost Al-Cr-Fe-Mn-Mo-Ni-Ti system and extended to general corrosion resistant CCA design principals.

11:35 AM

Mechanical, Corrosion Properties and Industrial Application of CoCrFeNiTi-based Multiprincipal Element Alloys Achieved by a Combination of Additive Manufacturing and Heat Treatment: *Tadashi Fujieda*[1]; Hiroki Sugawara[1]; Toshimi Miyagi[1]; Yuzo Daigo[1]; Kousuke Kuwabara[1]; Hiroshi Shiratori[2]; [1]Proterial, Ltd; [2]Hitachi, Ltd

CoCrFeNiTi-based multiprincipal element alloys (MPEAs) are proposed to meet the demands of high mechanical strength and corrosion resistance in additively manufactured products. First, the effectiveness of applying L-PBF to this MPEA was compared with that of using EB-PBF. The higher solidification rate during L-PBF promoted a fine uniform microstructure with no coarse precipitates, which led to superior tensile properties and a higher pitting potential in comparison to the EB-PBF specimens. In addition, the ultimate tensile strength of the L-PBF specimens increased over 1500 MPa and the corrosion rates in boiling 10% H2SO4 decreased to less than 1mm year by the microstructure control in the solution and aging heat treatments. Furthermore, the higher cobalt and chromium content of the proposed CoCrFeNiTi-based MPEA demonstrated their effectiveness in retarding acid corrosion. We will also report the applicability of the die steel coated this MPEA by L-DED to the hot forging mold.

11:55 AM

Refractory Element Free High Entropy Alloy with Exceptional Oxidation Resistance at Elevated Temperature: Pooja Jangra[1]; Aditya Balpande[1]; Ananya Chattree[1]; *Akshit Dutta*[1]; Saurabh Nene[1]; [1]Indian Institute of Technology Jodhpur

High temperature oxidation of metallic alloys is inevitable during service. However, aerospace and aeronautical components demand delayed oxidation kinetics of alloys used in them to avoid their sudden failures during service. In line of that, here we present a next generation Ni-Co-V-Fe-Cr-Si containing high entropy alloy (OR-HEA) displaying very sluggish oxidation kinetics after exposing to 1050 C up to 100 hrs in muffle furnace atmosphere. The weight gain appears to saturate at 10 hrs of exposure and showed negligible increase in weight even after 100 hrs of exposure to 1050 C. The resultant high temperature oxidation behavior is exceptional when compared with the conventional IN-718 super alloy and much better than the newly designed refractory containing HEAs in similar temperature range and corrosive atmospheres. Thus, development of OR-HEA is not only providing cost friendly but also weight-effective pathway for designing high temperature alloys of future.

Characterization of HEAs III

Tuesday AM **Room: William Penn Ballroom**
November 14, 2023 **Location: Omni William Penn**

Session Chair: To Be Announced

9:00 AM Introductory Comments

9:05 AM Invited

Robert Ritchie_INVITED PLACEHOLDER: *Robert Ritchie*[1]; [1]University of California, Berkeley

Abstract submission missing, please contact programming@tms.org with details and topic area.

9:35 AM

Predicting the Strength of Multi-principal Element Alloys: A Mechanistic Data-driven Approach: *Ali Rida*[1]; Markus Sudmanns[2]; Yanfei Wang[3]; Zhuocheng Xie[4]; Xiaolong Ma[5]; Wenxin Zhou[6]; Yejun Gu[7]; Jaafar El-Awady[1]; Huajian Gao[8]; [1]Johns Hopkins University; [2]RWTH Aachen University; [3]Peking University; [4]South China University of Technology; [5]City University of Hong Kong; [6]University of California, San Diego; [7]Agency for Science, Technology and Research; [8]Nanyang Technological University

Although Multi-principal element alloys (MPEAs) are still in their early stages of development, they have demonstrated great potential for significant improvement in material properties compared to conventional alloys. It was found that some alloys exhibit an impressive combination of strength and ductility. However, the variation in microstructure contrasts with empiric models such as the Hall-Petch relation, which aim to capture the basic trends using a few parameters. One significant challenge in developing robust physics-based models for predicting the yield stress is therefore to provide quantitative measures for the statistical uncertainty originating from the microstructural variation. Here, we present a combined mechanistic data-driven and experimental approach for predicting the yield strength in NiCoCr, NiCoV, and CrMnFeCoNi and quantify the influence of different microstructural features on the yield strength and its statistical distribution. We demonstrate the applicability of this probabilistic approach to guide the design of polycrystalline MPEAs with superior mechanical properties.

9:55 AM

Phase Decomposition in CrFeNiMn Under Thermal Aging: *Nina Perry*[1]; Anshul Kamboj[1]; Emmanuelle Marquis[1]; [1]University of Michigan

The understanding that high entropy alloys (HEAs) are stable solid solutions has been widely accepted since the discovery of these materials. However, recent studies have shown that this is often untrue, as they have revealed phase formation at high annealing temperatures. This suggests the possibility for extensive transformations at lower temperature and leaves the door open for further exploration. Indeed, our 9-week aging investigation of a CrFeNiMn alloy revealed complex phase evolution at a relatively lower annealing temperature through characterization with scanning electron microscopy, X-ray diffraction, transmission electron microscopy, and atom probe tomography. More specifically, this alloy separated into nanoscale distributions of an $L1_0$ Ni-Mn phase, an FCC Fe-rich phase, and a BCC Cr-rich phase. This microstructure is believed to be a result of two competing growth mechanisms: homogeneous nucleation and discontinuous decomposition. The findings imply that the range of properties obtainable by HEAs can potentially be expanded through microstructure tailoring.

10:15 AM

Computational Thermodynamics-guided Alloy Design and Phase Stability In Non-equimolar Cocrfemnni Multi-principal Element Alloys: An Experimental-theoretical Study: *David Silva*[1]; Gustavo Bertoli[2]; Nelson Neto[1]; Michael Kaufman[1]; Amy Clarke[1]; Francisco Coury[2]; Claudemiro Bolfarini[2]; [1]Colorado School of Mines; [2]Federal University of Sao Carlos

The formation of sigma phase (brittle and undesirable) is a real concern when engineering face centered cubic (FCC) alloys subjected to operation at elevated temperatures (600-1000 ˚C). Therefore, predicting its formation is essential in alloy design. Phase equilibria were studied in a wide range of compositions by the CALPHAD method in combination with two empirical methods for predicting sigma phase formation (valence electron concentration (VEC) and paired sigma-forming element (PSFE)). Isothermal aging treatments at 900 ºC, 1000 ˚C and 1100 ˚C for 20 h were selected, due to the fact that CALPHAD and Tsai criteria predictions for sigma phase formation diverged in some cases. Both prediction methods (CALPHAD and Tsai criteria) were compared with experimental characterization by a combination of synchrotron high energy X-ray diffraction (HEXRD) and electron backscattering diffraction (EBSD). This work will guide further studies of CoCrFeMnNi alloys potentially sensitive to sigma phase formation.

10:35 AM Break

10:55 AM

The Compositional Dependence of Deformation Mechanisms, Strength, and Ductility in a Pseudo-binary Cr-Co-Ni Alloy System: *Joshua Cicotte*[1]; Ying Yang[2]; Dunji Yu[2]; Ke An[2]; Weicheng Zhong[2]; Easo George[1]; [1]University of Tennessee - Knoxville; [2]Oak Ridge National Laboratory

We investigated the mechanical properties and deformation mechanisms off-equiatomic variants of the CrCoNi medium-entropy alloy, specifically the Co-rich alloys in the pseudo-binary Cr33-Co(x)-Ni(67-x) system. Based on neutron diffraction, we find that the Co33, Co40, and Co50 alloys are FCC solid solutions after quenching from elevated temperature whereas the Co57 alloy retains some martensitic HCP phase in an FCC solid solution. Tensile testing revealed that ductility decreases linearly with increasing Co content from a maximum in the equiatomic Co33 alloy. Ex-situ neutron diffraction of the fractured tensile specimens found significant amounts of deformation-induced HCP martensite formed during tensile testing in the Co40, Co50, and Co57 alloys. The elongation of these alloys shows a linear decrease with increasing HCP volume, directly tying the formation of HCP martensite to the reduction in ductility. Comparisons are also made to our Ni-rich pseudo-binary compositions where twinning rather than phase transformation occurs.

11:15 AM

Towards Design of Multifunctional High Entropy Alloy using Metastability Engineering: *Akshit Dutta*[1]; Ming-Hung Tsai[2]; Saurabh Nene[1]; [1]Indian Institute of Technology Jodhpur; [2]National Chung Hsing University

Conventional alloy design strategy aims to attain a specific property profile in a material and consequently gives rise to single material for single application (SMSA) analogy. Present work aims in modifying this analogy to single material for multiple application (SMMA) by designing alloys using high entropy alloy concept in synergy with metastability engineering. The main aim of the work is to attain harmonic combination of properties (at least five) in the designed alloy, giving rise to multifunctionality in it. The HEA system was formulated by choosing critical elements present in different categories of steels namely low-density steels, stainless steel, TRIP/TWIP steels and electrical steels such that the resultant alloy would show excellent strength-ductility synergy, corrosion resistance, electrical resistivity and formability. The resultant HEA out of Fe-Mn-Cr-Ni-Co-Si system demonstrated excellent combination of all proposed properties in comparison with the counter alloys thereby suggesting multifunctionality in it.

11:35 AM

Strength and Thermal Stability of Mechanically Driven Nanocrystalline High Entropy Alloys: Yuan Yao[1]; Luyan Li[1]; *Mostafa Hassani*[1]; [1]Cornell University

Nanocrystalline materials are featured by ultra-high strength but have strong tendency of grain coarsening, while high entropy alloys provide stable microstructures due to sluggish diffusion. Nanocrystalline high entropy alloys (nc-HEAs) are expected to combine the benefits of these two worlds, further pushing the performance limits of structural materials. Here we use forced mechanical mixing to fabricate a nc-HEA in solid state. Nanoindentation is used to measure the strength of the alloy and evaluate its strain rate sensitivity. The thermal stability of the alloy is also studied with isochronal and isothermal annealing experiments. We find significant contributions from grain boundary and solid solution strengthening and discuss the strain rate sensitivity of the nc-HEA in light of the interplay between the two mechanisms. We also find excellent grain size retention as well as some unexpected increase in the hardness after annealing which we attribute to the second phase precipitations in the material.

11:55 AM

Solid Solution Strengthening on CrCoNi-(Pd,V) Alloys: *Pedro Oliveira*[1]; Francisco Coury[1]; Claudemiro Bolfarini[1]; [1]Federal University of Sao Carlos

This study examined the impact of adding vanadium (V) and palladium (Pd) on the mechanical properties and deformation mechanisms of CrCoNi alloys. Pd and V (10% at) were added to the CrCoNi system, resulting in a face-centered cubic (FCC) solid solution. The addition of Pd led to a significant change in atomic mismatch, while the electronegativity of the system remained relatively unchanged. On the other hand, the addition of V aimed to create a notable difference in electronegativity without greatly affecting the atomic mismatch. Mechanical properties were assessed through hardness and tensile tests at room temperature. X-ray diffraction analysis using synchrotron radiation was performed during the tensile test to examine microstructural changes and understand deformation mechanisms. Fractured samples were analyzed using scanning electron microscopy and transmission electron microscopy. Results showed that V and Pd additions enhanced the hardness and mechanical properties compared to the equiatomic Cr33Co33Ni33 alloy.

Fundamental Theory and Modeling III

Tuesday PM **Room: Three Rivers**
November 14, 2023 **Location: Omni William Penn**

Session Chair: To Be Announced

1:40 PM Introductory Comments

1:45 PM Invited
Machine Learning Guided High Entropy Alloy Development: *John Sharon*[1]; Ken Smith[1]; Ryan Deacon[1]; Anthony Ventura[1]; Soumalya Sarkar[1]; GV Srinivasan[1]; [1]Raytheon Technologies Research Center

High Entropy Alloys (HEAs) with multiple principal elements have demonstrated enhanced properties that can rival or exceed conventional alloy systems. HEAs are typically comprised of 4 or more elements present from 5 to 35 at.% resulting in a large combinatorial composition space for which computational tools are vital to sort through combinations and identify the most promising candidates. A variety of analytical and other relatively fast computational models are available to help identify candidates. This talk will describe a machine learning framework assembled to assist in identifying candidates that leverages experimental data, published literature, as well as mechanistic models. Examples of using the framework to identify potential HEA candidates will be provided along with complementary experimental characterization and validation. Industry perspective on HEA maturation and adoption for engineering applications will also be discussed

2:15 PM
Grain Boundary Segregation in High Entropy Alloys: Theoretical Development and Mesoscale Simulations: *Fadi Abdeljawad*[1]; Milad Taghizadeh[1]; Malek Alkayyali[1]; [1]Clemson University

Owing to their far-from-dilute compositions, high entropy alloys (HEAs) exhibit unique properties that are not typically encountered in conventional alloys. Recent experiments revealed segregation of elemental species to grain boundaries (GBs) in several HEAs. Even minute amounts of alloys at GBs greatly influence boundary dynamics, including GB migration and grain coarsening. Herein, we present a theoretical and computational model of GB segregation in HEAs and its impact on GB migration. The model accounts for bulk thermodynamics and the interaction of various elemental species with GBs, and it captures various mass transport processes. Simulation results reveal a plethora of segregation behaviors, including synergistic co-segregation and induced de-segregation, that are dependent on alloy-alloy interactions within the GB. Our approach provides avenues to employ GB segregation engineering as a strategy to design HEAs with tailored microstructures.

2:35 PM
Developing CALPHAD Databases for High Entropy Alloys: Huahai Mao[1]; Martin Xing[1]; Reza Naraghi[1]; Qing Chen[1]; *Paul Mason*[2]; [1]Thermo-Calc Software AB; [2]Thermo-Calc Software Inc.

CALPHAD modeling of High Entropy Alloys presents unique challenges compared with that of conventional alloys due to the lack of a single principal element. It requires an accurate description for the entire composition range rather than just in the vicinity of the base element. Here we describe the approach taken in developing the TCHEA thermodynamic database, which contains 26 elements, where almost all underlying binary and over 500 ternary systems have been critically evaluated to capture the composition and temperature dependence. We also present the corresponding MOBHEA mobility database. The CALPHAD approach to describing composition and temperature dependence can also be extended to many other thermochemical or thermophysical properties such as density, viscosity, surface tension, thermal conductivity, and electrical resistivity. All these properties are modelled in the TCHEA database. Validation with experimental data for various HEAs and application examples will also be given.

2:55 PM
Phase-field Simulation of Phase Separation in MPEAs: *Kamalnath Kadirvel*[1]; Weisheng Cao[1]; Shuanglin Chen[1]; Yunzhi Wang[2]; Shalini Koneru[2]; Fan Zhang[1]; [1]Computherm LLC; [2]Ohio State University

MPEAs (Multi Principal Element Alloys) owing to the compositional complexity can have convoluted phase transformation pathways (PTPs). Understanding these PTPs is critical for tailoring the microstructure for specific engineering applications. We utilized the recently developed phase-field simulation tool (called PanPhasefield, https://computherm.com/panphasefield) that efficiently couples with CALPHAD databases for thermodynamic and kinetic data to simulate the spinodal decomposition in MPEAs. We studied kinetics of phase separation in Fe-Co-Mn-Ni-Cu alloy system using PanHEA database. Interestingly, the partitioning of Ni and Mn is much slower compared to other elements in the early stages of decomposition despite their relatively high atomic mobilities. However, at the later stages of decomposition, the concentration modulations of Ni and Mn were comparable to those of other elements such as Fe and Co. Simulated results were in qualitative agreement with experiments. Independent thermodynamic calculations were also performed to decouple the effect of free energy and atomic mobility.

