SYMPOSIUM PM04

High-Entropy Alloys
November 26 - November 28, 2018

Symposium Organizers
Easo George, Oak Ridge National Laboratory
Haruyuki Inui, Kyoto University
Dierk Raabe, Max Planck Institute for Iron Research
C. Cem Tasan, Massachusetts Institute of Technology

Symposium Support
JEOL USA, Inc.
Kyoto University
Thermo-Calc Software Inc.

* Invited Paper

SESSION PM04.01: Mechanical Properties and Cryogenic Phenomena
Session Chair: Peter Liaw
Monday Morning, November 26, 2018
Hynes, Level 1, Room 105

8:30 AM *PM04.01.01
Damage-Tolerance in Medium- and High-Entropy CrCoNi Alloys Robert O. Ritchie[1, 2], Jun Ding[2], Mark Asta[1, 2], Bernd Gludovatz[4], Easo P. George[3] and Qing Yu[5]; [1]Materials Science & Engineering, University of California, Berkeley, Berkeley, California, United States; [2]Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, California, United States; [3]Oak Ridge National Laboratory, Oak Ridge, Tennessee, United States; [4]University of New South Wales, Sydney, New South Wales, Australia; [5]Zhejiang University, Hangzhou, China.

Damage-tolerance is an essential characteristic of structural materials as it defines the combination of strength and toughness, properties that are often mutually exclusive. Certain medium- and high-entropy alloys, the equiatomic Cantor alloy CrMnFeCoNi and its derivatives such as CrCoNi, all of which are single-phase, fcc solid solutions, display exceptional combinations of strength (~1 GPa), ductility (~60-90%), and toughness (>200 MPa.m$^{1/2}$), properties which are further enhanced at cryogenic temperatures. *In situ* TEM observations of fracture at 293K and 93K identify multiple deformation mechanisms, associated with these alloys' high friction stress yet low stacking-fault energy (SFE), that are activated at different stages of deformation and act synergistically to contribute to strength, ductility and toughness. For example, TEM studies on CrCoNi show that a hierarchical twin network is established at 293K associated with its low SFE. This network generates substantial 3-D barriers to dislocation motion, contributing to high strength and marked strain hardening, yet at the same time, the network provides multiple pathways for the easy dislocation motion, which provides for ductility - the perfect ingredients for exceptionally high damage-tolerance. We further examine the fundamental origin of these exceptional damage-tolerant properties by focusing on the potential effect of local chemical ordering in these alloys. Although difficult to observe experimentally, our DFT-based Monte Carlo simulations show that variations in the state of local chemical order can have a profound effect on the SFE, the twin boundary energy, the energy difference between the face-centered cubic and hexagonal-close packed phases (which affects the occurrence of transformation-induced plasticity), and even the energy of formation of vacancies and interstitials, all features that can have a marked influence on the mechanical properties. These results highlight the possibility of "tuning order in disorder" to ultimately achieve the science-based design and optimization of new high-entropy alloy systems with specifically desired combinations of macroscale mechanical properties.

9:00 AM PM04.01.02
Low-Temperature Deformation Pathways of a High-Entropy Alloy by *In Situ* Neutron Diffraction Muhammad Naeem[1], Haiyan He[1], Bing Wang[1], Stefanus Harjo[2], Takuro Kawasaki[2], Si Lan[1], Zhenduo Wu[1], Hailong Huang[3], Fan Zhang[3], Zhaoping Lu[3] and Xun-Li Wang[1]; [1]Department of Physics, City University of Hong Kong, Kowloon, Hong Kong; [2]Japan Proton Accelerator Research Complex, Japan Atomic Energy Agency, Tokai, Japan; [3]State Key Laboratory for Advanced Metals and Materials, University of Science and Technology Beijing, Beijing, China.

High-entropy alloys, which consist of five or more alloying elements in equal molar ratios, are an intriguing new class of structural materials. Despite the complex chemistry, they can form a single phase solid-solution with an incredibly simple lattice. CrMnFeCoNi is a face-centered cubic (FCC), for example. Several deformation mechanisms are known to operate in high-entropy alloys. At room temperature, CrMnFeCoNi deforms like a conventional FCC alloy, showing clear stages of dislocation slip and dislocation entanglement. At liquid-nitrogen temperature, the dominant deformation mechanism changes from dislocation to twinning, leading to high strength and large ductility. Here we show that, at even lower temperature, the serrated deformation dominates. Deformation behavior of CrMnFeCoNi high-entropy alloy was studied at 15K by *in-situ* neutron diffraction, to obtain insights of the effect of low temperature on the underlying deformation mechanism and the corresponding evolution of structure. Due to the highly penetrating power of neutrons, the *in-situ* neutron diffraction is a powerful tool to capture changes in phase and deformation mode. The *in-situ* neutron diffraction data thus obtained clearly revealed crossover of different mechanisms and their demarcation points with deformation. The ultra-high strength of ~2.5GPa was achieved for the single phase CrMnFeCoNi high-entropy alloy with enhanced ductility at 15K mediated by serrated deformation, thus overcoming the strength-ductility trade-off, and showing the potential of this alloy for structural applications at low temperatures.

9:15 AM PM04.01.03
Peculiarities of Deformation of CoCrFeMnNi at Cryogenic Temperatures Aditya Srinivasan Tirunilai[1], Jan Sas[2], Klaus-Peter Weiss[2], Hans Chen[1], Dorothée Vinga Szabó[1, 3], Sabine Schlabach[1, 3], Sebastian Haas[4], David Geissler[5], Jens Freudenberger[5], Martin Heilmaier[1] and Alexander

Kauffmann[1]; [1]Institute for Applied Materials (IAM-WK), Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany; [2]Institute for Technical Physics (ITEP), Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany; [3]Karlsruhe Nano Micro Facility (KNMF), Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany; [4]Metals and Alloys, University Bayreuth, Bayreuth, Germany; [5]IFW Dresden, Dresden, Germany.

This contribution presents a comprehensive analysis of the low temperature deformation behavior of CoCrFeMnNi on the basis of quasistatic tensile tests at temperatures ranging from room temperature down to 4.2 K. Different deformation phenomena occur in this high entropy alloy in this temperature range. These include: (i) serrated plastic flow at certain cryogenic temperatures (4.2 K/8 K), (ii) deformation twinning (4.2 K/8 K and 77 K), and (iii) dislocation slip (active from 4.2 K up to room temperature). The importance of deformation twinning for a stable work-hardening rate over an extended stress range as well as strain range has been addressed through the use of comprehensive orientation imaging microscopy studies. The proposed appearance of å-martensite as well as a previously uninvestigated route of analysis, essentially a quantitative time-dependent, strain-dependent, and stress-dependent evaluation of the serrated plastic flow in CoCrFeMnNi is provided.

9:30 AM PM04.01.04
Strain Hardening in Face Centered Cubic High Entropy Alloys Feng He[1, 2], Zhijun Wang[2], Jincheng Wang[2] and C. Cem Tasan[1]; [1]Department of Materials Science and Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts, United States; [2]State Key Laboratory of Solidification Processing, Northwestern Polytechnical University, Xi'an, China.

High strain hardening rate plays a key role in enabling face centered cubic (FCC) high entropy alloys (HEAs) to have excellent ductility, high fracture toughness, and good ultimate tensile strength. Based on the alloy composition or thermo-mechanical processing, solid solution strengthening, precipitation strengthening, transformation-induced plasticity (TRIP) effect, twinning-induced plasticity (TWIP) effect can each contribute to strain hardening in FCC HEAs. The relative contributions of each of these mechanisms, however, have not been systematically investigated. In the current work, we designed two new FCC HEAs with high strain hardening rates but different solid solution strengthening levels. The deformation substructures of the two HEAs at specific strain levels were investigated by using electron channeling contrast imaging (ECCI) combined with electron backscatter diffraction (EBSD). The HEA with higher solid solution strengthening level showed not only higher strength but higher ductility as well. We attribute this abnormal solid solution strengthening effect to the different defect evolution behaviors of the two FCC HEAs. The origins of this observation were systematically studied and will be presented in this talk.

9:45 AM PM04.01.05
Microstructure and Mechanical Properties of Yttrium-Doped Bulk CrMnFeCoNi High-Entropy Alloys by Spray Forming Zhouran Zhang, Atsushi Sato and Patrick Grant; University of Oxford, Oxford, United Kingdom.

High-entropy alloys (HEAs), a new class of metallic system, have drawn worldwide considerable attention since firstly proposed in 2004. CrMnFeCoNi HEA (which is also called Cantor alloy), is the most extensively investigated one and exhibits many unique properties (e.g. good combination of strength and ductility down to 77 K, exceptional fracture toughness K_{JIc} > 200 MPa and irradiation resistance). However, in most of research, HEAs are only manufactured in laboratory scale, making mass production indispensable for further commercialization. Moreover, strengthening strategies are needed as Cantor alloys are not particularly strong at room and elevated temperatures.
In this research, spray forming is used to produce yttrium-free and yttrium-doped bulk Cantor alloy up to 15 kg as it offers the advantages of both casting (high mass flow rate) and powder metallurgy (refined microstructure) and is thus well-suited for manufacturing complex compositional alloys. Addition of yttrium together with oxygen source is known to form dispersed yttria, leading to grain refinement and oxide dispersion strengthening in alloys. Y- 24 wt.% Fe eutectic alloy was dropped into molten HEA, making final yttrium' composition 0.26 wt.%. As-sprayed alloys were subsequently swaged to rods and fully recrystallized microstructure was achieved after post annealing.
The yttrium-free and yttrium-doped (y-doped) Cantor alloys both displayed equiaxed FCC structure with average grain size of 10 and 5 μm respectively. A clear effect of trace yttrium's addition on grain refinement was observed, which contributed to 11% increase in yield strength while retaining similar ductility level. The corresponding yield strength, ultimate tensile strength and elongation are 385, 711 MPa and 41.5% and 430, 757 MPa and 32% respectively. After considering the effect of grain size on yield strength, both alloys show good combination of strength and ductility.
Nano scale yttrium oxides and chromium-rich particles were observed with bimodal size respectively in y-doped Cantor alloys. Whereas only chromium-rich particles with size of 150 nm were observed in Cantor alloys. Additional yttrium oxides serve as pinning points to dislocation movement, and further improve the strength. Moreover, good ductility of y-doped Cantor alloys, distinguished from the limited ductility of some precipitation-strengthened Cantor alloys, is likely to derive from uniformly distributed nano-scale subgrains with different crystal orientations inherent in the matrix. Some nano subgrains (orientated close to its slip planes) may play as preferential deformation site, further contributing to uniform deformation.
Bulk Cantor alloys were successfully manufactured through spray forming and yttrium oxides were introduced into Cantor alloys, exhibiting clear grain refining and strengthening effect. Further research will focus on investigating creep resistance and irradiation response of HEAs and y-doped HEAs.

10:00 AM BREAK

SESSION PM04.02: Local Structure and Mechanical Properties
Session Chair: Alice Hu
Monday Morning, November 26, 2018
Hynes, Level 1, Room 105

10:30 AM *PM04.02.01
Universal Relation Between Critical Resolved Shear Stress and Mean Square Atomic Displacement in Random High Entropy Alloys Shigenobu Ogata[1, 2], Haruyuki Inui[3] and Vei Wang[4]; [1]Osaka University, Osaka, Japan; [2]ESISM, Kyoto University, Kyoto, Japan; [3]Kyoto University, Kyoto, Japan; [4]Xi'an University of Technology, Xi'an, China.

High-entropy alloys (HEAs), are multi-component random solid solution alloys with nearly an equiatomic composition, have been receiving tremendous attention due to the excellent cryogenic temperature ductility, superior mechanical strength and good wear resistance, exceptional damage tolerance. Design and development of new HEA having further excellent mechanical properties is one of the challenges in these days. Since trial and error methods take long time and need cost, a general rule predicting mechanical response based on computable value by first-principles is truly desired. In our current study, we focus on critical resolved shear stress (CRSS) of HEA. It is well-known that CRSS of HEA is much higher than single element pure metals. Using molecular dynamics (MD) simulations with root-mean-square atomic displacement (RMSAD) tunable Jennard-Jones potential, we computed a

normalized CRSS by shear modulus as a function of a normalized RMSAD by Burgers vector length for different concentration and component of random alloys at zero temperature. The results uncover that almost linear one to one relation between the normalized CRSS and RMSAD, which stands over very wide RMSAD range, in addition the relation depends quite weakly on the concentration and component of alloys. The universality of relation is also confirmed by MD using more realistic EAM potential and available actual experimental data. This implies that RMSAD computable by first-principles can be a general CRSS predictor of random alloys, that may strongly support high-throughput design of high strength random alloys.

11:00 AM PM04.02.02
Property Targeted Quantitative Design of Complex Concentrated Alloys Hyunseok Oh[1], SangJun Kim[1], Khorgolkhuu Odbadrakhk[4], Wookha Ryu[1], Kooknoh Yoon[1], Sai Mu[2], Fritz Körmann[3], Yuji Ikeda[3], C. Cem Tasan[5], Dierk R. Raabe[3], Takeshi Egami[2, 6] and Eun Soo Park[1]; [1]Seoul National University, Seoul, Korea (the Republic of); [2]Oak Ridge National Laboratory, Oak Ridge, Tennessee, United States; [3]Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany; [4]Joint Institute for Computational Sciences, University of Tennessee and Oak Ridge National Laboratory, Oak Ridge, Tennessee, United States; [5]Massachusetts Institute of Technology, Cambridge, Massachusetts, United States; [6]University of Tennessee, Knoxville, Tennessee, United States.

Despite their unique combinations of mechanical and functional properties the property targeted quantitative design of complex concentrated alloys (CCAs) is difficult due to the complex local atomic environment. Here we present an effective quantitative design approach predicting the solid solution strength of complex concentrated alloys based on the quantum mechanically driven atomic level pressure approximation. We show that the dominant factor for the solid solution strengthening in single phase face-centered cubic complex concentrated alloys consisting of 3d transition metal elements is the variation in the atomic level pressures and discuss (i) which alloy constituents dominate the atomic level pressure, and (ii) how to rationalize configurational fluctuations of the atomic-level pressure. Finally, we establish a design recipe which uses elemental atomic-level information without explicit electronic structure calculations as an efficient vehicle for more systematic and constitutive structure-property design of CCAs.

11:15 AM PM04.02.03
Variable Chemical Order Opens a New High-Entropy Playground Qing-Jie Li[1], Howard Sheng[2] and Evan Ma[1]; [1]Johns Hopkins University, Baltimore, Maryland, United States; [2]Department of Physics and Astronomy, George Mason University, Fairfax, Virginia, United States.

High-entropy alloys (HEAs) were presumed to have a configurational entropy as high as that of ideally mixed solution of multiple elements in near-equal proportions. However, inevitable enthalpic interactions render such chemically disordered solid solution (SSs) rare and metastable, except at very high temperatures. Here we highlight a different “high entropy” signature that sets HEAs apart from traditional solvent-solute SSs. We show that HEAs can be defined as concentrated SSs offering an unusually large configurational space for *(local) chemical ordering* (LCO) and hence rich property possibilities. Our atomistic simulations with realistic empirical interatomic potentials for NiCoCr demonstrate that at a given overall composition the LCO changes conspicuously with alloy processing. The variable LCO gives rise to a broad spectrum for any generalized fault energy, in terms of both its sample-average and spatial variation (local fault energy on nanometer scale), significantly influencing the dislocation mechanisms and strength. As such, the partial chemical order in a single-phase HEA opens a vast playground not accessed by either random SSs or ordered intermetallics.

11:30 AM PM04.02.04
Tunable Stacking Fault Energies by Tailoring Local Chemical Order in CrCoNi Medium-Entropy Alloys Jun Ding[1], Qin Yu[1], Mark Asta[1, 2] and Robert O. Ritchie[1, 2]; [1]Lawrence Berkeley National Laboratory, Berkeley, California, United States; [2]University of California, Berkeley, Berkeley, California, United States.

High-entropy alloys (HEAs) are an intriguing new class of metallic materials due to their unique mechanical behavior. Achieving a detailed understanding of structure-property relationships in these materials has been challenged by the compositional disorder that underlies their unique mechanical behavior. Accordingly, in this work, we employ first-principles calculations to investigate the nature of local chemical order and establish its relationship to the intrinsic and extrinsic stacking fault energy (SFE) in CrCoNi medium-entropy solid-solution alloys, whose combination of strength, ductility and toughness properties approach the best on record. We find that the average intrinsic and extrinsic SFE are both highly tunable, as the degree of local chemical order increases. The state of local ordering also strongly correlates with the energy difference between the face-centered cubic (*fcc*) and hexagonal-close packed (*hcp*) phases, which affects the occurrence of transformation-induced plasticity. This theoretical study demonstrates that chemical short-range order is thermodynamically favored in HEAs and can be tuned to affect the mechanical behavior of these alloys. It thus addresses the pressing need to establish robust processing-structure-property relationships to guide the science-based design of new HEAs with targeted mechanical behavior. This work was supported by DoE-BES-DMSE, under Contract No. DE-AC02-05CH11231.

11:45 AM PM04.02.05
Lattice Distortion Measurement Using HR-STEM Yi Chou[1], Chanho Lee[2], Peter K. Liaw[2] and Yi-Chia Chou[1]; [1]Department of Electrophysics, National Chiao Tung University, Hsinchu, Taiwan; [2]Department of Materials Science and Engineering, The University of Tennessee, Knoxville, Tennessee, United States.

High entropy alloys (HEAs) have attracted attention for its excellent mechanical properties, such as very high yield strength even at elevated temperature or radiated condition,[1] which can be applied to high temperature (up to 1000 celsius degree) casting and nuclear application. HEA are alloys containing 5 or more elements in equal or near equal atomic percent to maximize the mixing entropy. Lattice distortion results from the atomic configuration of HEAs is expected to contribute effects on mechanical properties.
In this paper, we examine and measure the lattice distortion two HEAs, NbTaTiV and NbTaTiVZr. Average lattice distortion factor is the commonly used factor to describe the magnitude of lattice distortion, and it is related to effective distance of arbitrary two atom d_i^{eff} and the average of effective distance d^-. Both d_i^{eff} and d can be obtained from theoretical calculations. The measurement can be carried out in synchrotron or neutron diffraction, where d^- is the experimental data collected from diffraction peaks. Here we perform the imaging in STEM and the measurements from STEM images to evaluate the average lattice distortion factor.
The STEM samples were prepared using FIB equipped with in-situ pick up system, and the thin HEAs were attached to grids with platinum deposition to fix the position for reducing the drift. HR STEM HAADF images were taken when the drift rate is below 0.5 Å/min and fitted with 2D Gauss equation to specify the atomic position and intensity. The intensity guides to calculation of the Z contrast of HAADF images, and it clarifies that the atoms distributes randomly. The atomic position provides the guide to measure the lattice distortion by calculating the atomic displacement from two orthogonal plane which was defined as d_i^{eff}, and the standard deviation was taken from the displacement which in turn was the average lattice distortion u^{-D}. With the method, average lattice distortion is directly obtained from STEM images. The average lattice distortion factor of NbTaTiV and NbTaTiVZr are in good agreement with theoretical and synchrotron diffraction results.
Reference:
[1] Granberg, F. et al. Mechanism of Radiation Damage Reduction in Equiatomic Multicomponent Single Phase Alloys. Phys Rev Lett 116, 135504, doi:10.1103/PhysRevLett.116.135504 (2016).

[2] Yeh, J.-W. Recent progress in high-entropy alloys. Annales de Chimie Science des Matériaux 31, 633-648, doi:10.3166/acsm.31.633-648 (2006).

SESSION PM04.03: Elementary Deformation Mechanisms
Session Chair: C. Cem Tasan
Monday Afternoon, November 26, 2018
Hynes, Level 1, Room 105

1:30 PM *PM04.03.01
***In Situ* TEM Characterization on Deformstion of NiCrCo Alloy at Room and Cryogenic Temperature** Qian Yu[1], Robert O. Ritchie[2], Easo P. George[3], Scott X. Mao[4], Hongbin Bei[3] and Bernd Gludovatz[2]; [1]Zhejiang University, Hangzhou, China; [2]University of California Berkeley, Berkeley, California, United States; [3]Oak Ridge National Laboratory, Oak Ridge, Tennessee, United States; [4]University of Pittsburgh, Pittsburgh, Pennsylvania, United States.

NiCrCo alloy shows good combination of strength and ductility at both room and cryogenic temperature. To understand how the strength-ductility trade-off can be defeated, we apply in situ, and aberration-corrected scanning, transmission electron microscopy to examine deformation mechanisms in the medium-entropy alloy CrCoNi that exhibits one of the highest combinations of strength, ductility and toughness on record. We find that a three-dimensional (3D) hierarchical twin network forms from the activation of three twinning systems. This serves a dual function: conventional twin-boundary (TB) strengthening from blockage of dislocations impinging on TBs, coupled with the 3D twin network which offers pathways for dislocation glide along, and cross-slip between, intersecting TB-matrix interfaces. The stable twin architecture is not disrupted by interfacial dislocation glide, serving as a continuous source of strength, ductility and toughness. However, as temperature deceases, multiple deformation mechanisms are activated which was thought unlikely since reduce of temperature usually increase the competition between different deformation modes.

2:00 PM PM04.03.02
***In Situ* TEM Straining Experiments in A3S and Cantor's HEA Alloys at Liquid Nitrogen and Room Temperature** Marc Legros[1], Michal Mroz[2] and Anna Fraczkiewicz[2]; [1]CEMES CNRS, Toulouse, France; [2]Ecole des Mines de Saint Etienne, Saint-Etienne, France.

The yield stress of a non-equiatomic HEA from the CoCrFeMnNi family (A3S® grade) is significantly increased compared to the equiatomic (Cantor's) alloy of the same family. This behavior comes from a stable nanostructure, easily formed in the material after classical hot thermomechanical treatment (forging and annealing).
In situ TEM straining experiments were carried out in both alloys at liquid nitrogen and room temperature. Dislocations movements are analyzed with respect to the applied stress that is measured locally using dislocation curvature. Size effects due to the thin foil configuration are discussed. Strengthening mechanisms arise from classical dislocation/ obstacle (grain boundary, forest dislocations, twinning) interaction, but also from local distortions of the lattice that are probed by the moving dislocations. This effect seems to affect both partial and perfect dislocations.

2:15 PM PM04.03.03
TEM/STEM Investigations of the TRIP Effect in a Dual-Phase High-Entropy Alloy Wenjun Lu, Zhiming Li, Christian H Liebscher, Gerhard Dehm and Raabe Dierk; Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany.

The transformation induced plasticity (TRIP) effect is an ideal deformation mechanism for designing and tuning high-strength and yet ductile metallic materials. A recently developed dual-phase high entropy alloy (HEA) with a nominal composition of $Fe_{50}Mn_{30}Co_{10}Cr_{10}$ (at.%) shows an extraordinary combination of strength and ductility mainly owing to its TRIP effect, i.e. a sequential displacive transformation from the face-centered cubic (FCC) matrix to the hexagonal close-packed (HCP) phase [1-3]. In this study, we reveal the fundamental mechanisms of the displacive transformation in the dual-phase HEA at atomic scales. A combination of transmission electron microscopy (TEM), scanning TEM (STEM) and *in-situ*experiments unravels the detwinning and formation of hierarchical nanolaminated structures in the dual-phase HEA. The *in-situ* experiments conducted under low angle annular dark-field (LAADF)-STEM imaging reveals that the detwinning effect, i.e. formation of incoherent $\sum 3$ boundaries, induces a displacive transformation preferrably at coherent $\sum 3$ boundaries. In addition, owing to the positive and yet very low stacking fault energy of this specific dual-phase HEA (~5.2 mJm^{-2}), reversible displacive transformation from the HCP back into the original host FCC phase can also be induced during mechanical loading, in addition to the forward transformation from the FCC to the HCP. This complex sequence associated with the forward and backward transformation creates a hierarchical nanolaminated structure, which is strengthening the HEA without sacrificing any ductility.

[1] Zhiming Li, Konda Gokuldoss Pradeep, Yun Deng, Dierk Raabe, Cemal Cem Tasan. "Metastable high-entropy dual-phase alloys overcome the strength-ductility trade-off". Nature. 2016, 534, 227–230.

[2] Silva Basu, Zhiming Li, Konda Gokuldoss Pradeep, Dierk Raabe, "Strain Rate Sensitivity of a TRIP-Assisted Dual-Phase High-Entropy Alloy" May 2018, Frontiers in Materials 5

[3] Zhiming Li, Dierk Raabe, "Strong and Ductile Non-equiatomic High-Entropy Alloys: Design, Processing, Microstructure, and Mechanical Properties" JOM. 2017, 69, 2099-2106.

2:30 PM PM04.03.04
Light Weight High Entropy Alloys for Cryogenic Applications Kooknoh Yoon, Hyunseok Oh and Eun Soo Park; Seoul National University, Seoul, Korea (the Republic of).

High entropy alloy (HEA) has been studied due to its great mechanical properties such as strength, toughness and so on. Moreover, it is reported that Cantor alloy, FCC HEA, shows extremely high toughness at cryogenic temperature due to nano-size twins that is formed under dynamic stress. In this context, many researchers are trying to utilize this novel material under cryogenic environments such as the Arctic, the outer space and so on. Meanwhile, cryogenic applications are highly related with weight-lightening, because materials for LNG carrier, space shuttle are used for transportations. Thus, in this study, we will report about an alloy design of TWIP/TRIP HEAs by controlling the stacking fault energy (SFE). In addition, to achieve lighter weight while maintaining the excellent mechanical properties, aluminum which is one of the lightest metal was alloyed and the plasticity of the light weight HEA will be analyzed systematically. Indeed, our results provide a useful guideline how to improve mechanical properties by weight lightening as well as

TWIP/TRIP behavior in HEAs.

2:45 PM PM04.03.05
Multiscale Modeling of Mechanical Behavior of AlxCrCoFeNi High-Entropy Alloy Yu-Chia Yang[1], Cuixia Liu[2], Chun-Yu Liu[1], Jeffrey Lloyd[3] and Zhenhai Xia[4, 1]; [1]University of North Texas, Denton, Texas, United States; [2]Xi'an Technological University, Xi'an, China; [3]Impact Physics, U.S. Army Research Laboratory, Aberdeen, Maryland, United States; [4]Northwestern Polytechnical University, Xi'an, China.

High-entropy alloys (HEAs) have shown exceptional properties, including remarkable fracture toughness, high strength, and excellent resistance to fatigue. These properties of the HEAs result from their 5- or more equiatomic components that lead to relatively high configurational entropy, relatively large lattice strains, and unique deformation mechanisms. However, the atomic-scale complexity presents challenges to explore the underlying mechanisms through computer simulation due to a lack of effective potentials. In this work, we have developed a multiscale modeling approach for the simulations of mechanical behavior of HEAs. In the first step, the vacancy energy and stacking fault energy are calculated with density functional theory (DFT) methods. Based on the DFT calculations, we have developed an accurate embedded atom model (EAM) potential for large-scale molecular dynamics simulation of $Al_xCrCoFeNi$ HEAs. The DFT calculation results for $Al_{0.1}CrCoFeNi$ HEAs show that there is a large variation in stacking fault energy in a range of -79 to 46 mJ/m^2, depending on the local atomic environments. The origin of the negative stacking fault energy is discussed from the thermodynamic metastability of FCC stacking sequence. The nano-twin generation and interactions during deformation are also explored preliminarily with the EAM potential.