3:15 PM Break

3:35 PM
A Computational Thermodynamics Framework with Intrinsic Short-range Order: Chu-Liang Fu[1]; *Bi-Cheng Zhou*[1]; [1]University of Virginia

CALPHAD is a leading method for modeling and calculations of phase equilibria in materials. However, the prevailing solution model used in CALPHAD, the sublattice model, is an empirical mean-field model based on the ideal entropy approximation, which makes CALPHAD inadequate for describing chemical short-range order (SRO) in alloys. Here we develop a hybrid framework by marrying advantages from the Cluster Variation Method and CALPHAD through incorporating chemical SRO into CALPHAD with a novel cluster-based solution model. We have put more physics into CALPHAD, while maintaining its practicality and efficiency. The configurational and non-configurational (vibrational, elastic, electronic) contributions to free energy are modeled separately, gaining insights into their respective effects on phase stability. Phase diagrams of representative alloy systems are calculated, showing great comparison with experiments. This hybrid CVM-CALPHAD framework represents a new methodology for thermodynamic modeling that enables SRO to be exploited for the design of novel complex concentrated alloys.

3:55 PM
Prediction of Atomic Distribution in Solid Solutions via CALPHAD-based Models: *Shalini Roy Koneru*[1]; Kamal Kadirvel[2]; Hamish Fraser[1]; Yunzhi Wang[1]; [1]Ohio State University; [2]Computherm LLC

With the advent of HEAs, there is an increased interest over the prediction of solid solution phase properties. The atomic distribution in solid solutions, i.e., if it is truly random or not, can affect the mechanical, electrical and magnetic properties. Thus, researchers attempt to predict the atomic distributions in solid solutions through calculation of interatomic interaction energies via atomistic simulations. However, the interatomic interaction energies are also inherently present in the CALPHAD databases. Thus, we developed a CALPHAD module to predict the atomic distributions by directly utilizing the existing commercial databases. Here, we extended the de Fontaine's theory and utilized the inverse of the Hessian of the free energy of the solid solution (in the single solid solution region above any miscibility gap) to calculate the pair correlation functions and thereby short-range order (SRO) parameters. We will demonstrate the model via SRO prediction in different binary and ternary alloys.

4:15 PM

Rapid Design of Eutectic and Ordered HEAs using The Alloy Optimization Software (TAOS): *Nicholas Ury*[1]; Aurelien Perron[1]; Brandon Bocklund[1]; Thomas Voisin[1]; Vincenzo Lordi[1]; Joseph Mckeown[1]; [1]LLNL

High entropy alloys (HEAs), or multi-principal complex alloys (MPEAs) unlock the composition space from traditionally single-element rich alloys and offer a vast landscape of undiscovered alloys. However, when applying constraints during the alloy design process, the actual composition space becomes much smaller. Furthermore, finding this subset of compositions as well as optimizing an alloy for certain properties by hand becomes tedious. The Alloy Optimization Software (TAOS) was designed to overcome this issue by leveraging Calphad-based software packages such as Thermo-Calc and pycalphad coupled to blackbox optimizers. TAOS allows many types of objectives and constraints to be used for optimization. Two case studies focusing on eutectic and ordered HEAs are shown and the design process, lessons learned, and experimental results of the new alloy compositions will be discussed.

4:35 PM

Thermodynamics of Refractory Compositionally Complex Alloys: *Eric Lass*[1]; [1]University of Tennessee-Knoxville

From high temperature materials that may replace Ni-based superalloys to lightweight structural alloys, refractory compositionally complex alloys (R-CCAs) containing elements from Groups IV through VI of the periodic table represent an exciting new class of alloys for future exploitation in next generation technologies. R-CCAs are most often single-phase BCC, or a majority BCC also containing secondary phases such as B2, Laves, and others. BCC alloys behave fundamentally different than FCC-based alloys, such as Al- or Ni-based superalloys, including the thermodynamically higher-order BCC-B2 phase relationship and thermally activated dislocation motion governing plastic deformation even at room temperature, which leads to the ductile-to-brittle transition exhibited by most BCC materials. This work explores the thermodynamics of these materials, including the implications of the higher-order nature of the BCC-B2 transformation on precipitation strengthening and the effects of thermodynamics on plastic deformation and transformation-induced plasticity (TRIP) behavior.

4:55 PM

Design of High Hardness Carbide Reinforced High-entropy Alloys: *Joshua Berry*[1]; Yunus Azakli[1]; Olivier Messe[2]; Katerina Christofidou[1]; Iain Todd[1]; [1]University Of Sheffield; [2]Oerlikon AM Europe GmbH

High Entropy Alloys (HEAs) present an opportunity for the design and development of new wear resistant hardmetals, to replace the conventional WC-Co cemented carbides, used in demanding metal forming applications. Suitable alloy systems require high hardness and wear resistance, including at high temperatures, while retaining ductility for damage tolerance. To streamline the search for a new high-entropy alloy system capable of satisfying the design constraints, a combined machine learning and CALPHAD approach has been undertaken, targeting FCC systems. A set of nine of the hardest predicted FCC solid solution forming HEA compositions from the machine learning model were selected and fabricated, from which four demonstrated suitable microstructure for further carbon reinforcement. Mechanical and thermal assessment of these carbide reinforced alloys will be presented and rationalised through CALPHAD.This work was supported by Oerlikon AM Europe GmbH, Engineering and Physical Sciences Research Council UK [EP/S022635/1] and Science Foundation Ireland [18/EPSRC-CDT/3584].

Powders and Additive Manufacturing I

Tuesday PM
November 14, 2023

Room: William Penn Ballroom
Location: Omni William Penn

Session Chair: To Be Announced

1:40 PM Introductory Comments

1:45 PM Invited

Refractory Metal Based HEAs for Medical Purposes: *Karin Ratschbacher*[1]; [1]Gfe Metals and Materials GmbH

Zr-Ti-Ta-Nb based HEAs provide a great range of mechanical properties, that can be used to optimize the characteristics of medical implants to their application. An alloy development approach based on data, taken from the literature was applied. The manufacturing of fully alloyed powder is required to benefit from the advantages additive manufacturing offers to produce tailored medical implants. The manufacturing route for powder will be introduced, as well as the properties of the resulting powder. A first alloy for this application has been produced and thoroughly characterized. Samples manufactured through different powder-based methods are evaluated concerning their chemical composition, crystal structure, mechanical properties.

2:15 PM

Leveraging Metastability in High Entropy Alloy Design for Grain Refinement in Additive Manufacturing: Akane Wakai[1]; *Atieh Moridi*[1]; [1]Cornell University

The use of additive manufacturing (AM) techniques enables the fabrication of intricate structures with customized properties. However, the presence of coarse grains during solidification restricts the mechanical performance of AM-produced components. This study aims to exploit the metastable phase transformations within high entropy alloys (HEAs) to enhance grain refinement during AM without the need for post processing. Specifically, by varying the Mn content in a FeMnCoCr HEA, we can systematically evaluate the effect of solidification pathway on microstructure and properties. This comprehensive exploration combines thermodynamic modeling, operando synchrotron X-ray diffraction, multiscale microstructural analysis, and mechanical testing to develop advanced HEAs for AM. These findings provide insight into the solidification fundamentals of HEAs and help establish an alloy design guideline to enhance mechanical properties in AM and contribute to pushing the boundaries of AM technology.

2:35 PM

Designing Complex Concentrated Alloys for Additive Manufacturing: Expanding the Scope of Alloy 3D Printing for Resource-constrained and Location-specific Applications: *Wei Xiong*[1]; [1]University of Pittsburgh

Additive manufacturing has emerged as a highly effective approach for fabricating intricate structures with enhanced design flexibility. Expanding upon this methodology, we investigate the potential of laser-based additive manufacturing techniques, including directed energy deposition and laser powder bed fusion, for fabricating complex concentrated alloys. Specifically, we explore the feasibility of employing a powder mixture comprising the commonly used stainless steel 316L (SS316L) and Inconel 718 (IN718) to achieve exceptional print quality. This study not only addresses the demands of resource-constrained environments but also caters to the requirements of location-specific design objectives. The resulting complex concentrated alloy exhibits a refined grain structure, showcasing remarkable stability even under conditions of high-temperature homogenization. Moreover, using alloy CALPHAD-based ICME design (ICME: Integrated Computational Materials Engineering), we discovered a new composition demonstrating superior precipitation strengthening, yielding comparable strength to IN718 while reducing manufacturing costs through increased iron content.

2:55 PM

Additive Manufacturing as a Processing Pathway for Refractory BCC+B2 Alloys: *Kaitlyn Mullin*[1]; Sebastian Kube[1]; Carolina Frey[1]; Sophia Wu[1]; Tresa Pollock[1]; [1]University of California Santa Barbara

Emulating the nickel-base superalloy gamma+gamma-prime microstructure in BCC+B2 refractory multi-principal element alloys (RMPEAs) is a promising alloy design strategy to achieve strength and ductility at high temperatures. Ru-based B2 precipitates have shown exceptional thermal stability and can even persist to melting, making traditional solutioning and aging pathways difficult. Though the rapid solidification velocities inherent to additive manufacturing (AM) may suppress B2 formation upon solidification, these conditions introduce extreme thermal stresses that often lead to microcracking in precipitation-strengthened superalloys. To investigate AM as a possible processing strategy for BCC+B2 RMPEAs, a selection of HfRu and TiRu based BCC+B2 compositions with different solvus temperatures are exposed to laser track experiments. The cracking behavior and solidification morphologies are characterized as a function of composition and process parameters. B2 precipitate morphologies in the melt pools are characterized after subsequent aging treatments.

3:15 PM Break

3:35 PM

Rapid Solidification Behavior of Refractory Multi-principal Element Alloys: *Megan Le Corre*[1]; Kaitlyn Mullin[2]; Ruben Ochoa[1]; Adriana Eres Castellanos[1]; Tresa Pollock[2]; Amy Clarke[1]; [1]Colorado School Of Mines; [2]University of California, Santa Barbara

Additive manufacturing (AM) of high temperature refractory alloys and new refractory multi-principal element alloys (RMPEAs) promises to circumvent potential fabrication challenges associated with traditional manufacturing processes like thermomechanical processing. While recent studies of RMPEAs by AM have revealed promising results, much work remains to evaluate the foundational solidification behavior associated with and responsible for the resulting microstructures and properties. Thermal gradients and solidification velocities produced by laser processing parameters in single track melts of refractory alloys were determined using heat transfer modeling and computational fluid dynamics software. These characteristics are then correlated to predicted microstructural morphologies using the Ivantsov Marginal Stability model, the Hunt modification to the Gaümann columnar to equiaxed transition model, and the Scheil-Gulliver model. Agreement or discrepancy between microstructural predictions and experimentally observed microstructures can be used to calibrate solidification models, thereby enabling tailored microstructures and properties in these alloys.

3:55 PM

Development and Characterisation of a New TiVNbMo-based Refractory High Entropy Alloy for High Temperature Applications.: *Lucy Farquhar*[1]; Robert Snell[1]; Iain Todd[1]; Russell Goodall[1]; [1]University Of Sheffield

Refractory high entropy alloys (RHEAs) offer an interesting opportunity to tailor specific material properties and especially to retain high strength at elevated temperatures. Additive manufacturing (AM) has also been successfully utilised to make these difficult to process RHEAs with increased strength and refined microstructures, though few alloys have yet been specifically developed with this process in mind. Therefore, in this work the development of a new AM-processable TiVNbMo-based RHEA is presented from theoretical design and modelling stages, experimental weld tracks, to the resulting alloy manufactured by laser powder bed fusion (LBPF). These LPBF builds were completed using both bespoke pre-alloyed powder and off-the-shelf elemental powder, with a comparison between the two feed stocks and the resulting microstructures of the parts built. The thermal and mechanical properties and oxidation behaviour of the alloy are then characterised and compared with the properties of some conventional alloys.

4:15 PM

High-throughput Computation and Process Design for Metal Additive Manufacturing: Exploring the Fe-Co-Cr-Mn-Ni System as a Case Study: *Sofia Sheikh*[1]; Brent Vela[1]; Pejman Honarmandi[1]; Peter Morcos[1]; David Shoukr[1]; Abdelrahman Kotb[1]; Raymundo Arroyave[1]; Ibrahim Karaman[1]; Alaa Elwany[1]; [1]Texas A&M University

High entropy alloys (HEAs) have gained interest for their exceptional properties, while additive manufacturing (AM) enables the fabrication of intricate HEA structures. However, AM exploration of HEAs is limited. Determining optimal processing conditions is crucial to produce defect-free parts. Surveying the printability of alloys in terms of composition and processing is challenging through experiments alone. Thus, high-throughput (HTP) computational frameworks are essential for guiding the search for printable alloys and processing parameters. In this work, various criteria for process-induced defects are considered, properties are predicted using CALPHAD, processing parameters are determined, and melt pool profile are obtained by thermal models. We verify the framework by constructing printability maps for the CoCrFeMnNi system. Furthermore, the framework searches for alloys in the Co-Cr-Fe-Mn-Ni HEA constrained-space to reduce the formation of macroscopic defects. This framework enables systematic investigation of HEA printability and serves as a valuable tool for AM-centered alloy design in HEAs.

4:35 PM

Cold Spray Additive Manufacturing of Refractory High Entropy Alloys using Elemental Powder Blends: *Matthew Dunstan*[1]; Isaac Nault[1]; Frank Kellogg[2]; [1]US Army Research Laboratory; [2]Survice Engineering

In cold spray additive manufacturing (CSAM) three dimensional components are produced by spraying powder materials onto a substrate at supersonic speeds which causes the material to deform and create bonds on impact. CSAM has many benefits including high deposition rates, large build volumes, and solid-state processing. Due to many refractory high entropy alloys (RHEA) having high strength and low ductility producing these alloys in complex geometries can be challenging. In order to enable complex geometries of these alloys this work investigates the use of elemental blends of RHEAs with CSAM to produce green compacts which are subsequently sintered in order to homogenize and densify the alloy. By using elemental blends, CSAM can take advantage of the higher sprayability of the base elements (e.g., Al, Cr, Nb, Ti) in order to spray non-sprayable elements (e.g., Mo, W) and ultimately produce a refractory high entropy alloy.

4:55 PM

Enhanced Reduction of Stable Oxides: A Synergistic Effect for Processing of a High Entropy Alloy: *Wookyung Jin*[1]; Prince Sharma[1]; Animesh Kundu[1]; Ganesh Balasubramanian[1]; Helen Chan[1]; [1]Lehigh Unversity

High entropy alloys can be successfully fabricated by the reduction of the constituent oxide powders. During the processing of Cantor alloy CoCrFeNiMn using this technique, it was found that even highly stable oxides such as Cr_2O_3 and MnO could be partially reduced by annealing in 3% H_2 -Argon, at temperatures 1000 – 1250 °C. In addition to the entropy contribution (ΔS_{ss}), it is proposed that reduction is enhanced due to the negative enthalpy of solid solution (ΔH_{ss}) of the metal in the HEA composition. A series of binary, ternary and quaternary alloys (derived from the elemental set - Co, Cr, Fe, Ni, Mn) were processed by oxide reduction. In each case, the composition of the metallic phase, as well as the microstructure and overall extent of reduction were determined. These results will be discussed in the context of predictions based on values of ΔH_{ss} and ΔS_{ss} calculated from first principles.

High-throughput and Machine Learning I

Tuesday PM **Room: Riverboat**
November 14, 2023 **Location: Omni William Penn**

Session Chair: To Be Announced

1:40 PM Introductory Comments

1:45 PM Invited
BIRDSHOT: An Accelerated Program for the Discovery and Optimization of Refractory High Entropy Alloys: *Raymundo Arroyave*[1]; Brent Vela[1]; Danial Khatamsaz[1]; William Trehern[1]; Ibrahim Karaman[1]; Weiwei Zhang[2]; Douglas Allaire[1]; Paul Mason[2]; Duane Johnson[1]; Prashant Singh[3]; Axel van de Walle[4]; Miladin Radovic[1]; Ankit Srivastava[1]; [1]Texas A&M University; [2]ThermoCalc; [3]Ames National Laboratory; [4]Brown University

The Refractory High Entropy Alloy (RHEA) space is vast and it is impossible to explore using conventional approaches to materials discovery. In this talk, we present the Batch-wise Improvement in Reduced Design Space using a Holistic Optimization Technique (BIRDSHOT) framework. BIRDSHOT incorporates the strengths of ICME and combinatorial methods, while addressing all their drawbacks, as it: (i) employs novel machine learning (ML) and data-driven search algorithms to identify efficiently the feasible regions amenable to optimization; (ii) exploits correlations to fuse simulations and experiments to obtain efficient ML models for predicting PSPP relations; (iii) uses Bayesian Optimization (BO) to make globally optimal iterative decisions regarding which region in the RHEA space to explore/exploit, leveraging existing models and data; (iv) is capable of carrying out multiple optimal parallel queries to the design space. We show how we have been using BIRDSHOT to search for next generation refractory alloys for turbine engine applications.

2:15 PM
Automated Characterization and Bayesian Prediction of High Strength Multi-principal Element Alloys: *Eddie Gienger*[1]; Maitreyee Sharma Priyadarshini[2]; Denise Yin[1]; Lisa Pogue[1]; Justin Rokisky[1]; Paulette Clancy[2]; Christopher Stiles[2]; [1]JHU APL; [2]Johns Hopkins University

Multi-principal element alloys (MPEAs) are an active research area for their desirable corrosion resistance, strength-to-weight ratios and high temperature survivability. However, design of new MPEAs with tailored performance is complex, and traditional Edisonian discovery methods are slow. AI-guided discovery is promising for these materials, but there is limited training data. Here, we demonstrate a high-throughput characterization pipeline enabling registration of mechanical properties from nano-indentation with material microstructure. These results, combined with literature data, are used to inform a novel physics-based material discovery framework, PAL 2.0. This new method leverages the advantages of Deep Learning with Bayesian Optimization, making it accessible to the data-scarce field of MPEAs. MPEA recommendations from PAL2.0 are synthesized and characterized to determine yield strength and hardness. This "in-the-loop" computational-experimental approach is one of the first of its kind and has a disruptively attractive potential in the field of materials discovery.

2:35 PM
Yield Strength-plasticity Trade-off and Uncertainty Quantification in ML-based Design of Refractory High-entropy Alloys: *Stephen Giles*[1]; Debasis Sengupta[1]; Hugh Shortt[2]; Peter Liaw[2]; [1]CFD Research Corp; [2]University of Tennessee, Knoxville

Development of process-structure-property relationships in materials science is an important and challenging frontier which promises improved materials and reduced time and cost in production. Refractory high entropy alloys (RHEAs) are a class of materials that are capable of excellent high-temperature properties. However, due to their multi-component nature, RHEAs have a vast composition space which presents challenges for traditional experimental exploration. Here, quantitative models of compressive yield strength and room-temperature plasticity are developed through a deep learning approach. Uncertainty quantification is performed through a variety of statistical validation techniques. Model predictions are experimentally validated through collection of recent literature and the synthesis and experimental characterization of two new, unreported RHEAs: AlMoTaTiZr and Al0.239Mo0.123Ta0.095Ti0.342Zr0.201. Finally, through the application of model interpretability, features having the greatest impact on both the mechanical property and uncertainty of the deep learning models are revealed, and shown to agree well with current physics and materials science theory.

2:55 PM
Accelerating the Discovery of Lightweight High Entropy Alloys for Extreme Conditions: *Michael Miller*[1]; Jianliang Lin[1]; Mirella Vargas[1]; John Macha[1]; [1]Southwest Research Institute

High entropy alloys (HEAs) represent a vast, largely unexplored space of material systems with potentially revolutionary combinations of properties such as strength at high temperatures and resistance to oxidation and corrosion. Compositions in these material systems have the potential to surpass the operational temperature limits of current state of the art high temperature alloys. However, the search space for candidate alloys is huge, making efficiency and optimization of the exploratory process crucial. A multifaceted alloy discovery approach has been undertaken that couples advanced computational materials modeling, synthesis of combinatorial thin-film libraries, and high throughput experimentation to rapidly assess the properties of synthesized alloys and provide feedback loops to further refine future modeling and alloy synthesis. The present focus is on discovering lightweight high entropy alloys (LHEAs), a subset of HEAs with potentially unique properties. By including elements with low atomic numbers, we have discovered LHEAs exhibiting stable, single phase domains.

3:15 PM Break

3:35 PM

Fusing Analytical Models and Hardness Experiments for Accelerated Optimization of Yield Strength in RHEAs: *Brent Vela*[1]; Danial Khatamsaz[1]; Cafer Acemi[1]; Prashant Singh[2]; Douglas Allaire[1]; Raymundo Arroyave[1]; Ibrahim Karaman[1]; Duane Johnson[2]; [1]Texas A&M University; [2]Ames Laboratory

Refractory high entropy alloys (RHEAs) have gained attention as potential replacements for Ni-based superalloys in gas turbine applications. Improving their properties, such as their high-temperature yield strength, is crucial to their success. Unfortunately, exploring this vast chemical space using only experimental approaches is impractical due to the cost of testing of candidate alloys at operation-relevant temperatures. The lack of reasonably accurate strength models makes traditional Integrated Computational Materials Engineering (ICME) methods inadequate. We address this challenge by combining machine-learning models, easy-to-implement physics-based models, and inexpensive proxy experiments to develop robust and fast-acting models via Bayesian-updating. The framework combines data from one of the most comprehensive databases on RHEAs with a widely used physics-based strength model for BCC-based RHEAs into a compact predictive model that is significantly more accurate that the state-of-the-art. This model is amenable to ICME frameworks that screen for RHEAs with superior high-temperature properties.

3:55 PM

Charge-density Based Convolutional Neural Networks for Stacking Fault Energy Prediction in Concentrated Alloys: Jacob Fischer[1]; Gaurav Arora[2]; Serveh Kamrava[3]; Pejman Tahmasebi[3]; *Dilpuneet Aidhy*[1]; [1]Clemson University; [2]Fermi Lab; [3]Colorado School of Mines

A descriptor-less machine learning (ML) approach based only on charge density extracted from density functional theory (DFT) is developed to predict stacking fault energies (SFE) in concentrated alloys. Often, in ML models, textbook physical descriptors such as atomic radius, valence charge and electronegativity are used which have limitations because these properties 'adjust' in concentrated alloys due to varying nearest neighbor environments. We illustrate that, within the scope of DFT, the search for descriptors can be circumvented by charge density, which is the backbone of the Kohn-Sham DFT and describes the system completely. The descriptors are captured by charge-density inherently. The model is based on convolutional neural networks (CNNs) as one of the promising ML techniques. The performance of our model is evaluated by predicting SFE of concentrated alloys with an RMSE and R2 of 6.18 mJ/m2 and 0.87, respectively, validating the accuracy of the approach.

4:15 PM

Design Metastability in High-entropy Alloys by Tailoring Unstable Fault Energies: Chenyang Li[1]; Xing Wang[2]; Wei Xiong[2]; *Wei Chen*[1]; [1]Illinois Institute of Technology; [2]University of Pittsburgh

Metastable alloys with transformation-/twinning-induced plasticity (TRIP/TWIP) can overcome the strength-ductility trade-off in structural materials. Originated from the development of traditional alloys, the intrinsic stacking fault energy (ISFE) has been applied to tailor TRIP/TWIP in high-entropy alloys (HEAs) but with limited quantitative success. Here, we demonstrate a strategy for designing metastable HEAs and validate its effectiveness by discovering seven alloys with experimentally observed metastability for TRIP/TWIP. We propose unstable fault energies as the more effective design metric and attribute the deformation mechanism of metastable face-centered cubic alloys to unstable martensite fault energy (UMFE)/unstable twin fault energy (UTFE) rather than ISFE. Among the studied HEAs and steels, the traditional ISFE criterion fails in more than half of the cases, while the UMFE/UTFE criterion accurately predicts the deformation mechanisms in all cases. The UMFE/UTFE criterion provides an effective paradigm for developing metastable alloys with TRIP/TWIP for an enhanced strength-ductility synergy.

4:35 PM

High Throughput Multi-objective Optimization of FCC Complex Concentrated Alloys for Extreme Conditions: *Ibrahim Karaman*[1]; Raymundo Arroyave[1]; James Paramore[2]; Brady Butler[2]; Trevor Hastings[1]; Danial Khatamsaz[1]; Daniel Lewis[1]; Mrinalini Mulukutla[1]; Nicole Person[1]; Daniel Salas[1]; Wenle Xu[1]; Matthew Skokan[1]; Douglas Allaire[1]; George Pharr[1]; [1]Texas A&M University; [2]Army CCDC Army Research Laboratory

The FCC Complex Concentrated Alloys (CCA) compositional space is very broad, making it almost impossible to cover using conventional approaches to materials discovery. This talk will present an implementation of a framework combining an iterative multi-constrain multi-objective Bayesian optimization technique with CALPHAD-based phase stability predictions and machine learning-based modeling. This framework has been implemented for efficiently exploring the compositional space of FCC CCAs containing three or more elements among Co, Cr, Fe, Ni, V and Al, searching for alloys with the most optimum mechanical properties under extreme conditions. A total of 5 iterations (80 alloys) were produced and characterized in less than 9 months. These 80 alloys, which are only 0.15% of the total pool of 53124 alloys, were sufficient for achieving a clear picture of the objective mechanical properties Pareto front, demonstrating the high efficiency of the applied framework as compared to traditional approaches to materials discovery.

4:55 PM

High-entropy Materials Design by Integrating the First-principles Calculations and Machine Learning: A Case Study in the Al-Co-Cr-Fe-Ni System: *Guangchen Liu*[1]; Songge Yang[1]; Yu Zhong[1]; [1]Worcester Polytechnic Institute

The first-principles calculation is widely used in high-entropy materials. However, this approach may consume many computational resources for complex systems, limiting the development of property maps for the related materials across the whole composition range. This work chooses the most prevalent Al-Co-Cr-Fe-Ni system (FCC and BCC) for our investigation. A comprehensive database of properties (e.g., phase stabilities and elastic properties) was established by combining the first-principles calculation results and machine learning: starting from unary, binary, ternary, and quaternary, then extending into quinary systems. A comparable software program was also developed by utilizing this database. Furthermore, the information/mechanism that underlies the database was thoroughly studied by screening and statistical analysis.

Wednesday Plenary

Wednesday AM **Room: William Penn Ballroom**
November 15, 2023 **Location: Omni William Penn**

Session Chair: To Be Announced

8:00 AM Introductory Comments

8:10 AM Plenary
Designing Chemical Inhomogeneities in Concentrated Complex Alloys to Circumvent The Strength-ductility Trade-off: *Evan Ma*[1]; [1]Xi'an Jiaotong University

In HEAs, the chemical inhomogeneity has two prongs that can be present separately, but sometimes co-exist: i) concentration fluctuation/undulation that can be intentionally enlarged and manipulated [1]); ii) local chemical order [2] that arises from the varying chemical affinity among the constitutent species. Both aspects roughen the atomic and energy landscape, making it easy for the deformation carriers (dislocations and twins) to stall, multiply and accumulate, such that HEAs have an unusal ability to work-harden on the fly with increasing strain. These dynamic effects on defect evolution help delocalize the plastic strain, making it practical to achieve pure-metal-like ductility simultaneously with gigapascal yield strength, including in BCC refractory HEAs [3] that normally suffer from low tensile ductility. [1] H. Li et al., Nature, 604 (2022) 273-279; [2] X. Chen et al., Nature, 592 (2021) 712-716; [3] L. Wang et al., Nature Mater. (2023) April 10.

8:50 AM Break

Processing, Microstructure, and Properties of HEAs II

Wednesday AM **Room: Three Rivers**
November 15, 2023 **Location: Omni William Penn**

Session Chair: To Be Announced

9:00 AM Introductory Comments

9:05 AM Invited
Controlling the Sources of Interstitial Constituents in Refractory Complex Concentrated Alloys: Calvin Belcher[1]; Sakshi Bajpai[1]; Vivek Verma[1]; Benjamin MacDonald[1]; *Diran Apelian*[1]; Enrique Lavernia[1]; [1]University Of California Irvine

Recent findings reveal that interstitial constituents, especially oxygen and nitrogen, inadvertently introduced in refractory complex concentrated alloys (RCCAs) significantly contribute to, and convolute observations of, ductility and strength of the alloys at room temperature. Plasma arc melting (PAM) has facilitated the quest for RCCAs showcasing remarkable blends of strength and ductility. In this work, we studied the composition and chemistry of residual gases in the PAM chamber environment during arc melting using a mass spectrometer to better quantify methodologies utilized to control sources of oxygen and nitrogen, in arc melted RCCAs. Moreover, thermodynamic mechanisms of the absorption of interstitial constituents was investigated by arc melting MoNbTaW and NbTiZr RCCAs. With respect to interstitial constituents, the RCCAs were characterized using electron microscopy and atom probe tomography. Correlations between the microhardness and microstructures of the RCCAs aided elucidation of the influence of the interstitial constituents on the mechanical properties of the RCCAs.

9:35 AM
Complex Concentrated Alloys with Architectured Microstructures: A New Design Strategy for High-temperature Applications: *Jean-Philippe Couzinie*[1]; Loic Perriere[1]; Ines Crouzet[1]; Regis Poulain[1]; Frederic Prima[2]; Guy Dirras[1]; [1]CNRS; [2]IRCP

Over the last two decades, efforts have been made to break with the conventional alloy design and the concept based on multi-principal elements has raised a lot of attention. Thanks to their capacity to maintain high strength properties for T>1000°C, refractory complex concentrated alloys (RCCAs) have received attention for high-temperature (HT) applications. Promising compositions are found in alloy systems with intermetallic B2 phase together with disordered BCC phase. However, and in addition to the microstructural instability, most of those materials have been observed to lose their HT strength above $0.6T_m$. Another way to push the boundaries is the formation of architectured microstructures in these complex alloys. To do so, an option is the use of interface-driven microstructures with finely distributed phases. In that way, the development of eutectic RCCAs can meet with this challenge and the design strategy will be discussed in light of recent results gathered by our consortium.

9:55 AM
Deformation Behavior and Damage Evolution in AlCoCrFeNi2.1 Eutectic High Entropy Alloys: *Cal Siemens*[1]; Jidong Kang[2]; David Wilkinson[1]; [1]McMaster University; [2]CanmetMATERIALS

The AlCoCrFeNi2.1 eutectic HEA (EHEA) is a duplex casting alloy exhibiting high strength and moderate ductility. However, there is currently little work published on mechanisms controlling damage and fracture for this EHEA. A series of EHEAs were fabricated including as-cast and hot rolled variants, plus one with increased Fe content (termed the Fe-EHEA). In-situ techniques involving micro-digital image correlation and x-ray computed tomography were used to characterize the distribution of deformation and damage evolution at the microscale while under strain. These methods were paired with scanning electron microscopy and fracture toughness measurements to determine phase composition and defect sensitivity. Micro-crack nucleation and early strain localization were found to be controlling fracture mechanisms for the cast alloys. The Fe-EHEA was found to exhibit improved phase co-deformation and elongation to fracture, while maintaining tensile strength, when compared to the base EHEA composition. This work showcases fine-tuning HEA composition to tailor mechanical properties.