3:00 PM BREAK

SESSION PM04.04: Microstructure Control for Mechanical Properties
Session Chair: Xun-Li Wang
Monday Afternoon, November 26, 2018
Hynes, Level 1, Room 105

3:30 PM *PM04.04.01
Microstructure Control and Resultant Change in Mechanical Properties in High Entropy Alloys Nobuhiro Tsuji[1, 2], Tilak Bhattacharjee[2], Yu Bai[1], Nokeun Park[3], Shu Kurokawa[1], Pinaki Bhattacharjee[4], Rajeshwar R. Eleti[1] and Shuhei Yoshida[1]; [1]Department Materials Science and Engineering, Kyoto University, Kyoto, Japan; [2]Elements Strategy Initiative for Structural Materials, ESISM, Kyoto University, Kyoto, Japan; [3]School of Materials Science and Engineering, Yeunggnam University, Gyeongsan, Korea (the Republic of); [4]Department Metallurgical and Materials Engineering, Indian Institute of Technology Hyderabad, Hyderabad, India.

High entroly alloys (HEAs) have a large capability for microstructure control through thermo-mechanical processing, since they are mainly composed of solid solution phases that are stable and deformable at wide range of temperatures. However, HEAs have been mostly studied in their as-cast or even as-homogenized states. In this presentation, some examples of microstructure controls in several kinds of HEAs are introduced. For example, fully-recrystallized ultrafine grained microstructures with mean grain sizes of 200-400 nm could be obtained in CoCrFeMnNi and CoCrNi alloys. Such fine grain sizes are interesting from a viewpoint of nucleation of recrystallization. The ultrafine grained HEAs showed very high yield strength compared with their coarse-grained counterpart, still maintaining excellent strain-hardening ability after yielding, which led to nice combinations of high strength and large tensile ductility. We have also succeeded in microstrctucre control in an eutectic HEA, AlCoCrFeNi2.1, through various thermo-mechanical processes and in enhancing the strength keeping adequate ductility.

4:00 PM PM04.04.02
Design of Non-Equiatomic FeNiCoAl-Based High Entropy Alloys with Heterogeneous Lamella Structure Towards Strength-Ductility Synergy Cheng Zhang[1], Chaoyi Zhu[1], Tyler Harrington[1] and Kenneth Vecchio[1, 2]; [1]Materials Science and Engineering Program, University of California San Diego, La Jolla, California, United States; [2]Department of NanoEngineering, University of California San Diego, La Jolla, California, United States.

Two non-equiatomic FeNiCoAl-based high entropy alloys (HEA) with heterogeneous lamella (HL) structures are fabricated through conventional thermomechanical processing. In the HL microstructure, fine-grain regions result from inhibited grain growth due to Zener pinning of boundaries by NiAl (B2) precipitates, while of coarse grained regions originate from grain growth within large deformation bands in the absence of precipitates. A back-stress strengthening mechanism, unique to deformation of heterogeneous microstructures, is verified through electron backscatter diffraction enabled geometrically necessary dislocation (GND) density analysis. Macroscopically, back-stresses in the current two HEAs with HL structures are measured from the loading-unloading-reloading experiment. This mechanism gives rise to the combination of both high strength and high ductility in HL-HEAs.

4:15 PM PM04.04.03
Microstructural Design to Improve the Mechanical Properties of an Interstitial TRIP-TWIP High-Entropy Alloy Jing Su, Z. Li and Dierk R. Raabe; Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany.

High-entropy alloys (HEAs) have drawn considerable attention nowadays not only due to their massive solid solution structures and partly good mechanical properties but also for the reason that the concept uncovers a vast compositional space for future alloy development. Here we present a novel strategy of employing deformation-driven hierarchical microstructure design to enhance the mechanical properties of an interstitial carbon doped HEA. This is to combine the benefits of designing specific microstructure features with the compositional advantages of HEAs. The as-cast alloy was subjected to a sequence of thermo-mechanical processing including hot-rolling, homogenization, cold-rolling and tempering/annealing. A single FCC phase bimodal grain structure was obtained in the tempered specimen containing nano-grains (~50 nm) and large parent grains (10-35 μm) with pre-existing nano-twins. Trimodal microstructures were produced upon annealing characterized by small recrystallized grains (<1 μm) associated with shear bands, medium-sized grains (1-6 μm) recrystallized through subgrain rotation or coalescence of parent grains and retained large un-recrystallized grains. A superior yield strength of 1.3 GPa with an acceptable ductility (~14%) was achieved in the bimodal microstructure owing to the presence of nano-sized grains and nano-twins. In the trimodal microstructures, the ductility was dramatically improved (~60%) compared to the bimodal structures due to the appearance of a multi-stage work hardening behavior. This important strain hardening sequence was attributed to the sequential activation of transformation-induced plasticity (TRIP) and twinning-induced plasticity (TWIP) effects as a result of the wide variation in phase stability promoted by the grain size hierarchy.

4:30 PM PM04.04.04

Pressure-Induced Phase Modifications in Al-Based High-Entropy Alloys $Al_xCoCrFeNi$ (x=0.1, 0.3, 0.75, 1.5) Chenxu Wang[1], Cameron L. Tracy[1], Sulgiye Park[1], Chien-Hung Chen[1], Tengfei Yang[2], Congyi Li[2], Yugang Wang[3], Yong Zhang[4], Wendy L. Mao[1] and Rodney C. Ewing[1]; [1]Stanford University, Stanford, California, United States; [2]The University of Tennessee, Knoxville, Knoxville, Tennessee, United States; [3]Peking University, Beijing, China; [4]University of Science and Technology Beijing, Beijing, China.

Pressure-induced structural modifications in high-entropy alloys with varying Al content, $Al_xCoCrFeNi$ (x=0.1, 0.3, 0.75, 1.5), have been investigated at pressures up to ~50 GPa by synchrotron X-ray diffraction and transmission electron microscopy (TEM). In $Al_xCoCrFeNi$ compounds with $x \leq 0.3$, all of which exhibit initial pure fcc structures, the proportionality between the Al content and the transformation pressure is observed. This is attributed to the large size of Al atoms relative to those of the other constituent elements, which leads to more structural distortion in $Al_{0.3}CoCrFeNi$ and subsequently an increase in the formation energy of the stacking faults. High-resolution TEM results show the variation of the stacking sequence from ABCABC (fcc) to ABABAB (hcp) in $Al_{0.1}CoCrFeNi$ following exposure to high pressure. In $Al_{0.75}CoCrFeNi$, which exhibits an initial dual-phase structure, the result again shows the transformation to an hcp phase despite its higher Al content, which might be due to the presence of the bcc phase that is more amenable to the pressure-induced phase modification. However, the trend of transformation inhibition by increasing Al content is again observed, with $Al_{1.5}CoCrFeNi$ retaining its initial structures up to the highest pressure achieved. High-pressure processing of this class of high-entropy alloys might allow for improvement and producing phases that are otherwise inaccessible.

4:45 PM PM04.04.05
Structural Screening of FCC and BCC Thin-Film HEAs Using Compositional Gradient Samples Azin Akbari, Artashes N. Ter-Isahakyan and John Balk; University of Kentucky, Lexington, Kentucky, United States.

Combinatorial thin film samples of CrMnFeCoNiCu and TiVNbMoW were prepared by simultaneous magnetron sputtering of the alloying elements onto silicon wafer substrates. This arrangement yielded a wide composition gradient in the films and resulted in the formation of multiple phases. Some film regions exhibited the desired single-phase high-entropy alloy (HEA), albeit with non-stoichiometric compositions. In order to determine the extent of phase stability for these potential HEAs, multiple characterization techniques were utilized. Microstructure and composition of thin film samples were characterized via scanning electron microscopy and x-ray energy dispersive spectroscopy. Single-phase FCC and BCC regions were detected in the samples by x-ray diffraction and electron backscattered diffraction analysis. Mechanical properties of these alloys were screened across the composition range as well, using nanoindentation. Based on the results of this combinatorial approach, potential single-phase FCC and BCC HEAs were determined. Additionally, these alloys were cast in bulk form via arc-melting followed by thermomechanical processing, which yielded a homogeneous HEA in the FCC CrMnFeCoNiCu system.

SESSION PM04.05: Poster Session
Session Chairs: Easo George, Haruyuki Inui and Dierk Raabe
Monday Afternoon, November 26, 2018
8:00 PM - 10:00 PM
Hynes, Level 1, Hall B

PM04.05.01
Microstructure, Mechanical Properties and Wear Performance of Ultrafine-Grained CrFeNi-Based Medium Entropy Alloys Fuzeng Ren, Dingshan Liang, Weiwei Zhu and Cancan Zhao; Department of Materials Science and Engineering, Southern University of Science and Technology, Shenzhen, China.

Distinct from traditional alloy design strategy, metallic alloys with nearly equiatomic multi-principle elements, frequently referred to high-entropy alloys (HEAs), have attracted considerable interests in the materials science community as a new class of engineering materials with the unique mechanical properties. However, most of the present HEAs consist of coarse grained microstructure. Here, we have fabricated an ultrafine-grained (UFG) equiatomic medium entropy alloy (MEA) CrFeNi by a combination of mechanical alloying and spark plasma sintering. The obtained bulk CrFeNi consists of 98% FCC-based solid solution phase with an average grain size of ~ 740 nm and 2% BCC Cr-rich precipitates with the grain size of ~ 450 nm located at the grain boundaries. A close examination further reveals that the FCC-matrix consists of a Ni-rich zone and a Cr-rich zone. Such UFG CrFeNi alloy has tensile yield strength of ~ 650 MPa with elongation to ~ 30%. To further enhance its mechanical properties, 5 at% Nb was added to the CrFeNi matrix after which the strength was significantly increased to ~ 800 MPa and the hardness was increased from 390 HV to 540 HV. We then systematically investigated the tribological performance of the two alloys at elevated temperatures. The fabricated CrFeNi based MEAs have shown a comparable high temperature wear performance to that of the Inconel 718 superalloy. Based on an in-depth characterization on the worn surface morphology, wear debris and subsurface microstructure formed during wear, the wear mechanism was discussed. Due to an excellent combination of strength, plasticity and high temperature wear performance, the fabricated UFG CrFeNi-based MEAs are promising candidates as a new class of high temperature alloys.

PM04.05.02
Bicontinuous BCC HEA/Cu Nanocomposite Made by Liquid Metal Dealloying Process Kooknoh Yoon, Ilhwan Kim and Eun Soo Park; Seoul National University, Seoul, Korea (the Republic of).

Due to its high melting point, high sputtering resistance, low deuterium/tritium retention, and high thermal conductivity, tungsten has been recognized as the most promising candidate of plasma facing materials (PFMs) for fusion reactors. Meanwhile, copper based alloys have been proposed as the heat sink materials behind the plasma facing material due to its excellent thermo-mechanical properties. The joining of W to copper based heat-sink (CuCrZr) remain a main problem in the development of plasma facing component (PFC) due to the large difference in the coefficient of thermal expansion (CTE) between these two materials.
On the other hand, Refractor high entropy alloys(RHEA) containing W, Nb, Mo, Ta etc. is reported recently. This multi-component system exhibits higher strength than pure W due to solid solution strengthening as well as high resistivity against neutron irradiation damage.
In this research, therefore, we fabricated composites of RHEA and Cu by liquid metal dealloying (LMD) process. To utilize this technique, we prepared a precursor material which contains elements having positive and negative enthalpy of mixing with Cu simultaneously, and we immersed it into high-temperature liquid copper to form bi-continuous composite material. Finally, we analyze strength and thermal conductivity of the composite systematically.

PM04.05.03
Spacegroup Monte Carlo Method Applied on Configurational Entropy of High Entropy Alloys Yu Cheng Chen[1], Guan-Rong Huang[2], J.P Chou[3],

Peter K. Liaw[4], J.W. Yeh[5] and Alice Hu[3]; [1]Department of Materials Science and Engineering, National Chiao Tung University, Hsinchu, Taiwan; [2]Physics Division, National Center for Theoretical Sciences, Hsinchu, Taiwan; [3]Department of Mechanical and Biomedical Engineering, City University of Hong Kong, Hong Kong, Hong Kong; [4]The University of Tennessee, Knoxville, Knoxville, Tennessee, United States; [5]Department of Materials Science and Engineering, National Tsing Hua University, Hsinchu, Taiwan.

Researchers have calculated alloy configurational entropy with ideal gas mixing formula regardless the intrinsic structure symmetry. How to define configurational entropy precisely for multi-component crystalline system is a tough question. The commonest topic related to such problem is Ising model which has only two kinds of states (spin up/down) in the system. However, it becomes much more difficult to solve if we have more states in a system such as complicated compositions in high entropy alloys (HEAs). How can we deal with it? Here we develop an innovative method to solve this troublesome problem. By utilizing the concepts in group theory and discrete mathematics, we can simplify the question into Pólya counting problem. We also implement Monte Carlo method which speeds up computation time with just a little deviation from exact solution. And we will demonstrate how to apply this method to distinguish the configurational entropy for different structures of HEAs.

PM04.05.04
Tailoring Strength and Ductility of Non-Equiatomic Ti-V-Nb-Ta-Mo High Entropy Alloys SangJun Kim, Hyunseok Oh and Eun Soo Park; Seoul National Univ, Seoul, Korea (the Republic of).

Recently, high entropy alloys (HEAs) with BCC structure composed of group-4 to group-6 elements (Ti, Zr, Hf, V, Nb, Ta, Cr, Mo and W) were reported to exhibit superior mechanical properties at high temperature above 1000 C comparing Ni-based superalloy. However, it is known that the HEAs containing group-6 refractory elements (Mo and W) suffer from poor ductility at room temperature, while HEAs without group-6 refractory elements have high ductility at room temperature but show poor strength at high temperature. In this study, we investigated mechanical behavior of HEAs depending on the composition to develop HEA with high strength at high temperature and favorable ductility at room temperature. It is known that valence electron concentration (VEC) of BCC alloys has negative relationship with ductility, but elements with high valence electron (Mo and W) are responsible for high strength of the alloy. To balance the strength and ductility, Ti-V-Nb-Ta-Mo system, whose VEC is 5.0 in equiatomic composition, was selected. HEAs in equiatomic and non-equiatomic composition in the system were predicted to form single BCC phase by CALPHAD (calculation of phase diagram) approach, and experimentally confirmed to have single BCC phase. Mechanical properties of the HEAs were quantitatively analyzed in terms of VEC and solid solution hardening. The results could provide an effective guideline for tailoring mechanical properties of high entropy alloy with bcc structure, and developing promising HEAs for high temperature structural materials.