10:15 AM
Microstructure and Mechanical Properties of Mo-Nb-Ti-V-W-Zr Refractory High Entropy Alloys Developed using a Data-driven Inverse Alloy Design approach: *Lavanya Raman*[1]; Marcia Ahn[1]; Arindam Debnath[1]; Shuang Lin[1]; Adam Krajewski[1]; Shunli Shang[1]; Wesley Reinhart[1]; Allison Beese[1]; Bed Poudel[1]; Zi Kui Liu[1]; Shashank Priya[1]; Wenjie Li[1]; [1]Pennsylvania State University

The concept of heterogeneous/composite microstructure has proved as an effective approach in achieving an optimum combination of high strength and ductility. In MoNbTaW-containing refractory high entropy alloys, adequate strength and ductility are reported by the addition of V and Zr by tailoring the microstructure. Our work generates the desired compositions using high-throughput computational, machine-learning models, and inverse design. The selected compositions based on elements Mo-Nb-Ti-V-W-Zr are manufactured utilizing vacuum arc melting and field-assisted sintering technology. The phase formation is correlated using CALPHAD. ML models are used to predict the mechanical properties of the alloy and are validated with experimental mechanical data obtained from the three-point bend and compression tests. The deformation of different phases is also understood from nanoindentation studies. The effect of the synthesis route on the phase formation and mechanical data is also established. The interactive design strategy adopted is applicable to other materials systems including HEAs.

10:35 AM Break

10:55 AM
Effect of Rapid Solidification Process on Microstructure, Transformation Temperature and Superelastic Properties of (TiZrHf)50Ni25Co10Cu15 HESMAs: *Izaz Rehman*[1]; Yeon-wook Kim[2]; Tae-hyun Nam[1]; [1]Gyeonsang National University; [2]Keimyung University

The effects of the rapid solidification process on microstructure, transformation temperatures and superelastic properties of multi-component (TiZrHf)50Ni25Co10Cu15 high-entropy shape memory alloy (HESMAs) were investigated. Two ingots of (TiZrHf)50Ni25Co10Cu15 HESMAs were prepared by arc-melting. As-spun fibers from (TiZrHf)50Ni25Co10Cu15 alloy ingot were prepared by a rapid solidification process. The microstructure of the solution-treated (TiZrHf)50Ni25Co10Cu15 alloy specimen consisted of a (NiCoCu)-rich matrix and (TiZrHf)2(NiCoCu)-type phase while the microstructure of as-spun (TiZrHf)50Ni25Co10Cu15 fiber specimen consisted of (TiZrHf)-rich matrix. The (TiZrHf)2(NiCoCu)-type phase is dissolved in the matrix of as-spun fibers due to the rapid solidification process. The martensitic transformation start temperature of (TiZrHf)50Ni25Co10Cu15 alloy increased from 53.5 to 91.5 after the rapid solidification process. Both solution-treated (TiZrHf)50Ni25Co10Cu15 alloy and as-spun (TiZrHf)50Ni25Co10Cu15 fiber specimens showed clear superelasticity and the total recovered strain of (TiZrHf)50Ni25Co10Cu15 alloy increased from 4.6 % to 5.7% after rapid solidification process.

11:15 AM
High-throughput Design, Synthesis, and Characterization of Refractory High Entropy Alloys (RHEAs): *Cafer Melik Ensar Acemi*[1]; Eli Norris[1]; William Trehern[1]; Brent Vela[1]; Raymundo Arroyave[1]; Ibrahim Karaman[1]; [1]Texas A&M University

Refractory alloys are promising for high-temperature applications because of their high strength at elevated temperatures, high thermal conductivity, low thermal expansion coefficient, and operability under oxidizing conditions. One hundred twenty-five refractory high entropy alloys (RHEAs) have been designed to exhibit single BCC phase at elevated temperatures, target yield strength (>200 MPa) at 1300°C, density (<9 gr/cc), thermal conductivity (>9 W/mK), linear thermal expansion (<2%) between ambient and 1300 , and narrow solidification range for additive manufacturability. Designed compositions are synthesized with high-throughput vacuum arc melting and characterized via electron microscopy (SEM/EDX), XRD, Vickers microhardness, nanoindentation, compression, tension, thermal transport, and thermal expansion experiments. In as-cast state, all samples had BCC phase with dendrites. Homogenization heat treatments at 1800°C and 1925°C are performed based on diffusion calculations centered around the compositional difference and dendrite arm spacing. Compression/tension experiments are then performed at high temperatures to compare with the predicted high-temperature properties.

11:35 AM
The Fundamentals of Recrystallization in Binary Niobium Alloys: *William Waliser*[1]; [1]Colorado School Of Mines

Nb3Sn superconductor wires are the leading option for next-generation particle accelerator magnets, which require heat treatment. Additions of Hf to Nb precursor alloys assist in maintaining finer grain sizes, which result in increased superconductor performance. However, increased demand and reliance on constrained resources such as Hf poses sustainability concerns for future projects, i.e. Future Circular Collider and the development of refractory multi-principal element alloys (RMPEAs). To identify cost effective alternatives, a series of binary Nb-X alloys, including X=Ti, Zr, Hf, V, Ta, Mo, W, and Re, were fabricated and cold rolled to observe the effects of composition and deformation energy on recrystallization and grain growth processes. Samples were heat treated and resulting microstructures were characterized. Thermomechanical processability and mechanical properties of the alloys were also assessed. These results will inform the development of RMPEAs for superconductor and aerospace applications.

11:55 AM
Lightweight Refractory High Entropy Alloy with Extreme Ductility: *Saurabh Nene*[1]; Aditya Balpande[1]; Akshit Dutta[1]; [1]Indian Institute of Technology Jodhpur

Refractory high entropy alloys (R-HEAs) have gained enormous attention owing to their extreme chemical stability and high strength at elevated temperatures. However, they exhibit very limited formability at room temperature (RT) and extremely high cost and density thereby limiting their applications. Here we present a refractory Ti58-x-yZr16V16Nb10AxMoy high entropy alloy (Ti-HEA) having a very low density of 5.6 g/cc and extreme tensile ductility of 50 % at RT along with the yield strength of 1.1 GPa. The excellent property profile of Ti-HEA is attributed to the smart design strategy adopted for Ti-HEA which involves combination of HEA, valence electron configuration theories thereby activating slip dominated deformation in single phase -b.c.c. equiaxed micro-structure in-as-cast state.

Performance in Extreme Environments I

Wednesday AM
November 15, 2023

Room: William Penn Ballroom
Location: Omni William Penn

Session Chair: To Be Announced

9:00 AM Introductory Comments

9:05 AM Invited
Complex Alloys for Extreme Aerospace Environments: *Austin Mann*[1]; Ali Yousefiani[1]; Timothy Smith[2]; Harikirshnan Rajendran[1]; Atsushi Sato[3]; Pimin Zhang[3]; Yining He[3]; David Crudden[3]; [1]Boeing Research & Technology; [2]Nasa Glenn Research Center; [3]Alloyed Ltd

Desire for ultra-high capability aerospace vehicles and systems operating in extreme environments, and the increasing maturity level of cutting-edge manufacturing technologies is quickly advancing the sophistication of component design. However, high performance designs for harsh service conditions place additional demand on the materials of construction, and can potentially outpace current state-of-the-art material capabilities. Our team has been addressing this challenge by developing complex concentrated alloys/composites and their associated powder-based methods of manufacturing for extreme environment aerospace components, specifically topologically optimized heat exchangers and turbine blades. These new classes of disruptive and ultra-high-performance material solutions are being developed in pursuit of continuous operation under moderate to high sustained stresses at temperatures ranging from 1500°F to 3300°F (with active/passive cooling), for minutes to tens of thousands of hours. Applications of these complex alloys and simulated service testing will also be described.

9:35 AM

Discovery and Development of Novel, Ultrahigh-temperature Alloys and Coatings for Jet Engine and Industrial Gas Turbine Applications: *Philseok Kim*[1]; Pankaj Trivedi[1]; Ashok Gidwani[1]; Toni Marechaux[1]; Christian Vandervort[1]; Peter de Bock[1]; [1]ARPA-E, Department of Energy

An introduction to Advanced Research Projects Agency – Energy (ARPA-E)'s Ultrahigh Temperature Impervious Materials Advancing Turbine Efficiency (ULTIMATE) program as well as the program findings to date will be presented and discussed. The ULTIMATE program aims to develop ultrahigh temperature materials for gas turbines used in power generation and aviation industries, enabling them to operate continuously at 1300°C (2372°F) in a stand-alone material test environment, or with coatings, enabling gas turbine inlet temperatures of 1800°C (3272°F) or higher. The successful materials must be able to withstand not only the highest temperature in a turbine but also the extreme stresses imposed on turbine blades. Manufacturing processes for turbine components using these novel alloys are concurrently developed, enabling complex geometries that can be seamlessly integrated in the system design. Progress in environmental barrier coatings and thermal barrier coatings will also be presented.

9:55 AM

The Mechanical Properties and Tribological Performance of High Entropy $(AlCoCrNiSi)_{100-x}N_x$ Thin Films: *Tongyue Liang*[1]; Sima Alidokht[2]; Richard Chromik[1]; [1]McGill University; [2]Memorial University of Newfoundland

Thin films of $(AlCoCrNiSi)_{100-x}N_x$ were deposited on silicon wafers using pulsed DC magnetron sputtering technique, with nitrogen gas flow ratios (R_{N2}) of 0, 0.33, and 0.50. The structure and properties of the films were analyzed for elemental composition, surface and cross-sectional morphology, microstructures, roughness, and mechanical properties. Using nanoindentation, the coating deposited at R_{N2} = 0.50 had the highest hardness (10.7±0.5 GPa) and reduced modulus (176±5 GPa). Microtribology testing was conducted using a 20 µm radius spherical diamond tip under ambient air, applying six loads ranging from 0.5 mN to 9 mN. The worn surfaces were characterized using atomic force microscopy. The coefficient of friction was evaluated to investigate the elastic and plastic behaviors of the coating using Schiffman's model. The coating without nitrogen displayed a predominant plastic behavior during the initial cycles, while the coating deposited at R_{N2} = 0.33 demonstrated a more elastic behavior, particularly at lower loads.

10:15 AM

Novel High-entropy Metal-ceramic Composites with Superior Mechanical Properties: *Bai Cui*[1]; Xin Chen[1]; Fei Wang[1]; Xiang Zhang[1]; Shanshan Hu[2]; Xingbo Liu[2]; Samuel Humphry-Baker[3]; Michael Gao[4]; Lingfeng He[5]; Yongfeng Lu[1]; [1]University of Nebraska-Lincoln; [2]West Virginia University; [3]Imperial College London; [4]National Energy Technology Laboratory; [5]North Carolina State University

A new concept of high-entropy metal-ceramic composites (HEMCC) has been proposed that combines the outstanding physical properties of both high-entropy alloy (HEA) and high-entropy ceramic (HEC). As the first HEMCC system, to the best of our knowledge, TiTaNbZr-(TiTaNbZr)C, has been developed by a powder metallurgy process. Both the HEA and HEC phases with non-equimolar compositions exhibit body-centered cubic (BCC) and rock-salt B1 crystal structures, respectively, and both have non-equimolar compositions. With the increase of the HEC phase in HEMCC, the hardness is enhanced while the density and fracture toughness are decreased. HEA50C shows a favorable combination of flexural strength and fracture toughness at room temperature and a high compressive strength at 1300 ºC. The optimized mechanical performance of HEMCC might be attributed to the combination of the ductile HEA and strong HEC phases, smaller grain size, and crack trapping at HEC/HEA interfaces.

10:35 AM Break

10:55 AM

Effects of Si and B Contents on the Microstructure and Mechanical Properties of Boron Enhanced Complex Concentrated Silicides: *Willian Pasini*[1]; Adelajda Polkowska[1]; Rafa Nowak[1]; Wojciech Polkowski[1]; [1]Krakow Institute of Technololgy

Designing and developing new high-temperature structural materials surpassing Ni superalloys limitations is a significant challenge in materials science. Boron Enhanced Complex Concentrated Silicides (BECCSs) – a novel concept of high entropy-derived ultra-high temperature materials combines the concepts of RM-Si-B silicides, RCCAs, and ultra-high-temperature borides building a bridge between lightweight, oxidation-resistant but brittle silicides and high-strength, refractory metallic alloys. A Central Composite Design (CCD) were employed to explore the effect of Si and B additions on BECCSs microstructure, mechanical response and performance. Nine different compositions (NbMo0.9W0.2Ta0.4Ti1.8)1-x-ySixBy, have been manufactured by arc-melting, while their SEM/EDS/EBSD, micro-indentation methods, were used to evaluate the microstructure and mechanical properties at room temperature. The results allow for the identification of specific phase constituents, and it has also been demonstrated that switching from BCC solid solutions to intermetallic-based alloys results in a significant increase in hardness.

11:15 AM

Sulfidation Behavior of NbTiCr Multicomponent Alloy: *Isabela Dainezi*[1]; Brian Gleeson[2]; Carlos Rovere[1]; [1]Federal University of Sao Carlos; [2]University of Pittsburgh

The new properties of multicomponent alloys show promising results that are relevant to various applications, such as strategic industries. Currently, one challenging aspect in area of materials for harsh service environments is to design alloys that are resistant to sulfidation at high temperatures. Sulfur is one of the most common corrosive contaminants in high-temperature industrial environments, including fuel and feedstocks. The principal aim of this study was to investigate the sulfidation behavior of a NbTiCr alloy in the as-cast and hot-isostatically pressed (HIP) conditions in a reducing H2S/H2 gas mixture at different temperatures. The sulfidation behavior of NbTiCr was compared to as-received HAYNES 188 at temperatures between 600 and 1100°C and exposures for 20 to 100 hours. The preliminary results show that the multicomponent alloy has significantly superior sulfidation resistance compared to the conventional 188 alloy. The modes of degradation will be compared and assessed in this presentation.

11:35 AM

Influence of the Fabrication Process on the Corrosion Behavior of Two High Entropy Alloys in Molten Solar Salt: *Paula Olmos*[1]; Rita Carbajales[1]; Celia Sobrino[1]; [1]Universidad Carlos III de Madrid

One field where the development of materials resistant to extreme environments is crucial is advanced power generation systems, such as Solar Concentrated Power (CSP) plants, which employ molten salt (solar salt: 40% KNO3/60% NaNO3) as a thermal storage medium. This study examines the feasibility of using HEAs as a material for components exposed to these solar salts, assessing their corrosion resistance in this medium. The study includes an original Co-free composition, FeCrMoAlTiNi,, and another eutectic composition, AlFeCrCoNi, previously reported to exhibit good corrosion results in marine environments. HEAs were produced using Arc Melting and Powder Metallurgy techniques. The latter processing route was chosen to achieve greater microstructural control, using rapid and ultra-rapid field-assisted sintering methods, such as thermomechanical sintering, Spark Plasma Sintering (SPS), and Electrical Resistance Sintering (ERS). The results provide insight into the effect of processing route on corrosion resistance, demonstrating an improvement over the reference material (stainless steel).

11:55 AM

Development of High Entropy Alloy based Coatings via Directed Energy Deposition (DED) Additive Manufacturing for Nuclear Applications: *Subhashish Meher*[1]; Mohan Nartu[1]; Chinthaka Silva[1]; Isabella van Rooyen[1]; Calvin Downey[2]; Luis Nunez[2]; Michael Maughan[3]; Yogesh Sighla[3]; [1]Pacific Northwest National Laboratory; [2]Idaho National Laboratory; [3]University of Idaho

Advanced coatings systems have been utilized to protect bulk components from extreme environments such as thermal and mechanical stresses, corrosion and irradiation in nuclear reactors. The current work focuses on development of new coating materials via advanced manufacturing (AM) techniques and their advanced characterization. Here, a powder-based directed-energy deposition (DED) technique is used to synthesize functionally graded high entropy alloys (HEAs) between three commonly industrial alloys: IN718, SS316L, and 70Co30Cr. The HEAs are of interest due to their possible high strength and hardness, wide operational temperature ranges, creep and diffusion resistance, and radiation resistance. Samples are fabricated with a 1:1:1 ratio of IN718, SS316L, and 70Co30Cr where IN718 is a source of nickel and chrome, SS316 is a source of iron and chrome, and 70Co30Cr is a source of cobalt and supplemental chrome. For each sample, overall build quality, microstructure, compositional distribution, phases analyses were studied by transmission electron microscopy.

High-throughput and Machine Learning II

Wednesday AM **Room: Riverboat**
November 15, 2023 **Location: Omni William Penn**

Session Chair: To Be Announced

9:00 AM Break

9:30 AM Introductory Comments

9:35 AM

Design Nb-Ta-Mo-W-Re-based Alloys with Enhanced Ductility: *Liang Qi*[1]; [1]University of Michigan

Body-centered cubic (bcc) refractory multicomponent alloys are of great interest due to their remarkable strength at high temperatures. Optimizing the chemical compositions of these alloys to achieve a combination of high strength and room-temperature ductility remains challenging. Many efforts have been made to include Group IV or other elements (e.g. Ti and Zr) to enhance their ductility. However, such alloying elements may reduce the melting points and high-temperature mechanical properties. In this study, we focus on the manipulation of alloy chemical compositions only in five common refractory elements (Nb-Ta-Mo-W-Re), First-principles calculations, regression surrogate models, and machine-learning interatomic potentials are applied to predict planar fault energies and elastic properties in these alloy systems. These results will be used to estimate the ductility of the corresponding alloys based on different types of ductility criteria (Pugh ratio, Rice-Thomson criterion, and Rice criterion) to guide the design of refractory multicomponent alloys with enhanced ductility.

9:55 AM

Designing High-entropy Alloys: Aluminum Refractory B2 Phases: *Diego Ibarra*[1]; Jie Qi[1]; Xuesong Fan[2]; Debashish Sur[1]; Rui Feng[2]; John Scully[1]; Peter Liaw[2]; Joseph Poon[1]; [1]University of Virginia; [2]The University of Tennessee, Knoxville

Ordered high-entropy body-centered-cubic (BCC) phases with the B2 structures, particularly those formed with refractory elements and aluminum (Al-RHEAs), are of interest due to their high strength, corrosion resistance, and oxidation resistance. The incorporation of Al lowers the density and promotes the long-range atomic ordering, which in turn stabilizes the B2 formation, and strengthens the material but usually deteriorates ductility. B2 Al-RHEAs are screened using machine learning (ML) models to predict B2 formation and toughness. High prediction accuracy is achieved. Several Al-RHEAs have shown large compression plasticity and high strength and exhibit some tensile ductility.

10:15 AM

Ab-initio Tensile Tests Applied to BCC Refractory Alloys: *Vishnu Raghuraman*[1]; Michael Widom[1]; Michael Gao[2]; [1]Carnegie Mellon University; [2]National Energy Technology Laboratory

Refractory metals exhibit high strength at high temperature, but often lack ductility. Multi- principle element alloys such as high entropy alloys offer the potential to improve ductility while maintaining strength, but we don't know a-priori what compositions will be suitable. A number of measures have been proposed to predict the ductility of metals, notably the Pugh ratio, the Rice-Thomson D-parameter, among others. Here we examine direct ab – initio simulation of de- formation under tensile strain, and we apply this to a variety of Nb- and Mo-based binary alloys and to several quaternary alloy systems. Our results exhibit a variety of ductility mechanisms including slip, stacking faults, transformation and twinning. We relate these deformations to otherpredictors of ductility, and we correlate these with each other.

10:35 AM Break

10:55 AM

ML-based High-throughput Search to Identify Refractory High Entropy Alloy with Trade-off Mechanical Properties: *Debasis Sengupta*[1]; Stephen Giles[1]; Hugh Shortt[2]; Peter Liaw[2]; [1]CFD Research Corp; [2]University of Tennessee, Knoxville

Identifying Refractory High Entropy Alloy (RHEA) compositions with desired high temperature strength and room temperature ductility/plasticity from the vast composition space is a challenging task. Generally, compositions with higher yield strength tend to have lower room temperature ductility or sometime show brittle behavior. In this work, we first present machine learning (ML) based models for compressive yield strength and room temperature plasticity. These models were extensively validated against experiments. The two completely independent models were able to reproduce the well-established fact that an increase in plasticity comes at a cost of reduction in strength. We then used the two models and applied the state-of-the-art sampling method to generated approximately 100,000 RHEA compositions, and computed their strengths and plasticities. We then designed a "Figure of Merit" to identify the promising compositions. Some selected compositions were synthesized and characterized for their mechanical properties.

11:15 AM

AI-accelerated Materials Informatics Method for the Discovery of Ductile Alloys: *Max Hodapp*[1]; Ivan Novikov[2]; Olga Kovalyova[2]; Alexander Shapeev[2]; [1]Materials Center Leoben; [2]Skoltech

In computational materials science, a common means for predicting macroscopic (e.g., mechanical) properties of an alloy is to define a model using combinations of descriptors that depend on some material properties (elastic constants, misfit volumes, etc.), representative for the macroscopic behavior. The material properties are usually computed using density functional theory (DFT). However, DFT scales cubically with the number of atoms and is thus impractical for a screening over many alloy compositions. Here, we present a novel methodology which combines modeling approaches and machine-learning interatomic potentials. Machine-learning interatomic potentials are orders of magnitude faster than DFT, while achieving similar accuracy, allowing for a predictive and tractable high-throughput screening over the whole alloy space. The proposed methodology is illustrated by predicting the room temperature ductility of the medium-entropy alloy Mo-Nb-Ta.

11:35 AM

Stability and Growth Kinetics of Deformation Twin Embryos in BCC Complex Concentrated Alloys: *Ganlin Chen*[1]; Liang Qi[1]; [1]University of Michigan

We employed computational tools to understand and further tune the effects of diffusionless phase transformations on twinnabilities in BCC complex concentrated alloys. First-principle calculations were firstly performed to study the atomic structures and energy stability of different metastable phases at their local-minimum states in different alloy compositions. Secondly, we applied atomistic simulations with classical interatomic potentials to further analyze the atomic structures of alloys at finite temperatures. Both first-principle calculations and atomistic simulation results are employed to construct the order parameters that can effectively describe the energy landscape and diffusionless phase transformation paths between multiple phases. Thirdly, with the aid of atomistic simulations and crystallographic theories, we investigate the energy landscape of the nucleation and growth dynamics of deformation twinning under external loading conditions at different temperatures and further explore how the diffusionless phase transformations affect the deformation twinning activities in BCC complex concentrated alloys.

11:55 AM

Investigation of Phase Equilibria and Growth Kinetics in Co-Cr-Ni Alloy System: *Vivek Verma*[1]; Sakshi Bajpai[1]; Calvin Belcher[1]; Diran Apelian[1]; Enrique Lavernia[1]; [1]University of California Irvine

Metallurgical characteristics are prominently observed in the diffusion structures of multiphase, multicomponent alloys. Nonetheless, the task of predicting phase equilibrium in systems with multiple components remains challenging due to the limited availability of thermodynamic data. Isothermal multiphase diffusion couples in complex concentrated alloys (CCAs) play a pivotal role in offering invaluable understanding of stable phases and their composition ranges within such systems.

CALPHAD thermodynamic calculations indicate that the equi-atomic Co-Cr-Ni alloy is likely to form Cr-rich sigma phase at temperatures below 690°C. However, there is lack of experimental evidence supporting the existence of sigma phase. Presence of the sigma phase, if present, could potentially have negative effects on mechanical properties of this alloy system. Thus, the present work utilizes multiphase diffusion couples to investigate phase stability, nucleation, and growth of sigma phase in FCC alloy at 550-690°C. Metallography and electron microscopy were used to examine diffusion zone's diffusion structure.

Powders and Additive Manufacturing II

Wednesday PM
November 15, 2023

Room: William Penn Ballroom
Location: Omni William Penn

Session Chair: To Be Announced

1:40 PM Introductory Comments

1:45 PM

Direct Ink Writing Printing and Microstructural Engineering of Lightweight Al10Co25Cr8Fe15Ni36Ti6 Micro-lattices: *Ming Chen*[1]; Dingchang Zhang[1]; Ya-Chu Hsu[1]; David Dunand[1]; [1]Northwestern University

Given its superior high-temperature strength and oxidation resistance, Al10Co25Cr8Fe15Ni36Ti6 is a promising alloy for high-temperature structural applications. Additive manufacturing provides high flexibility for fabrication of complex shapes, but, for Al10Co25Cr8Fe15Ni36Ti6, traditional AM approaches based on laser beam fusion/solidification induce cracking and warping due to high temperatures and thermal gradients. Here, we demonstrate 3D direct ink writing technique can fabricate lightweight Al10Co25Cr8Fe15Ni36Ti6 micro-lattices, enabling complex geometries with superior strength and ductility for applications in high-temperature structural components. Elemental powders are suspended, together with binder, into an ink which is 3D-extruded into thin struts, in air at ambient temperature. Printed green bodies are sintered at elevated temperatures to decompose binder and densify powders. We discuss various approaches to achieve high quality micro-lattices and mitigate oxidation and impurities issues during sintering; we also describe effects of compositions on morphologies and volume fraction of ' precipitates to achieve high strength at elevated temperatures.

2:05 PM

Exploring Thermomechanical Post-processing Techniques to Improve the Mechanical Strength of an SLMed CoCrFeMnNi: *Joseph Agyapong*[1]; Alexander Czekanski[1]; Solomon Boakye-Yiadom[1]; [1]York University

Abstract:This study investigates thermomechanical post-processing techniques, including deep cryogenic treatment and annealing heat treatment, to enhance the mechanical strength of a selective laser melted (SLMed) CoCrFeMnNi high-entropy alloy. The alloy exhibits high strength, corrosion resistance, and ductility, making it suitable for aerospace, automotive, and biomedical applications. The research utilizes SEM and TEM microscopy techniques for microstructural analysis. Fracture toughness is evaluated using SENB, while high strain rate impact and hardness tests assess dynamic behavior. The results provide insights into the effects of thermomechanical processing on the alloy's mechanical properties, contributing to the optimization of high-entropy alloys produced via selective laser melting. This study advances additive manufacturing knowledge and facilitates the development of robust metallic components for diverse industries.

2:25 PM
3D Ink Extrusion Printing of CoCrFeNi and (Zr0.50Ti0.35Nb0.15)80Al20 Microlattices: *Ya-Chu Hsu*[1]; [1]Northwestern University

The preparation of high-entropy alloys (HEAs) via 3D ink-extrusion printing has been increasingly used in the past few years. Green bodies with complex shapes can be printed layer by layer by using powder-loaded liquid ink at room temperature. This method offers flexibility in using elemental, oxide, or hydride powders and avoids the problems of residual stress and textured microstructure. In this work, microlattices with open channels are 3D ink-extrusion printed from inks containing a powder blend of oxides and graphite powders. Metallic CoCrFeNi alloy microlattices are then achieved by co-reduction in different atmospheres and sintering. Compression properties of sintered CoCrFeNi microlattices are measured at room temperature. Microlattices of the (Zr0.50Ti0.35Nb0.15)80Al20 alloy are created via 3D extrusion of inks containing ZrH2, Ti, Nb, and TiAl3 powders. Further hydride decomposition, elemental interdiffusion, homogenization, and densification of the struts of the microlattices were studied. Their compressive properties are measured at elevated temperatures.

2:45 PM
The "Commodity Approach": A Novel and Sustainable Method to Develop Non-equitomic CoCrFeNiMox High Entropy Alloys: *Jose Torralba*[1]; S. Venkatesh Kumaran[1]; Dariusz Garbiec[2]; Alberto Meza[3]; [1]Universidad Carlos III Madrid-Imdea Materials Institute; [2]Łukasiewicz Research Network – Poznań Institute of Technology; [3]IMDEA Materials Institute

One obstacle to developing HEAs is the need to use many alloying elements, which are considered critical and strategic and expensive metals. However, it has been demonstrated[1,2] that HEAs can be obtained from combinations of commodity alloys (e.g., nickel and cobalt-based superalloys or stainless steels). This possibility opens up the prospects for the development of HEAs using raw materials that can come from the recycling of commodity alloys, which are available sources of metals such as Ni, Fe, Co, Cr, or Mo, which, being available in the form of scrap, lose their critical character and offer a cheaper possibility than the direct use of pure metals. In this work, non-equiatomic high entropy CoCrFeNiMox alloys are developed from three PM routes: SPS, LBPF (additive manufacturing), and MIM. [1] J.M. Torralba, S. Venkatesh Kumarán, Mater. Lett. 301 (2021). [2] S. Venkatesh Kumaran, et al., Mater. Sci. Eng. A 878 (2023) 145207.

3:05 PM
Development of a Process Optimization Framework for Fabricating Fully Dense NiCoCr Medium Entropy Alloy using Laser Directed Energy Deposition: *Thaer Syam*[1]; Bilal Mansoor[2]; Ibrahim Karaman[1]; [1]Texas A&M University; [2]Texas A&M University at Qatar

Multi-principal alloys, such as medium entropy alloys (MEAs) show promise due to their superior mechanical properties such as high strength-to-weight ratios. Here, we report our initial results on laser-based Direct Energy Deposition (DED) of pre-alloyed NiCoCr - focusing on the challenges associated with achieving dense NiCoCr parts using this process. As a first step, basic single-track experiments were employed to chart the range of parameters including scanning speed, power and RPM, and a blend of geometric factors for hatch spacing and layer height was suggested to identify parameter combinations that accomplish desired build heights while minimizing the formation of porous regions. 19 parameter combinations were identified and prisms of 8mm by 8mm with variable target heights were printed for further analysis. Initial, printability maps were constructed based on the main process parameters, and criteria for hatch spacing, layer height and dilution limits as an output of the melt pool characteristics.

Performance in Extreme Environments II

Wednesday PM **Room: Three Rivers**
November 15, 2023 **Location: Omni William Penn**

Session Chair: To Be Announced

1:40 PM Introductory Comments

1:45 PM
A First-principles Study on the Structural-thermodynamics Properties of Tungsten-based High Entropy Alloys: *Jie Peng*[1]; David Cerecedar[1]; Yichen Qian[1]; [1]Villanova University

High entropy alloys (HEAs) are a class of materials promising for plasma-facing applications in fusion energy devices. Among them, Tungsten (W-) based HEAs have been considered as leading candidates due to remarkable properties including superior mechanical properties, a superior melting point (above 2873 K), enhanced radiation resistance to heavy ion irradiation, and negligible radiation hardening compared to pure W. However, there is a lack of understanding of how mechanical and thermodynamics properties of W-based HEAs are affected by temperature. In this work, we present a study on the temperature-dependent thermal properties of W-based HEAs. The first-principles density-functional-theory (DFT) calculations combined with quasi-harmonic approximation (QHA) theory is used to investigate electronic, structural, and thermal properties of HEAs in different chemical compositions as a function of temperature. Our work advances understanding of structural-mechanical-thermal relations in HEAs, thus providing insights on inverse design of candidate HEAs in fusion energy devices.

2:05 PM
Effect of Local Chemical Order on the Irradiation-induced Defect Evolution in Multi-principal Element Alloys: *Jun Ding*[1]; Zhen Zhang[1]; Chenyang Lu[1]; Robert Ritchie[2]; Evan Ma[1]; [1]Xi'an Jiaotong University; [2]University of California Berkeley

Multi-principal element alloys (MPEAs) have emerged as potentially suitable structural materials for nuclear applications, particularly as they appear to show promising irradiation resistance. However, the influence of local chemical order (LCO) on the irradiation response of MPEAs has remained uncertain thus far. In this work, we combine ion irradiation experiments with large-scale atomistic simulations to reveal that the presence of LCO, slows down the formation and evolution of point defects in MPEAs during irradiation. In particular, the irradiation-induced vacancies and interstitials exhibit a smaller difference in their mobility, arising from a stronger effect of LCO in localizing interstitial diffusion. This effect promotes their recombination as the LCO serves to tune the migration energy barriers of these point defects, thereby delaying the initiation of damage. These findings imply that local chemical ordering may provide a new variable in the design space to enhance the resistance of MPEAs to irradiation damage.