PM04.05.05
***In Situ* Grown Nanocystalline High Entropy Alloy Oxide Particles on Reduced Graphene Oxide as Hybrid Electrode Material for Supercapacitor** S. Ramaprabhu and Mamta Sham Lal; Department of Physics, Indian Institute of Technology Madras, Chennai, India.

Supercapacitors are considered as one of the most promising electrochemical energy storage device due to their high power density, large charge/discharge rates and long cycle life. A Hybrid electrode material is mainly a nanocomposite of carbon based nanomaterials and metal oxide nanoparticles. Reduced graphene oxide with high surface area and high conductivity shows electrical double layer capacitive behaviour whereas high entropy alloy oxides (HEAO) constructed with of five or more metal with equal or nearly equal quantities, shows pseudocapacitive behaviour. In this work, we successfully synthesized a novel hybrid electrode material, (CoCrCuNiAl) oxide nanoparticles uniformly embedded on reduced graphene oxide sheets (rGO) by simple in-situ sol-gel auto combustion method. The mixed (bcc and fcc) phase of the HEAO nanoparticles is confirmed from X-Ray Diffraction pattern while microstructure is studied using Transmission electron microscopy (TEM) wherein the average size of CCCNAO nanoparticle is ~20 nm. A solid-state supercapacitor with CCCNAO nanoparticle as electrode material is fabricated and the electrochemical energy storage performance is discussed.

PM04.05.06
Microstructure of a New Type of Co and Ni Based High Entropy Alloys Daniel Laipple, Andreas Stark, Marcus W. Rackel and Florian Pyczak; Helmholtz-Zentrum Geesthacht, Geesthacht, Germany.

One frequent definition for High Entropy Alloys (HEA) is a material of single phase, this single phase being a solid solution of four or more alloying elements which are mixed in nearly equal content. Probably, partly due to the difficulty of generating such single phase materials this concept is often not followed strictly, by allowing certain amounts of a second phase which is often of an ordered intermetallic type. Along similar lines as for the single phase HEAs consisting of ordered phases can be designed. Instead of the whole single phase being of equiatomic composition of all alloying elements in the ordered phase, the principle can be applied on the sublattices of the ordered phase. Then all alloying elements occupying one sublattice have to be present on this sublattice in nearly equiatomic content. The resulting alloys are termed MOCCA standing for Multiphase and/or Ordered Constitutionally Complex Alloy. For their design pre-knowledge about the partitioning behavior of alloying elements between the different phases but also between the different sublattices is necessary. We studied initially the characteristics of six different such MOCCA high entropy alloys: (1) 77Co-8Al-8W-7Ta, (2) 77Co-6Al-6W-6Ti-5Ta, (3) 38,5Co-38,5Ni-6Al-6W-6Ti-5Ta, (4) 77Co-10Al-13W, (5) 38,5Co-38,5Ni-10Al-13W and (6) 77Co-8Al-8W-7Ti which were all based on the $L1_2$-Co_3(Al,W) ordered phase. Information about partitioning between phases and sublattices is available from experimental and theoretical investigations and was used to design the alloys. The samples are manufactured by arc melting and were annealed at 1300°C for 12h under Ar atmosphere respectively. Due to the results of SEM investigations including EDX analysis, the compositions (3) and (6) were refined in a second step by (7) 36Co-39Ni-6,5Al-6W-6Ta-6,5Ti and (8) 77Co-7,5Al-9W-6,5Ti in order to achieve a single phase constitution. Again by evaluating the SEM results composition No (7) was refined in a third step by (9) 39Ni-37Co-7Al-7Ti-7Ta-3W.
Synchrotron X-ray diffraction at P07 (PETRA III at DESY, Hamburg, Germany)
confirmed in general the phase compositions expected by the SEM investigation.

PM04.05.07
High-Entropy Ceramics of Five-Component, Equimolar, Rare-Earth (RE) Oxides Kuo-Pin Tseng and Waltraud M. Kriven; Materials Science and Engineering, University of Illinois at Urbana-Champaign, Urbana, Illinois, United States.

To investigate the influence of cation radii on synthesizing high-entropy ceramics, a new system of five-component high-entropy oxides are reported here. Much research has been conducted in defining high-entropy alloys. However, the cation selection rules for high-entropy ceramics are still unclear. In this research, four rare-earth (RE) cations were selected and fixed. The fifth cation with larger radius was chosen from another set of eight different rare-earth (RE) cations. According to the rules of thermodynamics, each group of five cations were mixed in equimolar ratios to maximize the mixing entropy. Using the concept of atomic size difference (δ) in high-entropy alloys, the cation radii difference in this system ranges from 1.25 to 5.71. Synchrotron-sourced X-ray powder diffraction patterns were measured here. The results show that all of these eight rare-earth (RE) candidates change into simple disordered high-entropy oxides after heat treatment. This indicates that the well-distributed cations in cubic-bixbyite structure are established in each group of candidates.

Even though the radius of the largest cation is 1.16 times larger than that of the smallest one, all these cations still uniformly share the same lattice sites.

Meanwhile, high-entropy oxides have the ability to keep all the cations in the same oxidation states. As we all know in oxides, some of cations tend to transform between trivalent states and tetravalent states under different conditions of temperature and pressure. Surprisingly, the high-entropy configuration can prevent the same type of cation from moving and aggregating. As a result, the valence states of all the trivalent cations are retained. This research provides a preliminary guideline of cation selection for synthesizing high-entropy ceramics in order to explore the next generation of structure-stabilized ceramics.

PM04.05.09

Ordering in a Series of Al-Containing Refractory High Entropy Alloys Ta-Nb-Mo-Cr-Ti-Al Alexander Kauffmann[4], Hans Chen[4], Sascha Seils[4, 1], Torben Boll[4, 1], Sandra Kauffmann-Weiss[2], Ian Harding[3], Sharvan Kumar[3], Dorothée Vinga Szabó[4, 1], Sabine Schlabach[4, 1], Christian H Liebscher[5], Franz Müller[6], Bronislava Gorr[6], Hans-Jürgen Christ[6] and Martin Heilmaier[4]; [1]Karlsruhe Nano Micro Facility (KNMF), Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany; [2]Institute for Technical Physics (ITEP), Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany; [3]School of Engineering, Brown University, Providence, Rhode Island, United States; [4]Institute for Applied Materials (IAM-WK), Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany; [5]Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany; [6]Institut für Werkstofftechnik, Universität Siegen, Siegen, Germany.

High entropy alloys (HEAs) based on the Ta-Nb-Mo-Cr-Ti-Al system are expected to possess high creep and oxidation resistance as well as outstanding specific mechanical properties due to comparably low density. However, we recently reported that these arc-melted and subsequently homogenized alloys exhibited a lack of ductility up to 600 °C depending on the specific alloy composition [H. Chen et al. in Metall. Mater. Trans. A 49 (2018) 772-781 and J. Alloys Cmpd. 661 (2016) 206-215]. In this presentation, we provide the results of comprehensive microstructural characterization of a series of Ta-Nb-Mo-Cr-Ti-Al derivatives for assessing ordering as potential origin for the observed lack of ductility. Backscatter electron imaging (BSE), energy dispersive X-ray spectroscopy (SEM-EDX and STEM-EDX) and atom probe tomography (APT) were used to prove uniform element distribution after homogenization in these alloys. X-ray diffraction patterns (XRD) of the Ta-free derivatives indicated W prototype crystal structure without the presence of significant superlattice peaks, whereas TEM diffraction experiments confirmed B2 order. The presence of thermal antiphase domain boundaries (APDBs) suggested that order resulted from a disorder-order solid-state phase transformation during cooling from the homogenization temperature. In MoCrTiAl, these APDBs were enriched in Cr and depleted in Ti as confirmed by STEM-EDX line scans as well as APT analyses. Based on these results, we present an experimental approach to determine the site occupation factors in order to refine the experimental XRD patterns of these alloys. These refinements provide the basis for a critical discussion of the conflicting absence of superlattice reflections in XRD patterns in some HEAs while order is revealed by other techniques.

PM04.05.10

Possible Correlation Between Strength and Mean Square Atomic Displacement in Cr-Mn-Fe-Co-Ni High Entropy Alloys Makoto Asakura[2], Kodai Niitsu[2, 1], Norihiko L. Okamoto[3], Koretaka Yuge[2], Kyosuke Kishida[2, 1], Haruyuki Inui[2, 1], Takashi Fukuda[4] and Tomoyuki Kakeshita[4]; [1]Center for Elements Strategy Initiative for Structural Materials (ESISM), Kyoto University, Kyoto, Japan; [2]Department of Materials Science and Engineering, Kyoto University, Kyoto, Japan; [3]Institute for Materials Research, Tohoku University, Sendai, Japan; [4]Division of Materials and Manufacturing Science, Osaka University, Osaka, Japan.

High entropy alloys (HEAs) are equiatomic or nearly equiatomic solid solution alloys consisting of at least five elements, which crystallize into a single phase presumably due to the large contribution of configurational entropy to the Gibbs free energy. The equiatomic Cr-Mn-Fe-Co-Ni HEA with the face-centered cubic (FCC) structure has been reported to exhibit excellent ductility and exceptional fracture toughness at cryogenic temperatures. To date, these properties in HEAs have been explained within the framework of the classical theories of solid solution strengthening. However, the classical derivations for binary dilute alloys, such as Fleischer's and Labusch's models, are not applicable to HEAs because solute atoms in HEAs are no longer discernible. Very recently, Mean-Square Atomic Displacement (MSAD) is suggested to be a new parameter scaling the degree of solid solution strengthening. This is a value of lattice distortion averaged across whole crystal, and is evaluated by ab initio calculation with Special Quasi-random Structure (SQS) models. For polycrystalline equiatomic HEA and its derivatives, the positive correlation between their yield strength and $MSAD^{0.5}$ values was reported [1]. However, since the yield strength in the form of polycrystals is anticipated to be perturbed by the grain boundaries and textures, critical resolved shear stress (CRSS) of the HEA crystal should be assessed with single crystals. In the present study, we fabricated single crystals of Cr-Mn-Fe-Co-Ni HEAs and its derivatives with which the composition of only one element is changed and the other four elements' compositions are equiatomic by the Bridgeman method. Compression tests were performed on rectangular parallelepiped single crystals with the size of $2\times2\times5$ mm^3 with the [-123] loading axis at an engineering strain rate of 1.0×10^{-4} s^{-1} and at temperatures from 13K to 298K. MSAD values were calculated by ab initio method with SQS models. Bulk single crystals are successfully grown for all compositions. Positive linear relationship between CRSS and $MSAD^{0.5}$ is elucidated as is previously reported for the relationship between yield stress and $MSAD^{0.5}$ in the HEA polycrystals. In addition, this relationship is found to be applicable even for non-equiatomic HEA derivatives; MSAD is anticipated to be an essential parameter scaling the degree of solid solution strengthening of broader class of FCC multi-component alloys.

[1]Norihiko L. Okamoto, Koretaka Yuge, Katsushi Tanaka, Haruyuki Inui, Easo George, AIP Advances 6, 125008 (2016)

PM04.05.11

Anomalous X-Ray Scattering Study of the Local Structure of Mo Atoms in FeCoCrNiMox (x = 0.11 and 0.23) High Entropy Alloys Haiyan He[1], Bing Wang[1], Si Lan[1, 2], Jacob Ruff[3], Chain Tsuan Liu[4] and Xun-Li Wang[1]; [1]Physics, City University of Hong Kong, Hong Kong, Hong Kong; [2]Herbert Gleiter Institute of Nanoscience, School of Materials Science and Engineering, Nanjing University of Science and Technology, Nanjing, China; [3]Cornell High Energy Synchrotron Source, Cornell University, Ithaca, New York, United States; [4]Mechanical and Biomedical Engineering, City University of Hong Kong, Hong Kong, Hong Kong.

High entropy alloys which contain 5 or more elements often have a rather simple structure like body-centered-cubic (BCC) or face-centered-cubic(FCC). In spite of the simple average crystalline structure, the local atomic order of individual atomic species has remained an open question. In this study, anomalous X-ray scattering was applied to determine the local structure of Mo in FeCoCrNiMox (x = 0.11 and 0.23), a high entropy alloy with FCC lattice. At the Mo absorption edge, the intensity of all diffraction peaks decreased, by nearly identical amount. Detailed analysis of the experimental data confirms that Mo atoms are randomly distributed instead of locally segregated in the FCC lattice.

The work was supported by the grant from the Research Grants Council of the Hong Kong Special Administrative Region [CityU 11215917]. Anomalous X-ray scattering was conducted at station A2, Cornell University, Cornell High Energy Synchrotron Source.

PM04.05.12

Plastic Deformation of Single Crystals of a Cr-Co-Ni Equiatomic Medium Entropy Alloy Kazuki Ehara[1], Makoto Asakura[1], Kodai Niitsu[1], Kyosuke Kishida[1, 2] and Haruyuki Inui[1, 2]; [1]Department of Materials Science and Engineering, Kyoto University, Kyoto, Japan; [2]Center for Elements Strategy Initiative for Structural Materials (ESISM), Kyoto University, Kyoto, Japan.