2:25 PM
Radiation-induced Segregation in FCC Multi-principal Element Alloys: *Daniele Fatto Offidani*[1]; Emmanuelle Marquis[1]; [1]University Of Michigan - Ann Arbor

Multi-principal element alloys (MPEAs) have been proposed as potential structural material candidates for next-generation nuclear reactors because of their notable mechanical properties and environmental resistance. However, the effects of irradiation on the microstructural and chemical evolution of these alloys are still not fully understood. Grain boundaries are of particular interest due to their susceptibility to radiation-induced segregation (RIS), which by altering their chemistries can negatively impact the resistance of the materials to stress-corrosion. Focusing on the impact of alloy chemistry and the role of single elements on RIS, we systematically characterized the RIS behavior at grain boundaries in three ion-irradiated single-phase FCC Fe-Ni-Cr-Co-Mn based alloys. The results provide insights into the effects of dose, temperature, and alloy composition on RIS.

2:45 PM

Irradiation Effects in a Precipitation-hardened AlCuCrFeNi High Entropy Alloy: *Nathan Curtis*[1]; Bao-Phong Nguyen[1]; Junliang Liu[1]; Nate Eklof[1]; Adrien Couet[1]; [1]University Of Wisconsin - Madison

Interest in the nuclear industry surrounding high entropy alloys (HEAs) is fueled by their observed resistance to microstructural damage under irradiation. HEA compositions of interest were compiled and downselected by comparing their mechanical properties to current structural nuclear materials. An AlCuCrFeNi HEA has reported nanoscale L12 precipitate growth with thermal aging, resulting in a 70% increase in yield strength and an elastic limit an order of magnitude greater than code-certified materials. The presence of nano-precipitates also increases defect-absorbing sinks which, while employed in conventional alloys to increase irradiation resistance, have not been thoroughly explored in HEAs. To better understand the influence of these nano-precipitates, this work presents heavy-ion irradiation results in aged AlCuCrFeNi HEAs. Transmission electron microscopy and nano-indentation techniques were used to characterize the irradiation-induced changes in microstructure and mechanical properties.

3:05 PM

Characterization and Comparison of Radiation Damage in HfMoNbTaTi and HfMoNbTaZr Refractory High Entropy Alloys by Multi-energy Helium Ion Irradiation: *Pin-Haung Chiu*[1]; Jenq-Horng Liang[1]; Der-Sheng Chao[1]; Che-Wei Tsai[1]; Jien-Wei Yeh[1]; Peng-Wei Chu[1]; [1]National Tsing-Hua University

Refractory HEAs (RHEAs), which consist of high melting point metallic elements, demonstrate exceptional mechanical properties even in extremely high-temperature conditions. However, it remains unclear whether these superior mechanical properties are still true in high-radiation environments. To address this issue, two RHEAs, HfMoNbTaTi and HfMoNbTaZr, were selected and multiple energy helium ion irradiation was adopted to introduce radiation damage within the alloy in this study. The mechanical properties and microstructures of RHEAs samples were examed by several characterization methods, such as nanoindentation and GIXRD method, etc. The results showed that the hardness of both compositions decreases after He^+ irradiation. The lattice parameter of HfMoNbTaTi remains almost unchanged, while that of HfMoNbTaZr slightly declines by a ratio of 0.74%. It can be expected that this study would be useful to evaluate the feasibility of RHEAs utilized in high-radiation environments and gain insights into the effects of alloy elemental components on radiation resistance.

Performance in Extreme Environments III

Wednesday PM
November 15, 2023

Room: Riverboat
Location: Omni William Penn

Session Chair: To Be Announced

1:40 PM Introductory Comments

1:45 PM

Influence of Ar Ion Irradiation on Precipitation Behavior of FCC-based $Al_{0.2}Co_{1.5}CrFeNi_{1.5}Ti_{0.3}$ High Entropy Alloy: *Chun-Hao Tseng*[1]; Jenq-Horng Liang[1]; Der-Sheng Chao[1]; Che-Wei Tsai[1]; Jien-Wei Yeh[1]; Peng-Wei Chu[1]; [1]National Tsing Hua University

This study aims to clarify the effects of radiation damage on precipitation-strengthened HEAs under various aging temperatures. In this study, the FCC-structured $Al_{0.2}Co_{1.5}CrFeNi_{1.5}Ti_{0.3}$ samples with different precipitate sizes were employed. Two different aging temperatures were utilized to obtain distinct microstructures, which exhibit coherent precipitates of $L1_2$ structure within the matrix. In addition, a separate set of cold-rolled samples was also prepared as the control group. In order to evaluate the radiation tolerance of the samples underwent different aging temperatures, the samples were irradiated by 190 keV argon ions to a fluence of 8.5E15 cm^{-2}. Then the mechanical properties, component distribution, and microstructures between the pristine and irradiated samples were compared to identify the effects of Ar ion irradiation on precipitation behavior. The results revealed that the sample with higher aging temperature has better radiation resistance. Further investigation is currently in progress to ascertain the ordering-disordering mechanism of nanoprecipitates.

2:05 PM

Defects in High Entropy Alloys: A Real Cocktail Effect: *Simon Middleburgh*[1]; Christopher Moore[1]; Jack Wilson[1]; Alexander Lin-Vines[1]; [1]Bangor University

The behavior of point defects in high entropy alloys differ from standard alloy systems due to the distribution of stabilities, readily assessed using modelling techniques such as atomic scale modelling. Not only are the formation of defects altered, but so too are the migration and recombination of defects initiated due to athermal effects such as radiation damage. A range of atomic scale techniques shall be presented that impact a various characteristics of high entropy alloys in use, including their use as corrosion barriers, neutron shielding materials and hydrogen storage materials. The ability to understand these atomic scale processes aids in the design of bespoke alloys, fit for specific purposes.

2:25 PM

Combined Experimental and Numerical Investigation of Ductile Fracture in the Cantor Alloy: *Ahmed Ataya*[1]; Joshua Herrington[1]; Shi-Hoon Choi[2]; Amine Benzerga[1]; [1]Texas A&M University; [2]Sunchon National University

The ductile fracture of the CoCrFeMnNi high-entropy alloy was investigated. Round notched and unnotched bars were deformed to fracture in tension in order to determine the influence of stress triaxiality. Some bars were interrupted near macrocrack initiation. Fractographic analysis reveals a failure mechanism dominated by void nucleation at second-phase particles, followed by growth to coalescence. Dimple size measurements were acquired in-plane and depth-wise using a profilometer. The finite element method was utilized to analyze notched bars using constitutive relations of porous material plasticity. With nearly no fitting damage parameters, the constitutive model allowed for a good prediction of failure strains. Furthermore, unit cell calculations were carried out for a periodic array of voids in a J2 matrix under remote triaxial loadings after calibrating the plasticity parameters. This simple approach allowed for a good prediction of the fracture locus as well as the deformed void dimensions.

2:45 PM
A CALPHAD Based Approach for Designing Precipitation-hardened High-entropy Alloys: Diego Santana[1]; Claudio Kiminami[1]; Amy Clarke[2]; Michael Kaufman[2]; *Francisco Coury*[1]; [1]Universidade Federal de São Carlos; [2]Colorado School of Mines

Designing precipitation-hardened high-entropy alloys with good mechanical properties is challenging due to the complexity introduced by composition and heat treatment temperatures. To address this, thermodynamic calculations based on the CALPHAD method were employed to analyze 11,235 compositions of Cr-Co-Ni-Al-Ti alloys. By applying specific filtering criteria, the remaining alloys were evaluated to estimate their solid solution hardening and maximum precipitation hardening contributions to yield strength. To validate the methodology, three alloys were selected, processed, and subjected to microstructural and mechanical characterization techniques. The results were compared with predictions made using CALPHAD and mathematical modeling, revealing a positive qualitative agreement. This approach shows promising potential in effectively identifying and developing new precipitation-hardened alloys with improved mechanical properties.

3:05 PM
Self-healing and Machinable Refractory High-entropy Alloys for Energy and Aerospace Applications: *Sal Rodriguez*[1]; [1]Sandia National Laboratory

Lathing, filing, drilling, slicing, polishing, and RHEA-to-RHEA welding were performed on SPS- and LENS-manufactured test pieces. RHEA combinations with the highest degree of machinability tended to be more ductile, but had a lower yield strength, and vice-versa. Of the selected RHEA combinations, most survived the extensive machining at room temperature (RT), though a few shattered. An analysis of the experimental data provides several insights regarding the continued development and improvement of higher-strength machinable compositions at RT.NbTaVW RHEA test pieces were manufactured via LENS to test for self-healing, and were subsequently irradiated at the Ion Beam Laboratory. High energy Au ions at 2.8 MeV at a dose of 1x1014 ions/cm2 resulted in 0.9 displacements per atom, while a dose of 1x1015 ions/cm2 resulted in 9 DPA. The average measured nanoindentation hardness of the irradiated RHEA increased 5 to 24%, comparatively less than Inconel 718 and 316 stainless-steel samples.

Wednesday Closing Plenary

Wednesday PM
November 15, 2023

Room: William Penn Ballroom
Location: Omni William Penn

Session Chair: To Be Announced

3:45 PM Plenary
Short-range Ordering and Its Effects on Mechanical Properties of High-entropy Alloys: *Zhaoping Lu*[1]; [1]University of Science and Technology Beijing

High-entropy alloys (HEAs) have opened up a new field for discovering un-explored mechanical properties and deformation behaviors. In this talk, experimental and theoretical verification of short-range orderings (SROs) in HEAs will be first reviewed, and then effects of SROs on mechanical properties and deformation behavior will be discussed. The main theme is to demonstrate that existence of SROs is a common yet key structural feature of HEAs, and tuning the degree of SROs is an effective way for optimizing mechanical properties of HEAs. In addition, the challenges concerning on formation mechanisms and experimental characterization of SROs in HEAs will be explored, and future research activities in this area will be proposed.

4:25 PM Concluding Comments

Contender High-entropy Alloy Coatings to Superalloy 720 for Hot-forging Dies: *Tanjore Jayaraman*[1]; Ramachandra Canumalla[2]; [1]United States Air Force Academy; [2]Weldaloy Specialty Forgings

Superalloy 720 is ubiquitous to a myriad of high-temperature applications, including weldoverlay coatings for hot-forging dies. Currently, high-entropy alloys, having a unique combination of ambient and elevated temperature properties, appear as potential competitors to superalloy 720 as coatings for conventional hot-forging die materials, e.g., Uddeholm Dievar or H13. We analyzed the refractory high-entropy alloys (RHEAs) available in the current literature by decision science-driven techniques, including multiple-attribute decision making (MADM), for sorting and ranking the RHEAs. The ranks assigned by several MADMs, viz. WEDBA (weighted Euclidean distance-based approach), ROVM (range of value method), ARAS (additive ratio assessment), etc., were consistent. Principal component analysis (PCA) consolidated the ranks, while hierarchical clustering (HC) discerned the similarities among the alloys. The investigation identified contender RHEAs having properties superior to superalloy 720, revealed their potential as coatings for hot-forging dies, and suggested directives for further development.

Custom-made Test Equipment for Measuring the Temperature Dependence of Hardness for High Entropy Refractory Alloys: *Ottó Krisztián Temesi*[1]; Chinh Nguyen Q.[2]; Lajos K. Varga[3]; [1]H-ION Ltd., Eötvös Loránd University; [2]Eötvös Lóránd University; [3]Wigner Research Center for Physics

The scope is the measurement of the highest working temperatures, Tc, for a given alloy. Tc will be determined in terms of the temperature dependence of the indentation hardness performed at a constant heating rate. Indentation is realized with a cylinder or cone-shaped measuring head loaded with a constant force and pressed into the sample placed in a tubular furnace. We measure the degree of indentation as a function of temperature. The main instrument parameters are the following: applied force: 0,1-5 kgf (10-50 N), maximum temperature: 1200 ˚C, displacement measurement sensitivity 0,1 micron, sample size: 2-10 mm thick plane-parallel cylinder or bar and 10 mm maximum diameter. The measurements are performed under an argon-protective atmosphere or in the air to check the oxidation resistance.At this stage, the instrument can determine the softening temperature, coefficient of thermal expansion of metal alloys, and the permanent flow (creep) parameters.

Design of High Entropy Superalloy FeNiCrAlCu with Stacking Fault Energy Modeling using Thermodynamic Calculations, First-principles, and Machine Learning: *Tria Achmad*[1]; Farrel Baskara[1]; Muhammad Aulia[1]; [1]Bandung Institute of Technology

High entropy superalloys (HESA) are promising materials with unique properties, but their development and optimization remain ongoing. This study focuses on Fe-based HESA FeNiCrAlCu and their stacking fault energy (SFE), a critical parameter influencing deformation mechanisms and creep resistance. Leveraging machine learning and computational thermodynamics, we propose a novel approach for predicting SFE using big data analysis. However, thermodynamic data of some rare elements like Zr is limited. Then, we use first-principles to investigate further the effect of adding Zr on elastic properties, SFE, and electronic structure. Our research establishes an optimal design guide for achieving desired SFE values: Ni (20-25 at%), Cr (15-36 at%), Al (5-20 at%), and Cu (9-20 at%). We achieve an impressive 0.98 accuracy in classifying SFE types by employing a deep learning neural network model. This work advances HESA design, provides valuable insights into their mechanical behavior, and improves creep resistance for demanding applications.

Design of High Entropy Superalloy FeNiCrCoAl using Molecular Dynamics, Computational Thermodynamics and Machine Learning: *Tria Achmad*[1]; Fauzi Sukma[1]; Putri Wibowo[1]; [1]Bandung Institute of Technology

The development of High Entropy Superalloy (HESA) with superior mechanical properties and affordable raw material raises the possibility of replacing superalloys. Designing a HESA frequently involves expensive and time-consuming processes of experimental. Even with the growth of computational studies, it still complicated to model multicomponent alloy systems. This study focuses on the compositional design simulation of HESA FeNiCrCoAl on lattice parameters, stacking fault energy (SFE), and compression strength using molecular dynamics (MD). We also propose a new approach to predict SFE using extensive data analysis by leveraging machine learning and computational thermodynamics. Then it is possible to explore the high-dimensional composition space much more efficiently. Increasing Al, Cr, and Co will decrease the SFE, while increasing Ni will increase the SFE. An optimal design guide for achieving desired SFE values: Ni (18-25 at%), Cr (24-30 at%), Al (5-15 at%), Co (20-35 at%), and Fe (20-35 at%). This work provides valuable insights into HESA mechanical behavior to improve creep resistance.

Effects of Specific Minor Elements on the Nanostructural Evolution of Quaternary Alcrfeni-based High Entropy Alloys and Their Consequent Influence on Mechanical Properties: *Elyorjon Jumaev*[1]; Amir Abidov[1]; Abdulla Khursanov[1]; [1]Almalyk Mining and Metallurgical Combine JSC

The AlCrFeNi eutectic HEAs have been designed by the introduction of 1, 3, 5 at% Mo and Ti, and their mechanical behaviors were investigated along with double-phase strengthening. The X-Ray Diffraction analysis demonstrated the presence of B2 and BCC dual phases. Compositional variation by the addition of minor elements such as Mo and Ti resulted in the formation of the eutectic structure. The high degree of coherence in dendritic and lamellar regions of the nanoscale Al-Ni-rich B2 phase and Cr-Fe-rich A2 phase was proven by the results of in-detail investigation of the nanostructural evolution of the alloy. Variation in the grain size highlights fraction combined with the addition of the minor elements exhibit good hardness behavior at elevated temperatures which highlights the enhancement of the mechanical properties of the new alloy.

Enhancing Hydrogen Storage with Laser Metal Deposition of AlCoCrMoFeTi/Ni High-entropy Alloy: *Morena Xaba*[1]; Nana Arthur[2]; Caroline Khoathane[1]; Sisa Pityana[2]; [1]Tshwane University of Technology; [2]Council for Scientific and Industrial Research, National Laser Centre, Pretoria, South Africa

Hydrogen has been extensively studied as a valuable energy source, with its production and storage being the focus of research for centuries. Metal hydrides possess the ability to store energy due to the presence of intermetallic phases in BCC and FCC structures. High-entropy alloys (HEAs) represent a novel group of alloys that exhibit exceptional and distinctive properties, such as incorporating multiple metallic elements as primary constituents. Additionally, these alloys possess a configurational entropy of f ΔSconf ≥ 1.5R, resulting in a unique crystal distortion that offers advantages for hydrogen storage phases. This study aims to explore the relationship between microstructure and hydrogen storage by investigating a series of AlCoCrMoFeTi/Ni alloys. Laser metal deposition, an additive manufacturing technique that utilizes a high-powered laser to build up layers of material from an excess pool of powder, will be employed to fabricate the HEA matrix with varying percentages of Fe and Ni atoms.