Medium/high entropy alloys are a class of multi-component solid solution alloys with (nearly) equiatomic compositions, which are considered to be stabilized because of the large contribution of configurational entropy to the Gibbs free energy. Some of these alloys exhibit exceptional mechanical properties such that their strength, tensile elongation and fracture toughness increase with decreasing temperature simultaneously. Among various medium/high entropy solid solution alloys discovered so far, the Cr-Co-Ni equiatomic solid solution alloy with the face-centered cubic (FCC) structure has been reported to exhibit both the highest strength and highest elongation in a polycrystalline form. However, the detailed mechanisms endowing the excellent mechanical properties to the Cr-Co-Ni equiatomic alloy remain unclear in many aspects mainly because of the lack of fundamental studies using single crystals. In the present study, we prepared single crystals of the Cr-Co-Ni equiatomic solid solution alloy by directional solidification in an optical floating zone furnace and investigated the deformation behavior of the [-123]-oriented single crystals under uniaxial tensile and compressive loading as a function of temperature (13K to 1073K). Temperature dependence of the activation volume were investigated by strain rate change compression tests (1×10^{-5} to 5×10^{-3} s^{-1}). Stress-strain curves obtained from tensile tests at low temperatures exhibit a widely extended easy-glide region (stage I) when it is compared to that for the Cr-Mn-Fe-Co-Ni equiatomic solid solution alloy. This is considered to reflect a relatively low stacking fault energy for the Cr-Co-Ni equiatomic alloy. The critical resolved shear stress (CRSS) of the Cr-Co-Ni equiatomic alloy is higher than that of the Cr-Mn-Fe-Co-Ni equiatomic alloy. The CRSS value increases significantly with decreasing temperature below room temperature and with increasing temperature above 873K. Activation volume of the Cr-Co-Ni equiatomic alloy is found to be much lower than those of binary FCC solid solution alloys.

PM04.05.13

Effect of Impurity Solute Atoms on Strength of α-Al (fcc) Single-Crystal Micropillars Soichiro Takeyasu, Naoki Takata, Asuka Suzuki and Makoto Kobashi; Department of Materials Process Engineering, Nagoya University, Nagoya-shi, Japan.

High-entropy alloys (HEAs) exhibit high ductility and strength and toughness with decreasing temperature, and it is widely known that CrMnFeCoNi is the fcc structure and maintains its single-phase, solid solution state at elevated temperatures. N. L. Okamoto et al. have recently demonstrated that single-crystal micropillars prepared from the HEA exhibit the size dependence of shear stress for the initial slip, which corresponds to pure fcc metals (Ni, Au and Cu). The study indicates the size dependence of strength would be independent of solid-solution atoms in fcc metals. In contrast, the size dependence of strength was scarcely reported in fcc solid-solution phases, whereby the influence of solid-solution atoms on the size dependence has not yet been elucidated even in fcc metals. In the present study, focusing on the commercial purity aluminum (2N purity) containing Fe and Si elements as impurity solute atoms, we have attempted to clarify the influence of trace solute atoms on the measured strength of microscale-sized pure aluminum. We have fundamentally examined the compression response of α-Al (fcc) single-crystal cylindrical micropillars with different diameters (approximately ranging from 1 to 10 μm) prepared on the sample surface of 4N and 2N purity Al sheets with the recrystallized microstructure. Micropillars were fabricated by FIB and compressed by the nanoindentation systems attached the flat punch (φ=20 μm). Slip systems were identified by crystal orientation analysis using electron back-scattering diffraction (EBSD) and scanning electron microscopy (SEM) observation. The compression tests for micropillars with various sizes demonstrated the flow stress of micropillars increases with decreasing pillar diameter. In the case of 4N purity Al, the observed size dependence of resolved shear stress for slip corresponds well to the previous studies on micropillars prepared from 5N and 3N purity Al sheets. The measured shear stress resolved onto a primary slip system (τ_i) scaled by shear modulus (G) and the pillar diameter (d) scaled by Burgers vector (b) show the following correlation: $(\tau_i/G) = 0.33(d/b)^{-0.63}$. In the case of 2N purity Al, the size dependence of resolved shear stress is smaller than that observed in higher purity Al (5N, 4N and 3N). The resolved shear stress shows the following correlation with the normalized pillar diameter: $(\tau_i/G) = 0.0062(d/b)^{-0.19}$. These results indicate that the impurity solute atoms in pure Al would reduce the size dependence of strength. In the presentation, we will present the dislocations inside the compressed micropillars observed by transmission electron microscopy (TEM) and discussed on the observed size dependence utilizing the single-arm dislocation source model. Furthermore, we will report the compression response of single-crystal micropillars of α-(Al, Mg) solid-solution phases.

PM04.05.14

Micropillar Compression Deformation of Single-Crystal in CrMnFeCoNi High-Entropy Alloy Norihiko L. Okamoto[2, 4], Shu Fijimoto[1], Yuki Kambara[1], Marino Kawamura[1], Zhenghao M. Chen[1], Hirokata Matunoshita[1], Katsushi Tanaka[3], Haruyuki Inui[1, 4] and Easo P. George[5]; [1]Kyoto University, Kyoto, Japan; [2]Tohoku University, Sendai, Japan; [3]Kobe University, Kobe, Japan; [4]Center for Elements Strategy Initiative for Structure Materials, Kyoto, Japan; [5]Ruhe University Bochum, Bochum, Germany.

High-entropy alloys (HEAs) comprise a novel class of scientifically and technologically interesting materials. Among these, equatomic CrMnFeCoNi with the face-centered cubic (FCC) structure is noteworthy because its ductility and strength increase with decreasing temperature while maintaining outstanding fracture toughness at cryogenic temperatures. However, plastic deformation behavior has not been fully characterized, due to the difficulty of obtaining large single crystals of the HEA. Recent years, a method for micro-compression testing of single-crystal pillars prepared by focused ion beam (FIB) machining, making further investigation of plastic deformation behavior in HEA possible, has been developed.

In the present study, we investigate the plastic deformation behavior of single crystals of the CrMnFeCoNi HEA by performing compression tests on micropillar specimens at room temperature as a function of specimen size and crystal orientation, in order to deduce its bulk CRSS value and orientation dependence. We also characterize deformation mechanisms at low homologous temperatures by investigating the deformation behavior of bulk polycrystals at room temperature and 77 K. Dislocation structure in a specimen deformed at 77K is investigated with Transmission electron microscopy (TEM). Stacking fault energy is thus deduced from the separation distance between the Shockley partials.

The critical resolved shear stress (CRSS) in room temperature with bulk size is estimated to be ~33–43 MPa, ~10 times higher than that of pure nickel. CRSS depends on pillar size with an inverse power-law scaling exponent of –0.63, which is within the range reported in FCC metals (-0.5 to -1.0) but close to the lower bound, and independent of orientation. The relatively low exponent of power-law in HEA corresponds to the high CRSS value, compared to those of the FCC metals. No orientation dependent is confirmed. Dislocations are smoothly curved without any preferred line orientation indicating no significant anisotropy in mobilities of edge and screw segments. Planar ½ < 110 > {111} dislocations dissociate into Shockley partials whose separations range from ~3.5–4.5 nm near the screw orientation to ~5–8 nm near the edge, yielding a stacking fault energy of 30 ± 5 mJ/m^2. Although the stacking fault energy in HEA is not particularly low, compared to certain FCC alloys (e.g. Cu-Al binaries), the separations can be relatively large, due to its relatively high shear modulus. The large separation distance may account for the difficulty in cross slip and for the occurrence of deformation twinning at low temperature. The shear-modulus-normalized CRSS of the HEA is not exceptionally high compared to those of certain concentrated binary FCC solid solutions. Its rough magnitude calculated using the Fleischer/Labusch models corresponds to that of a hypothetical binary with the elastic constants of our HEA, solute concentrations of 20–50 at.%, and atomic size misfit of ~4%.

PM04.05.15

Irradiation Behaviour and Response of High Entropy Alloys Honglun Fu[1], Maulik K. Patel[1], Anna Kareer[2], Karl Dawson[1] and Karl R. Whittle[1]; [1]University of Liverpool, Liverpool, United Kingdom; [2]Materials, University of Oxford, Oxford, United Kingdom.

High Entropy Alloys (HEA) have attracted interest within the nuclear context due to their predicted properties, and potential for tolerating radiation damage to high levels. The continued renaissance of nuclear energy, coupled with increased utilisation of fuel, and reactor materials requires continued development of materials capable of tolerating high levels of induced damaged within the core. Such increased utilisation of reactor materials, whether it be as cladding or as componentry within the core, can lead to enhanced operations of the reactor, with the potential for lifetime extensions of LWRs.

To this end we have studied four model HEAs $Co_{1.5}CrFeNi_{1.5}Ti_{0.5}Mo_{0.1}$, TaNbHfZrTi, $AlCoCrFeNiSi_{0.1}$ and CoCrCuFeNi, for use within reactor cores. The impacts of radiation damage have been examined using ions as proxies for neutron damage. After irradiation with Au, Ni and He, the degree of damage has been examined by electron microscopy (SEM, TEM and EDX) to elucidate the microstructural changes, and grazing incidence X-ray diffraction (GIXRD).

SESSION PM04.06: Fundamental Aspects of Entropy
Session Chair: Jun Ding
Tuesday Morning, November 27, 2018
Hynes, Level 1, Room 105

8:30 AM *PM04.06.01
High Entropy Alloys Beyond Configurational Entropy Jorg U. Neugebauer, Fritz Koermann, Blazej Grabowski, Yuji Ikeda and Tilmann Hickel; Max-Planck-Institut fuer Eisenforschung, Duesseldorf, Germany.

The name-giving entropy contribution in high entropy alloys is configurational entropy. However, configurational entropy is only one out of several entropic contributions. In a real alloy electronic, magnetic, vibrational entropy, as well as local chemical order or defects can also play a role. Presently, the relevance of these contributions for the phase stability of bulk alloys, but also for deformation mechanisms such as the formation of stacking faults or twins, remains largely unknown. Combining ab initio calculations with advanced thermodynamic methods and statistical sampling approaches we are able to accurately determine the various contributions. A detailed analysis of the results shows that the conventionally assumed dominance of the configurational entropy is in general not valid. Thus, for a realistic description of the bulk phase stability, but also to identify suitable process conditions or alloy compositions - e.g. by adding interstitial atoms such as C - the various entropic contributions have to be included. Examples of quinary magnetic high entropy alloys where this approach has been successfully employed will be given

9:00 AM PM04.06.02
From Symmetry to Entropy—An Inconvenient Truth of Crystal Configurational Entropy C.H. Hu[2], Yu Cheng Chen[3], K.Y. Fung[1], Peijun Yu[1], Peter K. Liaw[4], J.W. Yeh[5] and Alice Hu[1]; [1]City University of Hong Kong, Kowloon, Hong Kong; [2]National Taiwan University, Taipei, Taiwan; [3]National Chiao Tong University, HsinChu, Taiwan; [4]The University of Tennessee, Knoxville, Knoxville, Tennessee, United States; [5]National Tsing Hua University, HsinChu, Taiwan.

All along, researchers calculated configurational entropy with ideal gas mixing formula regardless which structure they are considering. However it is obvious that crystalline has symmetry while ideal gas does not. Therefore the very same ideal gas mixing value should not be assigned for all the other structures, such as body-centered-cubic (BCC), face-centered-cubic (FCC), hexagonal-close-packed (HCP), and others. Here we will show a precise definition how to determine configurational entropy for crystalline. Based on Burnside's lemma in combinatorial mathematics and crystalline rotation-point-group, we successfully present the configurational entropy difference between FCC and HCP. This is the first time in thermodynamic science that we know how to distinguish configurational entropy differences, which cannot be known from density functional theory, molecular dynamics, or any other computational method. Therefore this result will initiate a whole new revision of all the entropy related theorem in all kinds of disciplines including calculations of phase stability in thermodynamic physics, diffusion in material science, molecule symmetry in chemistry, DNA entropy in biology, and even statistical mechanics. Included this research, we apply our result to explain a crucial example that how high entropy alloy phase transformation starts at cryogenic temperature from nanoscale region. This also indicates conventional physical metallurgy theorem may require serious modification efforts before appropriate application on HEAs.

9:15 AM PM04.06.03
Entropy Contributions to Phase Stability in Random Solid Solutions Anus Manzoor[1], Shubham Pandey[2], Simon R. Phillpot[2] and Dilpuneet S. Aidhy[1]; [1]University of Wyoming, Laramie, Wyoming, United States; [2]University of Florida, Gainesville, Florida, United States.

High entropy alloys (HEAs) contain multiple elements in large proportions that make them prone to phase separation. In the overall vision of designing HEAs for structural applications, in this work, using density functional theory (DFT) calculations, we elucidate the contributions of various entropies, i.e., vibrational, electronic and configurational towards the phase stability of random alloys. Taking examples of various alloy systems, we show that the entropy contributions could be quantitatively comparable to the mixing enthalpy; as a result including the entropy contributions is critically important in correctly predicting the alloy phase stability. We also show that while the configurational entropy always favors phase stability by reducing the Gibbs free energy, the role of vibrational entropy is not predictable. The configurational and vibrational entropies can either compete to destabilize or can collectively contribute to stabilize the solid solutions. As a result, even those systems that have negative mixing enthalpy can show phase instability revealed as a miscibility gap; conversely, systems with positive mixing enthalpy can have stable phases due to the entropic contributions. Finally, we show that the contribution of electronic entropy is minor compared to the other two entropies. This work contributes towards the computational framework necessary for predicting the correct phase stability of HEAs.

9:30 AM BREAK

SESSION PM04.07: Mechanical Properties and High Temperature Phenomena
Session Chair: Marc Legros
Tuesday Morning, November 27, 2018
Hynes, Level 1, Room 105

10:00 AM *PM04.07.01
Deformation by Dislocations, Twinning, and Phase Transformations in Compositionally Concentrated FCC Solid Solutions C. E. Slone, J. Miao, M. Ghazisaeidi and Michael J. Mills; Department of Materials Science and Engineering, The Ohio State University, Columbus, Ohio, United States.