Formation and Physical Properties of New Superconducting High-entropy Alloys Prepared by Mechanical Alloying: *Rafal Idczak*[1]; Piotr Sobota[1]; Adam Pikul[2]; [1]Institute of Experimental Physics, University of Wroclaw; [2]Institute of Low Temperature and Structural Reaseach, Polish Academy of Sciences

In 2014, the first high-entropy alloy (HEA) superconductor, consisting primarily of 4d and 5d series elements, was found [1], revealing a new facet of the capabilities. A variety of studies have been performed on HEA superconductors since that time, to designate their potential for practical applications. Up to the present time, HEA superconductors are fabricated primarily through high-temperature arc-melting technique. A promising alternative for this method is mechanical alloying (MA). MA is a solid-state powder-processing technique involving repeated cold welding, fracturing, and re-welding of powder particles in a high-energy ball mill [2]. Physical properties of new superconducting HEAs prepared by MA will be presented. In particular, powders quality were verified by XRD and SEM. Critical superconducting parameters were determined from magnetization, electrical resistivity and specific heat data. [1] - P. Koželj et al., PRL (2014) 113.[2] - C. Suryanarayana, Progress in Materials Science 46 (2001) 1-184.

High Throughput Exploration of High Entropy MXenes using Neural Network Potentials: *Mohammed Wasay Mudassir*[1]; Sriram Goverapet Srinivasan[1]; Mahesh Mynam[1]; Beena Rai[1]; [1]TCS Research and Innovation

MXenes, a class of 2D materials of the general formula $M_{n+1}X_nT_y$(M = early 'd' block metal, X = C/N, T= O/OH/F) have shown promise as efficient materials for various applications ranging from electrocatalysis to battery anodes and supercapacitors. Configurational entropy driven stabilization was leveraged to synthesize multi-metallic MXenes recently. To explore the vast configurational and compositional space, density functional theory calculations were used to develop a neural network potential for Ti,Nb,V and Mo containing carbide MXenes. The potential, that was trained against equation of state and formation energies data, had a low RMSE of 6meV/atom in energy and 44meV/Å in forces. MC/MM simulations were carried out with this potential to construct the convex hull and identify stable MXenes of $(Ti_aV_bMo_cN_d)C_n$(a+b+c+d=n+1) stoichiometry. The MXenes at the vertices of the hull were further characterized in terms of the SRO parameters, inter-layer segregation parameters as well as the distribution of atomic neighborhoods.

Influence of Mo on Low Temperature Tensile Properties of As-cast CrFeCoNi-Mo High Entropy Alloys: *Toru Maruyama*[1]; Mei Fukuzawa[1]; [1]Kansai University

Annealed CoCrFeNi-Mo alloys show high tensile strength and no serious embrittlement occurred, although precipitation of the sigma phases, which are of concern for brittleness. However, tensile properties of as-cast CoCrFeNi-Mo alloys are currently not perfectly clarified, especially at low temperatures.Tensile tests of as-cast CoCrFeNi-Mo alloys (Mo at 4.9, 7.5, and 9.0 at%) were performed at room temperature and liquid nitrogen temperature. The as-cast specimens showed ruptured before plastic deformation occurred for the 7.5 at% Mo and 9.0 at% Mo alloys at both room temperature and liquid nitrogen temperature. These ultimate tensile strength were about 300 MPa. The 4.9at%Mo specimens at room temperature showed tensile strength of 645 MPa and elongation of 36.2%, and tensile strength of 934 MPa and elongation of 21.2% at liquid nitrogen temperature, suggesting that the high ductility at liquid nitrogen temperature was due to twin-induced plasticity.

Manganese-based A-site High-entropy Perovskite Oxides for Solar Thermochemical Hydrogen Production: Xingbo Liu[1]; Cijie Liu[1]; Dawei Zhang[2]; *Wei Li*[1]; Jamie Trindell[3]; Keith King[3]; Sean Bishop[3]; Joshua Sugar[3]; Anthony McDaniel[3]; Andrew Smith[3]; Peter Salinas[3]; Eric Coker[3]; Arielle Clauser[3]; Joerg Neuefeind[4]; Jingjing Yang[2]; Hector De Santiago[1]; Liang Ma[1]; Yi Wang[1]; Qiang Wang[1]; Wenyuan Li[1]; Qingsong Wang[5]; Qingyuan Li[1]; Hanchen Tian[1]; Ha Ngoc Ngan Tran[1]; Xuemei Li[1]; Boyuan Xu[6]; Brandon Robinson[1]; Angela Deibel[1]; Gregory Collins[1]; Nhat Anh Thi Thieu[1]; Jianli Hu[1]; Yue Qi[6]; Jian Luo[2]; [1]West Virginia University; [2]University of California San Diego; [3]Sandia National Laboratories; [4]Oak Ridge National Laboratory; [5]University of Bayreuth; [6]Brown University

High-entropy perovskite oxides (HEPO) have been studied as a new family of redox oxides for solar thermochemical hydrogen (STCH) production owing to their favorable thermodynamic properties. Here, we report a strategy of introducing A-site HEPO, (La1/6Pr1/6Nd1/6Gd1/6Sr1/6Ba1/6)MnO3 (LPNGSB_Mn), which shows desirable thermodynamic and kinetics properties, and excellent cycling durability. LPNGSB_Mn exhibits enhanced hydrogen production (~100 mmol moloxide–1) compared to LSM (~68) in 1-hour redox duration and high STCH and phase stability for 50 cycles. LPNGSB_Mn possesses moderate reduction enthalpy reduction (260–286 kJ (mol-O)-1), high reduction entropy (130–164 J (mol-O)-1 K–1), and fast surface oxygen exchange kinetics. All A-site cations do not show observable valence changes during the redox processes; however, STCH production correlates with the number of equimolarly mixed A-site elements. This research suggests a new A-site mixing strategy and a new class of A-site high-entropy perovskite oxides with a vast compositional space for tailoring properties for STCH.

Microstructure and Corrosion Behavior of Ti-Nb-Mo-Zr Containing Co and Ta High-entropy Alloys: *Rodinei Gomes*[1]; Bruno Alessandro Guedes de Lima[1]; Ricardo Alves[2]; Rafael Alexandre Raimundo[1]; Francisco Riccelly Feitosa[1]; [1]Universidade Federal da Paraiba; [2]Universidade Federal de Campina Grande

The microstructures and corrosion behavior of TiNbMoZr0.75Co and TiNbMoZrTa high entropy alloys (HEAs) were studied. The existing stable phases were predicted though simulations using Pandat software. The as-casted microstructure features including the solidified phases and phase fractions were simulated. It was found that the Ti–Zr–Nb–Ta–Mo HEAs showed a dendrite structure with two body-centered-cubic (BCC) solid solution phases. Ti-Zr rich BCC1 phase and Ti-Nb-Mo rich BCC2 phase. Furthermore, the highly-protective oxide films formed on the surface of Ti–Zr–Nb–Ta–Mo HEA resulted in the high corrosion resistance.

Oxygen Reduction Reaction on Pt- non PGM Transition Metal High Entropy Alloy Surface: Single Crystal Model Catalyst Study: *Toshimasa Wadayama*[1]; [1]TOHOKU University

Head-entropy alloys (HEA) are known as unique materials, exhibiting high mechanical strength and structural stability at high temperatures, anti-corrosion etc. Such unique properties have attracted much attention in the field of electrocatalysis, as the reduced free energy (ΔG) of HEAs should stabilize the topmost surface microstructures and thus increase the catalyst surface durability. However, at present, no study has been made on the correlations between HEAs electrocatalytic properties and lattice stacking structures, atomic-level distributions of constituent elements in the surface vicinity. In this study, we synthesized Pt-HEA(*hkl*) (*hkl* = 111, 110, 100) model catalyst surfaces by vacuum-deposition of a "Cantor alloy" (Cr-Mn-Fe-Co-Ni), followed by Pt layers on Pt single-crystal substrates in ultra-high vacuum ($<10^{-7}$ Pa). Then, we evaluated ORR properties of the Pt-HEA(*hkl*) surfaces and discuss the correlation between the topmost surface microstructures and electrocatalytic properties of the Pt-HEA.This study was supported by NEDO of Japan, JSPS KAKENHI (JP21H01645).

Predicting Properties of High Entropy Carbides from their Respective Binaries: *Mina Lim*[1]; [1]Gordon College

High Entropy Carbides (HECs) have been predicted the selection of candidate compositions with the phase stability from an entropy-forming-ability (EFA) descriptor from first principle. Using Density Functional Theory calculations, we address two questions: (1) to what degree can the properties of high entropy carbides created by equi-molar combinations of five of the set of eight refractory metals Hf, Nb, Mo, Ta, Ti, V, W, and Zr be predicted from their respective binaries compounds, and (2) can empirical relationships from properties of the binary compounds be used to predict phase stability for these materials. For the former question, it is found that lattice constant, binding energy and bulk modulus are well approximated by binary carbide averages. To address the second question, it is found that there is a correlation between EFA and the standard deviation of the distribution of bulk moduli of the constituent binaries.

Property and Microstructure Evaluation of Directed Energy Deposition High Entropy Alloys and Functionally Graded Materials: *Yogesh Singla*[1]; Luis Nunez III[2]; Calvin Downey[2]; Isabella Rooyen[3]; Michael Maughan[1]; [1]University of Idaho; [2]Idaho National Laboratory; [3]Pacific Northwest National Laboratory

The present work investigates the mechanical and microstructural properties of high entropy alloys (HEAs) and functionally graded materials (FGMs) manufactured with SS316L substrates using powder blown directed energy deposition. The HEAs and FGMs contain a mixture of commercially available IN718, SS316L and 70Co30Cr and the effect of compositional variation on hardness was studied using nanoindentation. Optical microscopy revealed the inclusion of unsintered particles and porosity. EDS analysis confirmed that unsintered particles consist of CoCr. Optical microscopy also showed that the layers are mechanically and metallurgically well bonded to each other. The samples were primarily crack-free, however, micro-cracks were observed in one of the FGM samples. Nanoindentation results from 1000 indents on each sample indicated that HEA has overall higher hardness compared to FGMs. In the FGMs a decrease in hardness was observed with the decrease of CoCr percentage.

Unleashing the Power of Machine Learning for High-Entropy Alloy Discovery: Phase Prediction: *Sima Alidokht*[1]; Ehsan Gerashi[1]; Armin Hatefi[1]; [1]Memorial University

High-entropy alloys (HEAs) have gained significant attention in materials science for their remarkable mechanical properties and extensive compositional versatility. Due to their high-dimensional chemical complexity, understanding their physical mechanisms and designing new HEAs is challenging. Predicting HEA phases can provide valuable insights, including mechanical properties anticipations. The conventional trial-and-error approach for discovering new HEAs is time-consuming and costly. To address the issue, we employ the power of machine learning methods to predict the phase of HEAs, reducing the effort required for HEA design. In this research, we propose various statistical and machine learning and artificial neural networks to model the HEAs phase responses, estimate the model parameters and explain the relationship between the HEAs phase features. Through extensive numerical experiments, we investigate the effects of design parameters in identifying various phases and evaluate the performance of the proposed models in estimating and predicting the HEA phases.

Unraveling the mechanisms of stability in $Co_xMo_{70-x}Fe_{10}Ni_{10}Cu_{10}$ high entropy alloys via physically interpretable graph neural networks: *James Chapman*[1]; Miguel Tenorio[1]; [1]Boston University

In recent years high entropy alloys (HEA) have become a topic of significant interest due to their combinatorial nature, showing promise for hypersonics and catalysts. In particular, the HEA system $Co_xMo_{70-x}Fe_{10}Ni_{10}Cu_{10}$ has been studied experimentally and computationally due to its reported superiority as a catalyst for ammonia decomposition. However, such catalytic reactions take place at elevated temperatures, leading to potential HEA instability and eventual phase separation at catalytically active temperatures. To this end, we combine density functional theory (DFT) calculations of mixing free energies, that include mixing and vibrational entropy terms, with physics-inspired graph neural networks (GNN) and consider binary (A B + C), ternary and quaternary decomposition routes. We show that by learning the mixing free energy with our GNN framework we can rank geometric and chemical HEA features to better understand which features are more important than others at stabilizing HEA stability at catalytically active temperatures.

Wick Transducers with High Entropy Alloys: Unveiling Novel Thermoelectric and Superparamagnetic Behaviors: Dani Cohn[1]; *Tami Pudina*[2]; [1]University of Tennessee Knoxville; [2]American Public University System

Wick Transducers, combining RF-driven nanocavities with HEA membranes, offer a platform for exploring classical thermodynamics, quantum mechanics, and quantum information processing. These devices hold promise for advancing quantum computing by enabling the study of quantum-inspired computations, transformations, and qubit behaviors. Continued research in this field can revolutionize quantum computing technology, leading to efficient and robust quantum computing systems.

Wire Arc Additive Manufacturing of Fe-rich CrMnFeCoNi High Entropy Tribological Alloy: *Ehsan Gerashi*[1]; Andrej Klapatyuk[2]; Alexandr Gaivoronskii[2]; Anatoliy Zavdoveev[2]; Richard Chromik[3]; Xili Duan[1]; Sima Alidokht[1]; [1]Memorial University of Newfoundland; [2]Paton Electric Welding Institute of NAS of Ukraine; [3]McGill University

High entropy alloys (HEAs) are alloys that contain five or more principal elements in approximately equal atomic percentages. These alloys, whether in the form of bulk materials or coatings, exhibit potential for harsh environment applications due to their exceptional combination of mechanical, thermal, and corrosion-resistance properties. This research aimed to develop Fe-rich CrMnFeCoNi HEA coatings using wire arc additive manufacturing (WAAM). Microstructural analysis, mechanical testing, and tribological evaluations were conducted to assess coating properties. The wear behavior of these coatings against a WC-Co countersphere was tested at room temperature. Various characterization techniques, including X-ray diffraction (XRD), electron backscatter diffraction (EBSD), and Raman spectroscopy for phase analysis, scanning electron microscopy (SEM) for cross-section microscopy and phase compositions, were employed. SEM was used to reveal surface morphologies and cross-sectional analysis of the wear track. Friction and wear behavior of additively manufactured parts were discussed in relation to their mechanical properties and microstructure.

A Proposed Structure of the Rhombohedral \956 Phase of FeNiMoW using Atomistic Calculations: *Sarah O'Brien*[1]; Matthew Beck[1]; [1]University of Kentucky

The multi-principal element alloy (MPEA) FeNiMoW contains three phases: FCC matrix ($Fe_{40}Ni_{40}Mo_{16}W_4$), BCC dendrites ($Mo_{40}W_{60}$), and rhombohedral \956 phase ($Fe_{13}Ni_8Mo_{13}W_5$). FeNiMoW demonstrates adiabatic shear banding in a lamellar structure of FCC and \956 phases. Previously Liu et al. highlighted the \956 phase's A_7B_6 crystal structure, e.g. Fe_7Mo_6. Experimental techniques like nanoindentation and XRD struggle to isolate the \956 phase in the lamellar structure due to it being a few microns wide and shallow. Atomistic calculations, like DFT and DFPT, thus become extremely useful tools for characterizing the \956 phase. Potential \956 phase structures have been proposed, including: a solid solution, ordered unit cells derived from Fe_7Mo_6 to maintain symmetry, and two sublattices based on Fe_7Mo_6, with a Fe and Ni solid solution sublattice and Mo and W sublattice. Here, we present results supporting the interlocking sublattice structure being the most stable and probable structure over a range of temperatures.