The equiatomic NiCoCrFeMn alloy is an fcc solid solution that exhibits intriguing characteristics including very large strain hardening rates, large fracture toughness, and strong dependence of the yield strength at low temperature. These characteristics are closely linked to dislocation-mediated plasticity, yet little experimental work has explored dislocation dissociation, stacking fault energy, or core structures in these alloys. In this study, these dislocation characteristics have been determined in the NiCoCrFeMn alloy using scanning transmission electron microscopy techniques. In addition, substructure development at larger strain has been explored as a function of strain, and compared with the ternary NiCoCr equiatomic alloy. While twinning is prevalent atlarger strains in NiCoCrFeMn, a transformation from the FCC structure to a fine-scale microtwin and hcp lath structure occurs in NiCoCr during large-strain deformation at room and cryogenic temperatures. In addition, first principles calculations using density function theory has been used to explore the relative phase stabilities and energy pathways for twinning and hcp phase formation. These modeling results are compared directly with atomic resolution scanning transmission electron microscopy evidence for these structures, and possible mechanisms by which they form will be presented. In addition, the relationship of this phase transformation to the strength and work hardening behavior in these two alloys will be explored.

10:30 AM PM04.07.02
Elastic Properties of Low, Medium and High Entropy Alloys with the FCC Structure Katsushi Tanaka, Takeshi Teramoto and Kazuki Yamada; Kobe University, Kobe, Japan.

Monocrystalline elastic constants of low, medium and high entropy alloys with the fcc structure have been analyzed systematically. Acording to our previous result, monocrystalline elastic constants of equiatomic quinary CrMnFeCoNi alloy show characteristic features indicating a relatively large elastic anisotropy and the existance of a strong directional interatomic interaction in the alloy. On the other hand, elastic constants of pure-Ni and FeNi low entropy alloy are analyzed as more metallic, that is a weaker directional interatomic interaction. In this study monocrystals of equiatomic low, medium and high entropy alloys with the fcc structure were grown by a modified Bridgeman method and the elastic constants were determined from liquid helium temperature to 1200 K using a ultrasound spectroscopy. The results show a systematic transition of the elastic properties from pure-metal to a high entropy alloy, though some scattering are observed depending on the alloying elements especially for midium entropy alloys.

10:45 AM PM04.07.03
Study of Pseudo-Binary Diffusion in Single-Phase High-Entropy CrFeCoNi Alloys Adeline Durand[1], Guillaume Laplanche[1], Ying Yang[2], Gunther Eggeler[1] and Easo P. George[2]; [1]Ruhr-Universität Bochum (RUB), Bochum, Germany; [2]Materials Science and Technology Div, Oak Ridge National Laboratory, Oak Ridge, Tennessee, United States.

High-Entropy Alloys (HEAs) are single-phase alloys composed of multiple principal elements in relatively high concentrations. Consequently, traditional notions of solvent and solute do not apply, and it is not clear how this affects diffusion kinetics of the constituent elements. Sluggish diffusion is said to be an important characteristic of HEAs; however, it has been increasingly contested in recent years. The goal of this study is to investigate and better understand interdiffusion processes in HEAs.

We adopted the pseudo-binary model introduced by Tsai et al. [1] in which only two elements are diffusing against each other while the others are kept at a constant concentration. According to Tsai, in this situation, the interdiffusion, intrinsic and self-diffusion coefficients are assumed to be equal. In our experiments, all the constituent pseudo-binaries were studied at the same time with the help of suitable diffusion multiples. The following are our major results and conclusions:

(1) Up-hill diffusion was observed, proving that interactions between all constituent elements exist and should not be totally ignored in contrast to what was claimed in the model of Tsai et al. [1]

(2) No significant Kirkendall effect (voids or shift of initial interface) was noted, confirming that interdiffusion and intrinsic diffusion coefficients are indeed equal.

(3) The systematic study of all pseudo-binaries showed substantial differences between the diffusion speeds of a given element in different pseudo-binaries, which invalidates the assumption that intrinsic and self-diffusion coefficients are equal.

(4) Thermodynamic simulations are currently under way to rationalize our experimental observations.

In conclusion, even though some aspects of Tsai's model have been disproven here and in the literature [2], the model still provides an efficient way to compare diffusion of elements in different conditions and can easily show the different interactions among them (e.g. whether certain elements enhance or slow down diffusion of others).

[1] K.-Y. Tsai, M.-H. Tsai, J.-W. Yeh, Sluggish diffusion in CoCrFeMnNi high-entropy alloys, Acta Materialia 61 (2013) 4887-4897
[2] M. Vaidya, K. G. Pradeep, B. S. Murty, G. Wilde, S. V. Divinski, Bulk tracer diffusion in CoCrFeNi and CoCrFeMnNi high entropy alloys, Acta Materialia 146 (2018) 211-224

11:00 AM OPEN DISCUSSION

11:15 AM PM04.07.05
Study of Oxidation Mechanisms in Refractory Mo-W-Ta-Ti-Zr HEA Using Periodic DFT and Atomistic Thermodynamic Modelling Eric Osei-Agyemang and Ganesh Balasubramanian; Lehigh University, Bethlehem, Pennsylvania, United States.

High-temperature strength, toughness and oxidation resistance are exhibited by Ni-based superalloys. However, increasing the application temperatures for such alloys become problematic due to melting temperatures of around 1350ºC. New class of materials that can withstand harsher conditions at elevated temperatures are therefore desirable.
High entropy alloys (HEA) based on refractory elements may achieve higher temperature operations with superior creep strength. At elevated temperatures, Mo based HEAs have been observed to exhibit good thermal and mechanical properties. Recently, a refractory Mo-W-Ta-Ti-Zr HEA was observed to exhibit greatly enhanced modulus of elasticity (3x at 300K) over near atomic cases and with higher moduli above 500K over commercial alloys (2.3x at 2000K).

In this study, periodic DFT and atomistic thermodynamic modelling is used to study the oxidation mechanisms in the Mo-W-Ta-Ti-Zr HEA. The special quasi-random structures (SQS) model was used to generate random structures in combination with the VASP DFT package. A Monte Carlo algorithm implemented in the ATAT package is used to match the correlation functions in the random structures for pairs up to the seventh nearest neighbor shells, triplets up to the fourth nearest neighbor shells and quadruplets up to the third nearest neighbor shells. The best representative random structure as shown in the figure below is used to create different surfaces and the most stable surface selected based on the calculated surface energy.
The stable facets are subsequently reacted with oxygen to gain a detailed understanding of the surface oxidation process. A link between theoretical and experimental conditions are established by using a thermodynamic approach to establish different temperature and pressure regimes on the oxidized surfaces at different oxygen coverages.

11:30 AM PM04.07.06
High-Temperature Nanomechanical Behavior of HEAs for Service Under Extreme Conditions Youxing Chen[1], Eric D. Hintsala[2], Nan Li[3], Douglas Stauffer[2], Bartosz Nowakowski[2] and Nathan Mara[1]; [1]University of Minnesota Twin Cities, Minneapolis, Minnesota, United States; [2]Bruker Nano Surfaces, Eden Prairie, Minnesota, United States; [3]Los Alamos National Laboratory, Los Alamos, New Mexico, United States.

The potential good high-temperature mechanical performance of high entropy alloys (HEAs) has attracted significant attention for demanding nuclear applications. Although abundant high-temperature mechanical behavior data exists for bulk HEAs, high-temperature correlation of microstructure and mechanical properties, especially after exposure to ion irradiation, requires more investigation in order to continue optimizing performance. In this talk, we investigate two types of HEAs with different microstructures: fcc FeCrNiMn and dual-phase FeCrNiMnAl HEAs with a mixed fcc/bcc structure. The mechanical properties of both materials were studied before and after Fe ion irradiation at 500 ºC with a peak damage level of ~ 50 dpa. High-temperature (up to 500 ºC) mechanical maps of HEA alloys achieved by elevated temperature nanoindentation under a vacuum atmosphere clearly demonstrate mechanical contrast from different grains and phases. With increasing test temperature, both fcc and bcc phases soften to different extents, and radiation hardening for the fcc and bcc phases exhibit marked differences. The combined effect of temperature and radiation damage on mechanical behavior will be discussed in terms of dislocation-based hardening models and resulting defect populations at elevated temperatures.

11:45 AM PM04.07.07
FeMnNiAlCr High Entropy Alloys (HEAs) and Their Native Oxide Solar Absorbers for Concentrated Solar Power Systems Eldred Lee, Margaret Wu, Sheppard Somers, Ian Baker and Jifeng Liu; Dartmouth College, Hanover, New Hampshire, United States.

Concentrated solar power (CSP) systems enable efficient solar energy harvesting and large-scale storage in the form of heat, allowing to supply solar electricity even when the sun does not shine. This capability can mitigate the intermittency issue of solar electricity. Carnot's Theorem dictates that a higher operation temperature of a CSP system lead to higher energy conversion efficiency. However, the maximal operation temperature of commercial CSP system is limited to 873K as common materials used for the tubing systems (e.g. stainless steel) cannot operate at higher temperatures due to challenges in mechanical & chemical stability. One challenge is the subpar creep resistance and excessive oxidation of currently used CSP tubing materials at high temperatures, leading to crack formation. Ni- & Ti-based and oxide-dispersion strengthened alloys can overcome the problems, but they are expensive. Another challenge is the receivers of CSP systems, where the sunlight is focused on solar selective absorber coatings. The receiver should absorb maximum solar radiation and convert it to heat with low thermal emittance loss at the IR regime. The conversion efficiency should ideally be >90% and stable at high temperatures (>973K). Yet the current coatings (e.g. Pyromark 2500) [1] have high emittance loss (>70%) & conversion efficiency below 90% under long-term at >973K with a likely delamination under the thermal cycles of CSP systems. To address these challenges, we grow native oxides on two- & three-phase FeMnNiAlCr HEAs to lower the thermal emittance loss (<50%), increase the solar absorptance (>92%), and enhance the conversion efficiency (~91% at 973K). The formation of Fe-Mn oxides and surface microstructures contribute to the drastic enhancement of optical performances at high temperatures, as previously found with externally applied Fe-Mn oxide nanoparticle-based coatings [2]. The native oxides also act as protective layers via diffusion limited oxide growth, thereby enhancing the corrosion-resistance of the HEAs. Furthermore, these HEAs have a yield strength twice that of 304 stainless steel at 973K and a good balance between strength and ductility. When annealed at 1173K, the Vickers microhardness increases considerably due to the fine NiAl-enriched precipitates. The precipitates are stable at 973-1073K, further enhancing the creep resistance of the HEA tubing materials for CSP applications. Because low-cost Fe & Mn constitute ~70 at.% of our HEAs, they are inexpensive compared to Ni- & Ti-based alloys. Therefore, the unique synergy between the mechanical & optical properties of surface-oxidized FeMnNiAlCr HEAs provides a promising solution to cost-effective tubing materials for future generations of high-efficiency CSP systems.

[1] http://www.tempil.com/specialty-Coatings/pyromark-High-Temperature-Paint/
[2] E. Lee, C. Xu, K. Kekalo, X. Wang and J. Liu, SPIE Optics and Photonics 2018: Nanoscience and Engineering Proceedings, 10730-10 (2018)

SESSION PM04.08: Mechanical Properties of FCC Alloys
Session Chair: Louis Santodonato
Tuesday Afternoon, November 27, 2018
Hynes, Level 1, Room 105

1:30 PM *PM04.08.01
Elementary Deformation Mechanisms in High- and Medium-Entropy Alloys Guillaume Laplanche[1], Joël Bonneville[5], Céline Varvenne[4], Aleksander Kostka[1], William A. Curtin[3] and Easo P. George[2]; [1]Institute for Materials, Ruhr-Universität Bochum, Bochum, Germany; [2]Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee, United States; [3]Institute of Mechanical Engineering, EPFL, Lausanne, Switzerland; [4]CINaM, Aix-Marseille University, Marseille, France; [5]Physics and Mechanics of Materials, Institut PPRIME, University of Poitiers, Chasseneuil-du-Poitou, France.

Recent progress in understanding the fundamentals of deformation in high- and medium-entropy alloys is reviewed. This presentation focuses on one of the most thoroughly investigated material systems, the fcc CrMnFeCoNi alloys. They have been shown to exhibit fascinating mechanical properties, including increasing strength and tensile ductility with decreasing temperature, with composition having a strong effect. Here, two model alloys from the CrMnFeCoNi alloy system are used to highlight key microstructural aspects responsible for strength, work-hardening rate, and ductility. Since the alloys deform by dislocation plasticity initially and mechanical twinning at higher strains, quantitative evolution of dislocation and twin densities, together with the magnitude and strain-dependence of activation volumes, are used to identify the elementary deformation mechanisms responsible for macroscopic mechanical behaviors. The activation volume at initial yielding is found to reflect the interaction of dislocations with solutes, in agreement with recent theoretical predictions, while its strong decrease upon straining is associated with forest hardening. The role of stacking fault energy on twinning is

discussed and related to deformation twinning, which enhances work hardening capability and ultimate tensile strength.

2:00 PM PM04.08.02
Phase Stability and Deformation Behaviors of High-Entropy Alloys Bing Wang[1], Muhammad Naeem[1, 2], Haiyan He[1], Si Lan[1, 2] and Xun-Li Wang[1]; [1]City University of Hong Kong, Kowloon, Hong Kong; [2]Herbert Gleiter Institute, Nanjing University of Science and Technology, Nanjing, China.

It is rather amazing that high-entropy alloys consisting of multiple alloying elements in equal molar ratios can form a single phase solid-solution with an incredibly simple lattice, e.g., face-centered cubic (FCC). We have conducted a systematic study of the phase stability and deformation behaviors of CrFeCoNiMox (x=0 – 0.3) FCC high entropy alloys, using in-situ neutron scattering techniques and electron microscopy. For x=0.3, measurements by small angle scattering show that high-entropy alloys are stable up to 800 C, beyond which significant growth of precipitates were observed, which is responsible for the reduced strength at high temperatures. At room temperature, the deformation of CrFeCoNi alloys are dominated by dislocation activities, from dislocation slip at small strains to dislocation entanglement at large strains (up to 40%). Analysis of the diffraction peak widths demonstrates that the dislocation substructures are responsible for the unusual three-stage hardening behavior observed in this alloy. At low temperatures, the alloys deform by serration, with a complicated deformation path which is fully captured by in-situ neutron diffraction measurements.