Assessing Additive Manufacturing Processability of Novel Refractory High Entropy Alloys Prior to Powder Manufacture: *Lucy Farquhar*[1]; Lova Chechik[2]; Alex Goodall[1]; Abdallah Reza[3]; Felix Hofmann[3]; Iain Todd[1]; Russell Goodall[1]; [1]University Of Sheffield; [2]Friedrich-Alexander-Universität Erlangen-Nürnberg; [3]The University of Oxford

Many high entropy alloys (HEAs) have been manufactured by additive manufacturing (AM), resulting in components with excellent build quality. However, AM processes require controlled feedstock materials, and screening HEAs for AM processability is time consuming and costly. For refractory HEAs especially, bespoke powders can also be difficult to manufacture with huge associated costs and lead times. This work presents an alloy processability assessment for the laser powder bed fusion (LPBF) process, to be used prior to welding trials or expensive powder manufacture. CALPHAD analysis is used along with Rosenthal based simulations to predict the alloy susceptibility to solidification and solid state cracking. These results are then compared with experimental weld tracks and LPBF of CoCrFeNi-based HEAs and with the cracking behaviour of some commonly processed commercial alloys. The method is then used to predict AM processability of some novel refractory HEAs, one of which is then successfully manufactured by LPBF.

Development of High-entropy Tribaloy Alloys for Wear Resistance Applications: Xueyao Wu[1]; *Siqi Li*[1]; Rong Liu[1]; Matthew Yao[2]; [1]Carleton University; [2]Kennametal Stellite

In this research, the material design concept of high-entropy alloy (HEA) is proposed for Tribaloy alloys, with three HEAs being created by mixing Co based T 800 and Ni-based T-700 Tribaloy alloys in different ratios, designated as MAT46, MAT55 and MAT73, and fabricated via spark plasma sintering. The phase transformation of the mixed powders is investigated with DSC analysis. The microstructures of the SPS specimens, detected by SEM, have similar characteristics, which all consist of FCC-Co, Mo and Ni solid solution with minor HCP-Co solid solution, various Laves phase, mainly Co3Mo2Si, CoMoSi and Ni3Mo2Si, and complex intermetallic compounds. The hardness and dry-sliding wear resistance of SPS HEAs are evaluated and compared with the initial alloys. The created HEAs exhibited hardness and wear resistance between T-800 and T-700. Among the new HEAs, MAT55 having an equal ratio of T 800 and T 700, with the largest configurational entropy (1.58R), displays the best wear resistance.

Effects of Heat Treatment on the Phase Evolution and Mechanical Properties of Arc Melted AlCuFeNiSi and AlCuFeNiTi High Entropy Alloys for Engineering Applications: *Modupeola Dada*[1]; Patricia Popoola[1]; DHLIWAYO Nhlanhla[1]; [1]Tshwane University of Technology

The idea of high entropy alloys (HEAs) has attracted interest because the alloys result in solid-solution phases despite containing five or more primary elements with identical or nearly equal atomic fractions and elemental concentrations ranging from five to thirty-five per cent (at%). Hence, High entropy alloys are now employed in several industries, including energy, nuclear, automotive, and aerospace, and are thought to be viable substitutes for conventional materials. In this study, AlCuFeNiSi and AlCuFeNiTi HEAs fabricated via arc melting with different atomic concentrations were examined for their phases and microstructural characteristics after heat treatment, as well as the impact of the Thermo-mechanical process on the nanomechanical, tribological and electrochemical properties for engineering applications. Studying the effect of heat-treatment on the properties of high entropy alloys is important for the control, optimization, and improvement of the properties of high entropy alloys for engineering applications.

Extensive Characterization of Precipitation Hardened CoCrFeNiTi0.2 High Entropy Alloy: *Ilan Prilutski*[1]; Noa Lulu-Bitton[2]; Yoav Snir[2]; Eli Brosh[2]; Louisa Meshi[3]; [1]Ben Gurion University in the Negev, and Israeli Atomic Energy Commision; [2]Nuclear Research Center in the Negev; [3]Ben Gurion University in the Negev

CoCrFeNi-based High Entropy Alloys (HEA) are at the center of researchers' attention due to their potential applications as structural materials where high ductility, fracture toughness, and resistance to corrosion, irradiation and hydrogen embrittlement are required. However, their low tensile strength impedes the usage. Precipitation hardening is one of themechanisms which may help to overcome this issue. Addition of Ti promotes precipitation of various phases, such as ' ((Ni,Co)3Ti-type, Pm-3m, a=0.36nm) and/or (Ni3Ti-type,P_63/mmc, a=0.51nm, c=0.83nm). To facilitate the usage of these HEAs, precise identification of the precipitate type as well as precipitation sequence is required. In the current research, the CoCrFeNiTi0.2 alloy was thoroughly characterized applying electron microscopy, microhardness and thermal analysis, and compared to CoCrFeNi which underwent the same thermo-mechanical treatments. As a result, the precipitation sequence and phase transition temperatures were determined. Experimental results agreed with theoretical calculations.

Impact of Thermal Processing on Microstructures and Mechanical Properties of Quaternary High Entropy Alloys: *Jakhongir Bakirov*[1]; Orifjon Mikhliev[1]; Sarvar Rozikhodjaev[1]; Elyorjon Jumaev[1]; [1]FDI "UzLITI Engineering" LLC

This study investigates the crystal structure and mechanical behavior of a quaternary AlCoCrNi-based high-entropy alloy. The alloy was prepared through vacuum arc casting and subsequently annealed at 873 K for 24, 72, and 192 hours. Body-centered cubic (BCC) crystal structure has been revealed in the as-cast sample by the XRD analysis, whereas heat-treated samples exhibited hexagonal close-packed (HCP) patterns. The microstructure of the alloys displayed dendritic and matrix regions. The dendritic area in the as-cast sample exhibited spherical particles, while the matrix area showed a basket-weave morphology. Upon annealing for various durations, grain growth occurred in the matrix area, and phase transformation took place in the dendritic area. This alloy demonstrated excellent compressive properties. Annealing resulted in the strengthening of the yield strength, however sacrificing the elasticity of the alloy.

Inferrable Bayesian Models for Process-structure-property Linkages in Complex Concentrated Alloys: *George Thoppil*[1]; Alankar Alankar[2]; Jian-Feng Nie[3]; [1]IIT Bombay-Monash University; [2]IIT Bombay; [3]Monash University

In this work we attempt to extract the effect of thermo--mechanical processing on the microstructure--mechanical property linkages of complex concentrated alloys (CCAs) by training machine learning (ML) models using processing parameters as features. The effect of processing on the phase morphology and the mechanical properties is studied. The stacking fault energy (SFE) predicted based on CCA composition is used as a benchmark to identify deformation mechanisms. This work presents a novel method that attempts to establish a framework using an assortment of Bayesian--learning models to generate process--structure--property (PSP) linkages that captures the evolution of phases, their volume fractions and grain sizes and the corresponding change in mechanical properties of a diverse set of CCA compositions as they undergo various processing conditions. The evolution of the mechanical property with grain size is captured as Hall--Petch relations as an example of possible PSP linkage representations.

Influence of Si on Latent Heat Release in Solidification and Microstructures of CrFeCoNi-Si Alloys: *Jinno Maika*[1]; Toru Maruyama[1]; [1]Graduate of Kansai university

Some high-entropy alloys (HEAs) like CrMnFeCoNi alloy show excellent low-temperature toughness due to TWIP resulting from their low stacking fault energy (SFE). Alloying Si into this type of HEAs has been expected to improve the balance between strength and ductility because first-principles calculations have shown SFE of the HEAs alloyed with Si locally increases.The influence of Si content on the phase transformation process and temperature was investigated to obtain fundamental knowledge for the preparation and understanding of this alloy.CrFeCoNi alloys with Si content of 13-20at% were prepared by the casting process. Two latent heat releases were detected from the thermal analysis curve during cooling. One at the high temperature side was the melting point, which decreased with increasing Si content. The other the formation of the second phase. It was almost constant regardless of Si content, suggesting that the latent heat release was caused by an invariant reaction.

Influence of the Powder Nature on Microstructure and Weldability of Al0.3CoCrFeNi Alloys Obtained by Spark Plasma Sintering: *Adrien Saviot*[1]; Sophie Le Gallet[1]; Pierre Sallamand[1]; Jean Marie Jouvard[1]; [1]Laboratoire ICB

In this study Al0.3CoCrFeNi alloys were produced by SPS from two different powders: a gas atomized powder and a mechanically activated mixture of pure element powders. Firstly, the microstructures of the powders and sintered pieces were analyzed by SEM and XRD to highlight the influence of the mechanical activation, which results in higher hardness and secondary phases contents. Secondly, weldability was investigated using laser fusion lines, varyingthe fibre spot, laser power and welding speed. The microstructural evolution and its influence on mechanical properties have also been investigated.

Mechanical and Tribological Properties of $(CoCrFeNiMn)_{1-x}$-Ti_x high-Entropy Thin Film Synthesized by Magnetron Sputtering: *Lin Wu*[1]; Tongyue Liang[1]; Richard Chromik[1]; [1]McGill University

Using Cantor alloy and Ti targets, $(CoCrFeNiMn)_{1-x}$-Ti_x (x = 0, 4, 12, 24 in at. %) high-entropy thin films were deposited by pulsed direct current magnetron sputtering on silicon wafers. The effect of Ti content on microstructure, mechanical and tribological properties were studied. Within the variation of Ti content, all films showed a columnar structure, but with increasing Ti content there was a trend from FCC crystalline structure (0 at. % Ti) to nearly amorphous (24 at. % Ti). Using nanoindentation, film hardness (H) and reduced elastic modulus (Er) were measured. The highest H/Er and H^3/Er^2 values, potential indicators of wear resistance, were found with the minor addition of Ti. The tribological properties of the $(CoCrFeNiMn)_{1-x}$-Ti_x films were evaluated by the micro-tribological test. The friction and wear behavior of the films were revealed, and the wear mechanism will be discussed.

Microstructure Evolution of Cobalt-containing High Entropy Alloy with Varying Tungsten Content Synthesized via Mechanical Alloying and Spark Plasma Sintering: *Xueyao Wu*[1]; Siqi Li[1]; Rong Liu[1]; Matthew Yao[2]; Xiaozhou Zhang[1]; [1]Carleton University; [2]Kennametal Inc.

A cobalt-containing high-entropy alloy (HEA) system with varying tungsten content, CoCrFeNiWx (x = 0.1, 0.2, 0.4, 1.0), is studied, with a focus on the influence of tungsten content on the microstructure, precipitation, hardness and wear resistance of the HEA. The alloyed powder is prepared through mechanical alloying (MA) and then examined by XRD. It is found that the alloying effect occurred in the milling process. The MAed powders are subjected to Differential Scanning Calorimetry (DSC) analysis to determine the melting points and to obtain cast-like bulk samples. The MAed CoCrFeNiW0.2 powder is also consolidated via spark plasma sintering (SPS). The experimental results show that increasing W content can promote precipitation and enhance entropy of CoCrFeNiWx HEA, resulting in an increase in hardness. The SPS specimens have higher hardness than the bulk samples from the DSC tests and exhibit comparable wear resistance to Stellite 6 fabricated via the same processing route.

Superconductivity in a New High-entropy Alloy Nb34Ti33Mo11Hf11V11: *Bartosz Rusin*[1]; Wojciech Nowak[1]; Michał Babij[2]; Rafał Idczak[1]; [1]Institute of Experimental Physics, University of Wroclaw; [2]Institute of Low Temepratures and Structural Research, Polish Academy of Sciences

High-entropy alloy (HEA) superconductors have attracted attention since the discovery of superconductivity in Ta34Nb33Hf8Zr14Ti11 in 2014 [1]. Superconducting HEA are the new category of disordered superconductors which exhibit great stability in high temperatures and robustness to high pressures and magnetic fields [2]. Their properties make them suitable for being used in extreme conditions, for example, as high field magnets. In this work, we present superconductive properties of a new HEA Nb34Ti33Mo11Hf11V11. High-entropy alloy was synthesized by arc melting. Physical properties of the system were characterized by means of X-ray powder diffraction, magnetization, electrical resistivity, and specific heat measurements. Experimental data revealed that Nb34Ti33Mo11Hf11V11 is a microscopically homogeneous mixture of the five constituent elements, crystalizes in body-centered cubic structure and exhibits type-II superconductivity at low temperatures. [1] P. Koželj et al., Phys. Rev. Lett. 113 (2014) 107001.[2] L. Sun, R. J. Cava, Phys. Rev. Mater. 3 (2019) 090301.

Synthesis and Characterization of High-Cr and High-Co Duplex High Entropy Alloys in the CrCoNiAl System: *Pedro Oliveira*[1]; Gabriel Leal[1]; Francisco Coury[1]; [1]Federal University of Sao Carlos

This study focused on duplex systems in High Entropy Alloys (HEAs), which are primarily composed of face-centered cubic (FCC) or body-centered (BCC) structures. However, limited information is available regarding HEAs containing both FCC and BCC phases. To address this gap, thermodynamic calculations were conducted to identify four non-equiatomic compositions in the CrCoNi and CrCoNiAl systems, enriched with high levels of Cr and Co, to form duplex structures (FCC/BCC). Incorporating aluminum Al expanded the duplex field by stabilizing the BCC phase, allowing for increased ductility by adding more cobalt to the alloys. The alloys underwent characterization in various conditions, including as cast, homogenized, cold rolled, and recrystallized states, using optical microscopy, X-ray diffraction (XRD), and Vickers micro hardness. The findings demonstrated that the alloys Co15Ni33.5Cr51.5, Co15Ni32Cr48Al5, and Co34Ni16Cr45Al5 exhibited a dual-phase structure. Conversely, the Co35Ni15.5Cr49 alloy did not possess a duplex structure, due to the narrow duplex field predicted by CALPHAD.

The Impact of Compositional Variations on Microstructure and Nanomechanical Properties of Additively Manufactured AlCuFeNiTi High Entropy Alloy: *Sandeep Khadka*[1]; Hubert Bilan[1]; Tao Ma[2]; Philip Yuya[1]; [1]Clarkson University; [2]University of Michigan

An equiatomic AlCuFeNiTi high entropy alloy (HEA) was successfully fabricated for the first time using the directed energy deposition method. The alloy's microstructure and nanoscale mechanical properties were characterized using microscopy techniques and nanoindentation to provide insight into the relationship between its microstructural and nanoscale mechanical properties. The microstructure mainly comprises a dendritic region with an ordered Heusler structure and an interdendritic region with FCC structure, which also shows traces of the C14 Laves region. Dendritic fragmentation occurs during solidification, resulting in the alloy mainly having equiaxed grains distribution. Nanoindentation revealed that the interdendritic regions present a soft zone, while the Laves phase presents the hardest region. The presence of laves phase within the grain boundaries also strengthens the region. This study demonstrates the synthesis of an equiaxed HEA with a high combination of elastic modulus and hardness values determined using nanoindentation.

Radiation Damage Resistance Dependent on Compositional Complexity in Molybdenum-Based Alloys: *Emily Hopkins*[1]; Annie Barnett[1]; Khalid Hattar[2]; Mitra Taheri[1]; [1]Johns Hopkins University; [2]University of Tennessee - Knoxville

Body-centered cubic refractory high-entropy alloys (RHEAs) are proposed for the next generation of materials suitable for fusion reactor components due to their outstanding high-temperature strength, and radiation tolerant properties. This study investigates compositionally gradient Mo-based alloys and explores radiation resistance dependent on chemical complexity using transmission electron microscopy techniques. Structural observations collected via in situ transmission electron microscopy (TEM) and precession electron diffraction automated crystallographic orientation mapping (PED-ACOM) reveal indicators of increasing radiation tolerance in alloys with increased complexity under high temperature conditions. By providing fundamental analysis of the impact of additional components on damage resistance, we approach a mechanistic understanding of grain boundary and matrix effects on defect accommodation in RHEAs.

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