2:15 PM PM04.08.03
Investigation of the Microstructure Evolution in $Al_{0.1}$CoCrFeNi High-Entropy Alloy Liu Zhichao and Chengwen Tan; Beijing Institute of Technology, Beijing, China.

The quantitative characterization of the microstructure evolution in high-entropy alloy (HEA) during deformation is of great importance to understanding its strain-hardening behavior. In the current study, in-situ high-energy synchrotron X-ray diffraction was employed to characterize the microstructure evolution in a $Al_{0.1}$CoCrFeNi HEA during a tensile test. The stacking fault probability and twin probability at different strain levels were analyzed by the Rietveld refinement method. $Al_{0.1}$CoCrFeNi HEA exhibits a high ultimate tensile strength with a superior uniform elongation and a high strain-hardening rate. The stacking fault energy (SFE) of the $Al_{0.1}$CoCrFeNi HEA by the synchrotron measurements was estimated to be 35mJ/m^2. The increased volume faction of nano-twins and twin-twin intersections, formed during deformation, has been confirmed by transmission electron microscopy analysis. The high strain-hardening rate can be attributed to the increased density of dislocations and nano-twins.

2:30 PM BREAK

SESSION PM04.09: Phase Stability
Session Chair: Alexander Kauffmann
Tuesday Afternoon, November 27, 2018
Hynes, Level 1, Room 105

3:00 PM *PM04.09.01
Solid Solution Limit in High-Entropy Alloys—Quantitative Prediction and Experimental Verification Ming-Hung Tsai[1, 2], Jian-Hong Li[1] and Ting Chang[1]; [1]National Chung Hsing University, Taichung, Taiwan; [2]National Tsing Hua University, Hsinchu, Taiwan.

The criterion for the formation of simple solid solution phases has been an important issue in the HEA community. Most of the existing criteria are semi-empirical, with the threshold values obtained from experimental data. Some of criteria are theoretical, the tendency of phase formation is obtained by the comparing different hypothetical thermodynamic states. In this work, a new thermodynamic-based theory is proposed to predict the solid solution limit (SSL) in simple solid solution HEAs. Then, the solid solution limits of various elements in a model FCC base alloy are experimentally measured. These experimental values are used to verify the accuracy of existing models and our model. The results show that existing models evidently overestimate the SSL in HEAs. Our model has significantly higher accuracy than existing models, which provides new insights to the behavior of these multi-component solid solutions.

3:30 PM PM04.09.02
Predictive Multiphase Evolution in Al-Containing High-Entropy Alloys Louis J. Santodonato[1, 2], Peter K. Liaw[3], Raymond R. Unocic[1], Hongbin Bei[1] and James R. Morris[1, 3]; [1]Oak Ridge National Laboratory, Oak Ridge, Tennessee, United States; [2]Advanced Research Systems, Macungie, Pennsylvania, United States; [3]Materials Science and Engineering, The University of Tennessee, Knoxville, Knoxville, Tennessee, United States.

The mixing of five or more elements, in near equimolar concentrations, to form disordered substitutional solid solutions is a central feature of the class of materials known as high-entropy alloys (HEAs). It is now becoming clear that the most promising HEAs for practical applications may actually be those which undergo phase transformations and separations during cooling. The present talk describes an approach to guide the development of multi-phase HEAs, using a simple Monte Carlo model with parameters derived from first-principles calculations. These high-throughput simulations are compared with neutron scattering, *in situ* microscopy, and calorimetry measurements. We demonstrate that the present technique captures not only the qualitative features, but also gives accurate quantitative results for the intermetallic phase formation and microstructure evolution of the Al-containing HEAs. Work is underway to generalize the approach and study a wider range of compositions.

3:45 PM PM04.09.03
Quantification of Solid-Solution Phase Stability and Short-Range Ordering in High Entropy Alloy from Atomistic Simulations Zhenyu Liu and Guofeng Wang; University of Pittsburgh, Pittsburgh, Pennsylvania, United States.

High entropy alloy (HEA, also known as compositionally complex alloy) refers to simple-phase solid solution alloy that contains multiple principal components in equimolar or near-equimolar ratios. To computationally address the complexities of this type of high-order alloy systems, we have performed atomistic simulations to predicte the solid-solution stability as well as the short-range ordering in CoCrFeNi and AlCoCrFeNi bulk alloys and CoNiRuRh nanoparticles. In our simulations, the interatomic interactions were described using a set of modified embedded atom method (MEAM) interatomic potentials for these alloy systems. First, we used atomistic simulation methods to examine solid-solution phase formation rules for CoCrFeNi high entropy alloy. Using the Monte Carlo (MC) simulations based on the developed MEAM potentials, we sampled the thermodynamically equilibrium structures of the CoCrFeNi alloy and further predicted that the CoCrFeNi alloy could form a solid solution phase with high configurational entropy of 1.329R at 1373 K. Then, we examined the stability of this solid solution phase of the CoCrFeNi alloy against the well-recognized solid-solution phase

formation rules by varying the MEAM potentials and thus tuning the atom size and mixing enthalpy in the alloy. Our simulation results revealed that it required atom size difference effect delta<0.05 and mixing enthalpy effect -10 kJ/mol < ΔH < 0 kJ/mol for the modeled CoCrFeNi alloy to remain a single solid solution phase. Furthermore, we studied the stability of solid-solution phase of AlxCoCrFeNi HEAs using the developed MEAM potentials and the atomistic MC simulation method. In our MC simulations, different constituent elements were allowed to exchange their positions and thus the modelled HEAs were relaxed to their thermodynamic equilibrium states after several millions MC steps at 1300 K. The mixing Gibbs free energy of the HEAs was calculated using adiabatic switching thermodynamic integration method. We predicted that the AlxCoCrFeNi HEAs would form a single fcc solid-solution phase when x<0. 21, a single bcc solid solution phase when x>1.08, whereas a mixture of fcc and bcc phases when 0. 21<x<1.08. Our theoretical results are quite consistent with experimental observation. Moreover, we investigated the formation of solid solution phase in $Co_{0.12}Ni_{0.14}Ru_{0.43}Rh_{0.30}$ nanoparticles with size ranging from 2 to 5 nm through a combined molecular dynamics (MD) and MC approach. Our simulation results indicated that the local severe lattice distortion could block the diffusion of atoms and hence lead to a stable solid solution phase during a carbothermal shock synthesis procedure. Consequently, we have demonstrated that atomistic simulation techniques as useful methods for understanding the composition-structure-property relation of novel high entropy alloys.

4:00 PM PM04.09.04
Accelerated Atomic-Scale Exploration of Phase Evolution in Compositionally Complex Alloys Alfred Ludwig[1, 2], Yujiao Li[2], Aleksander Kostka[2], Alan Savan[1] and Helge S. Stein[1]; [1]Institute for Materials, Ruhr-University Bochum, Bochum, Germany; [2]ZGH, Ruhr-Universität Bochum, Bochum, Germany.

Single-phase compositionally complex alloys (CCA) may decompose into multiple phases at elevated temperatures or reactive environments. We present a new methodology to investigate their phase stability in an accelerated way using a combinatorial processing platform[1] which enables: simultaneous synthesis of 36 identical atomic-scale-mixed films by combinatorial co-deposition of 5 elements on an array of 10 nm-diameter Si tips; rapid phase evolution in the formed nanoscale reactors upon processing; direct atomic-scale analysis of phase evolution after each processing step by atom probe tomography, complemented by transmission electron microscopy. Using this approach, we efficiently elucidate phase evolution by monitoring the redistribution of individual atoms upon annealing. Exemplaric results from nanocrystalline CrMnFeCoNi show that this alloy is unstable and already decomposes after 1 hour at low temperatures of around 300°C. The combinatorial processing platform was also used to explore the oxidation of this CCA. This concept will accelerate the design of novel structural and functional nanocrystalline multinary materials with superior properties, as the phase space of multiple principal element alloys can be more quickly and efficiently explored, resulting in the knowledge of which phases form or decompose at different processing conditions.

[1] Y. J. Li, A. Savan, A. Kostka, H. S. Stein, A. Ludwig (2018) *Accelerated atomic-scale exploration of phase evolution in compositionally complex materials*, Materials Horizons 5, 86 – 92

4:15 PM PM04.09.05
Combinatorial Exploration of High Entropy Alloys Sebastian A. Kube[1], David Uhl[2], Amit Datye[1], Apurva Mehta[3] and Jan Schroers[1]; [1]Yale University, New Haven, Connecticut, United States; [2]Southern Connecticut State University, New Haven, Connecticut, United States; [3]SLAC National Accelerator Laboratory, Menlo Park, California, United States.

High Entropy Alloys (HEAs) are compositionally complex and span a vast composition space with many compositions potentially forming single-phase solid solutions. The quantitative prediction of solid solution structure requires a basis of consistent experimental data covering a significant portion of the alloy space. Here, we create the basis for such predictions by fabricating and characterizing 2,478 quinary HEAs based on the elements Al, Cr, Mn, Fe, Co, Ni, and Cu through combinatorial co-sputtering and high-throughput EDX and synchrotron XRD. By mining the data, we show that the solid solution structure can be predicted through the atomic size difference and the content of BCC/FCC elements in the alloy. Also, we find that the BCC structure becomes increasingly favorable with increasing atomic size difference, because it accommodates atoms of various sizes more efficiently than FCC.

4:30 PM PM04.09.06
Electrochemical and Mechanical Properties of Al-Cr-Nb-Y-Zr Based Nitride Thin Films Kristina M. Johansson[1], Pavel Soucek[2], Aishwarya Srinath[1] and Erik Lewin[1]; [1]Uppsala University, Uppsala, Sweden; [2]Masaryk University, Brno, Czechia.

Recently multicomponent nitrides with five or more elements have attracted a lot of attention due to their excellent material properties such as high hardness, thermal stability as well as corrosion and oxidation resistance. These nitrides are based on the high entropy concept where the high entropy of mixing will favor the formation of a solid solution. In many cases, it has been shown that such nitrides can outperform their respective binary nitrides [1].

In this study, Al-Cr-Nb-Y-Zr-N thin films were synthesized to investigate the effect of nitrogen content on mechanical and electrochemical properties. The Al-Cr-Nb-Y-Zr system was chosen since binary and ternary nitrides based on Al, Cr, Nb and Zr have been extensively studied for their corrosion resistance and high hardness. Also, by addition of yttrium corrosion and oxidation resistance can be improved as previously studied for the Cr-Al-Y-N and Ti-Cr-Al-Y-N systems [2-3]. The films were synthesized by reactive dc magnetron sputtering, using elemental targets of the respective elements and a Ar/ N_2 gas mix. The ratio of gases was varied in order to obtain films with varying nitrogen content, from pure alloy to nitride material. The films with no nitrogen was amorphous. For high nitrogen contents only one crystalline phase with NaCl-type structure is observed, indicating a solid solution material in analogy with the high entropy materials. The hardness increased up to 32 GPa for the films with highest nitrogen content, about 40 at.%. Corrosion resistance, studied by polarization measurements between -0.2 V to +1.5 V in a 1.0 M HCl aqueous electrolyte, showed improved corrosion resistance for all the studied samples, i.e. increased corrosion potential and lower current densities, compared to an industrial stainless steel reference sample (hyper-duplex stainless steel). Furthermore, the films with highest nitrogen content showed higher corrosion resistance compared to the metallic films. Thus, this material system shows a potential for the use as protective coatings in harsh environments.

References
[1] Li et al., Mater. Res. Lett. 6, (2018)
[2] F. Rovere et al., Surf. Coat. Technol. 202 (2008)
[3] L.A. Donohue et al., Vacuum, 55 (1999)

4:45 PM PM04.09.07
Pseudo High Entropy Alloys Yonghua Meng, Jie Pan and Yi Li; Institute of Metal Research, Chinese Academy of Sciences, Shenyang, China.

High-entropy alloys (HEAs) are defined as an alloy with at least five principal elements and equiatomic or near-equiatomic composition. However, some so-called HEAs should be considered as pseudo-binary or ternary system due to similar properties of the constituent elements. Here we report our investigation of HEAs based on RE-Al-Co (RE = La, Ce, Pr, Nd Sm and Dy) elements with more than five principal elements. Our study shows that the microstructure changes from amorphous phase to multi-phases when the number of elements increases from 5 to 8. In addition, ZrTiHfTM (TM = Cu, Ni, Co and Fe) alloys exhibit the similar B2 structure with binary $Zr_{50}Cu_{50}$ alloy. These were attributed to possible decrease rather than increase in entropy because of mixing enthalpy of some elements (e.g. rare elements) is almost zero. In this regards, many of the HEAs should be considered as pseudo-HEAs.

SESSION PM04.10: Mechanical Properties of BCC Alloys
Session Chair: Katsushi Tanaka
Wednesday Morning, November 28, 2018
Hynes, Level 1, Room 105

8:30 AM *PM04.10.01
Theory of Strengthening in BCC High Entropy Alloys William A. Curtin and Francesco Maresca; Ecole Polytechnique Federale, Lausanne, Switzerland.

The refractory BCC High Entropy Alloys (HEAs) in the class of Mo-Nb-Ta-V-W are very strong (1-1.5 GPa) at room temperature and have exceptional retained strengths of 400-500 MPa at 1600C. The mechanistic origin of these outstanding properties is not yet understood, in spite of extensive experimental studies of these and related alloys. Here, we present a parameter-free theory for the strength versus temperature in this class of BCC HEAs based on the motion of edge dislocations through the random energy landscape created by the solute fluctuations. Excellent agreement with results from direct large-scale atomistic simulations at T=0K is achieved for a range of alloys. Moreover, very good agreement with experiments is achieved for the same alloys at T=300C, and for the two alloys MoNbTaW and MoNbTaVW that have been studied up T=1600C. The fundamental origins of the high retained strength are achieved because of large barriers to edge motion. The motion of screw dislocations is also considered, and are also strengthened but by different physical emerging from the high randomness in the alloy. The edge theory enables computationally-guided design of new alloy compositions aiming for the highest retained strengths and strength-to-weight ratios in this family of alloys, and several compositions are proposed.

9:00 AM *PM04.10.02
Body-Centered Cubic High-Entropy Alloys—Understanding of the Mechanical Properties and Associated Underlying Deformation Mechanisms Jean-Philippe Couzinié[1], Guy Dirras[2], Frederic Mompiou[3], Daniel Caillard[3] and Ivan Guillot[1]; [1]ICMPE CNRS-UPEC, Université Paris Est, Thiais, France; [2]LSPM CNRS, Sorbonne Paris Cité, Université Paris, Villetaneuse, France; [3]CEMES-CNRS, Toulouse, France.

Thanks to an attractive concept, high entropy alloys are actually among the most studied materials in the metallurgical field. In addition to the exploration of new materials, they also provide the opportunity to revisit the basic concepts of metallurgy. Among the most studied high entropy materials, those with body-centered cubic systems are particularly interesting as they mainly retain high mechanical properties and are candidates for structural applications under extreme conditions. The present talk provides an overview on the properties of single phase body-centered cubic high-entropy alloys. Analysis of the existing data from the available literature will be performed and trends relative to the mechanical behavior and underlying deformation mechanisms will be proposed. The emphasis will be put on recent experimental results aimed at bringing basic knowledges on the mobility of dislocations in such complex disordered solid solutions.

9:30 AM PM04.10.03
Development of Precipitation Strengthened CCAs in the AlCrFeNiTi System for High Temperature Structural Applications Silas Wolff-Goodrich, Thorsten Meiners, Christian H Liebscher and Gerhard Dehm; Max Planck Institute, Düsseldorf, Germany.

The need to make energy generation and conversion more sustainable and to reduce the emission of harmful gases requires the development of novel high temperature stable materials. Several of the so-called compositionally complex alloys (CCAs) have been shown to possess unique property combinations and, in some cases, exceptional mechanical properties. There is much promise in the development of cost-effective CCAs with the necessary properties for use in high temperature applications. In particular, alloys with high degrees of both solid solution strengthening and precipitation of creep resistant ordered phases, such as the $L2_1$-Heusler phase, can be realised under this alloy development strategy.

In the present study we are exploring the AlCrFeNiTi system for alloys exhibiting a BCC solid solution matrix and hierarchically arranged B2-NiAl and $L2_1$-Ni2TiAl precipitate phases. The goal is to obtain novel high temperature alloys with densities of approximately 6 g/cm^3 and mechanical stability up to 900 °C. Using arc melted samples containing 5-35 at.% of each component, we have begun screening the composition space in this system . More than 15 unique alloy compositions have been produced and characterised in the as-cast state using XRD, DSC, SEM, and micro-hardness measurements. One particularly promising alloy with a composition of 25Al-15Cr-30Fe-20Ni-10Ti (in at.%) has been further investigated using high resolution TEM and STEM. We have observed a wide compositional range of stability for the $L2_1$ and BCC phases, with a strong trend to form higher $L2_1$ phase fractions–up to ~70 vol.%– for increasing Al content. Alloys with Ti concentrations of >15 at.% tend to form large fractions of the Laves phase and for >25 at.% Ti are almost entirely comprised of the Laves phase.

The trends thus-far observed have guided us to the most promising region of the composition space in this system for the target application area, this region being (20-25)Al-(10-15)Cr-(30-35)Fe-(10-20)Ni-(5-10)Ti (in at.%). Upcoming work will include a comparison of results for arc melted compositions to results for thin film composition libraries, characterisation of vacuum-induction-cast (VIC) samples in both as-cast and heat treated conditions, as well as mechanical property testing, in particular creep testing. The methodology for alloy optimisation which is developed here will be applicable to future application oriented alloy discovery and optimisation.

9:45 AM PM04.10.04
Design of Advanced Light-Weight and Low-Cost High-Entropy Alloy Rui Feng[1], Michael Gao[2], Chuan Zhang[3], Wei Guo[4], Jonathan Poplawsky[4], Fan Zhang[3], Jeffrey A. Hawk[2], Joerg Neuefeind[4], Yang Ren[5] and Peter K. Liaw[1]; [1]The University of Tennessee, Knoxville, Knoxville, Tennessee, United States; [2]National Energy Technology Laboratory, Albany, Oregon, United States; [3]CompuTherm LLC, Middleton, Wisconsin, United States; [4]Oak Ridge National Laboratory, Oak Ridge, Tennessee, United States; [5]Argonne National Laboratory, Argonne, Illinois, United States.

High-entropy alloys (HEAs) with a vast alloy-design space have offered new avenues to explore novel low-cost, high strength-to-weight ratio structural

materials. However, to date, no satisfactory light-weight HEAs (LWHEAs) have been developed, due to the difficulty in balancing strength, ductility, and density. In this study, we investigate the phase stability and transformation behavior of a newly-designed light-weight $Al_{1.5}CrFeMnTi$ HEA. The coherent precipitation of the nano-sized $L2_1$ phase within the body-centered-cubic (BCC) matrix at intermediate temperatures was observed, and their size, shape, coherency, and spatial distribution can be tuned through selected annealing treatments. Moreover, the CALculation of PHAse Diagrams (CALPHAD) and first-principles calculations successfully optimize the compositions of light-weight HEAs with a coherent nano-sized $L2_1$ precipitate-strengthened BCC two-phase structure. With the support of the optimized CALPHAD database, first-principles calculations and experimental efforts, novel light-weight HEAs, featuring lower density and lower cost, have been designed for high-temperature and cost-effective light-weight applications.

Acknowledgments: We very much appreciate the support of the U.S. Army Research Office project (W911NF-13-1-0438) with the program managers, Drs. M. P. Bakas and D. M. Stepp and the National Science Foundation (DMR-1611180) with the program directors, Drs. G. Shiflet and D. Farkas. The present research used resources at the Nanophase Materials Sciences (CNMS) and Spallation Neutron Source (SNS), a DOE Office of Science User Facility operated by ORNL. Also, the present research used resources of the Advanced Photon Source, a U.S. DOE Office of Science User Facility operated for the DOE Office of Science by the Argonne National Laboratory under Contract No. DE-AC02-06CH11357.

10:00 AM BREAK

SESSION PM04.11: Refractory HEAs and Multiphase Alloys
Session Chair: Ian Mellor
Wednesday Morning, November 28, 2018
Hynes, Level 1, Room 105

10:30 AM *PM04.11.01
Solving the Strength-Ductility Trade-Off Dilemma of High-Entropy Alloys via Interstitial Hardening Zhifeng Lei, Xiongjun Liu, Yuan Wu, Hui Wang and Zhaoping Lu; University of Science and Technology Beijing, Bejing, China.

Oxygen, one of the most earth-abundant elements, often appears as an undesired interstitial impurity in metallic materials. Even when providing strengthening it renders metals brittle, causing the strength-ductility trade-off dilemma, i.e., increasing the strength leads to decreasing ductility. Here, we report an anomalous interstitial strengthening effect of oxygen in a family of single-phase refractory high-entropy alloys (HEAs) at ambient temperature. In contrast to conventional interstitial strengthening, strength and ductility are both substantially improved when doping a model TiZrHfNb HEA with 2.0 at.% oxygen, breaking the paradigm of the strength-ductility trade-off with an inexpensive and ubiquitous element. Alloying with oxygen leads to the formation of ordered oxygen complexes (OOCs) which pin dislocations and subsequently promote their cross slip and multiplication. This novel strain hardening mechanism improves work-hardening capability and thus ductility. This finding revises our current understanding of the effect of oxygen on the mechanical behavior of metallic materials and provides new pathways for the development of high-performance alloys which have the capability to access new performance regimes.

11:00 AM PM04.11.02
Development of Refractory High Entropy Alloys with Enhancing High Temperature Strength and Room Temperature Ductility Ilhwan Kim, Hyunseok Oh and Eun Soo Park; Seoul National University, Seoul, Korea (the Republic of).

As science and technology has been evolved, there exists an extreme environment where conventional materials are difficult to use. Refractory metals are one of the most promising candidates for extreme environment especially in high temperature condition. Tungsten is a widely used structural material exhibiting excellent physical properties in high temperature environment, with high melting point, high resistance against mechanical wear. For these properties, tungsten is currently being considered as structural materials in fusion power plants for plasma facing components (PFCs). However, refractory metals, including tungsten, have some drawbacks for using as structural materials. The first is dramatic softening phenomenon in high temperature range. Their high strength and hardness in low temperature range cannot be maintained in high temperature range due to its softening phenomenon. The other is brittle behaviour below room temperature. Operating temperature of structural materials is determined above the ductile-to-brittle transition temperature (DBTT) below the recrystallization temperature. Therefore brittle behaviour at room temperature limits the application of refractory alloys because refractory alloy should be used above room temperature. In particular, the DBTT of refractory alloy is increased by small amount of adding elements. It means orthodox alloying concept cannot be answer to increasing strength and ductility of refractory alloys. Thus, it is required to develop a new-type refractory alloy to tailor these mechanical properties. In the present study, maintaining good properties of tungsten, we developed novel refractory alloys to enhance mechanical properties by utilizing design concept of high entropy alloys (HEAs). To design materials having high temperature strength and room temperature ductility, we use two parameters, atomic size misfit parameter for solid solution hardening and valence electron concentration. Because of mixing effects among the elements, tungsten based HEAs had enhanced mechanical properties than pure tungsten. To evaluate the high temperature mechanical properties, we conducted compression test and thermal conductivity measurement at high temperatures. As a result, tungsten based HEAs were improved to strength and ductility simultaneously. This study offers an explanation of the tendency between physical properties and configurational entropy. Moreover, the mechanical and thermal properties database provides us a better understanding of refractory alloys, which can suggest guidelines for tailoring refractory alloys.

11:15 AM PM04.11.03
Boundary Micro-Cracking in a Metastable High-Entropy Alloy Shaolou Wei, Jinwoo Kim and C. Cem Tasan; Department of Materials Science and Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts, United States.

Mechanically-induced martensitic transformation can be a double-edged sword: depending on composition and processing it can either lead to various beneficial mechanical effects (e.g. transformation-induced plasticity, transformation-toughening), or cause local brittleness and damage nucleation. While several corresponding guidelines are present in steels research, controlling microstructure metastability has not been drawing attention in the fast-growing field of high-entropy alloys. In the present work, we investigated the damage mechanisms of a mechanically metastable $Fe_{45}Mn_{35}Co_{10}Cr_{10}$ high-entropy alloy under uniaxial tensile loading. Our integrated in-situ scanning electron microscopy / electron backscatter diffraction experiments revealed a twofold effect of the highly localized strain, induced by asynchronously transformed martensite, leading to boundary damage nucleation and dissimilarly oriented martensitic variant formation. The latter suppresses slip transfer between adjacent grains, further expediting the growth of the nucleated damage incidents. Based on these experimental observations and corresponding theoretical calculations, we discuss the underlying mechanisms and propose a sequence of micro-events that create the observed phenomena.

11:30 AM PM04.11.04
Carbon Supersaturated Refractory Multicomponent Nanostructured Coatings Stefan Fritze, Paulius Malinovskis, Lars Riekehr, Linus von Fieandt, Erik Lewin and Ulf Jansson; Uppsala University, Uppsala, Sweden.

The combination of ceramic hardness with high ductility is a major challenge in the design of protective thin films and high entropy alloys (HEAs) are a promising pathway to achieve new high-performance materials. While HEA thin films have been studied to some extent by experimental and computational materials science, there is only limited information available about the influence of carbon on HEA thin films, especially when prepared with physical vapor deposition techniques. In this study, we report on the influence of carbon on the structure and properties of two different HEA alloys in the CrNbTaTiW system. The metal composition of these alloys includes a near-equimolar alloy and a Ta/W-rich composition.
We have deposited Cr-Nb-Ta-Ti-W-C thin films by non-reactive magnetron sputtering. The material properties were strongly depending on the composition and the best results were observed for TaW-rich films which crystallise in a bcc structure with a strong (110) texture. TEM analysis revealed that the films exhibit coherent grain boundaries with specific crystallographic directions. The addition of 8 at.% led to the formation of a meta-stable bcc supersaturated solid-solution without the formation of carbide precipitates. The main effect of the carbon addition was a significant grain refinement reducing the column width from 35 to 10 nm, which resulted in an increase in hardness from 14 to 19 GPa while the reduced E-modulus was unaffected. The enhanced hardness will be discussed in terms of solid solution hardening and grain refinement strengthening. Nanoindentation deformation studies revealed that the addition of carbon significantly reduces the plastic deformation around the indents without showing any signs of crack formation which is explained by the special arrangement of the grain boundaries.
Finally, the effect of carbon addition on the corrosion properties was likewise investigated in 0.6 M NaCl environment. High pitting corrosion resistance was found for the $Cr_3Nb_{10}Ta_{38}Ti_3W_{38}C_8$ composition, with a corrosion potential of 0.23 V (vs. Ag/AgCl) and a transpassive region equal to hyper-duplex stainless steel (i.e. SAF3207HD).

11:45 AM PM04.11.05
Mechanical Behavior and Oxidation Resistance of a Particle-Reinforced Fe-Al-Cu-Ni-Ti Alloy Manja Krueger[2], Volodymyr Bolbut[1], Georg Hasemann[2], Katja Wollgarten[2] and Dmitry Naumenko[2]; [1]University of Magdeburg, Magdeburg, Germany; [2]IEK-2, Research Center Jülich, Jülich, Germany.

We introduce the compositionally complex alloy (CCA) $Fe_{32.3}Al_{29.3}Cu_{11.7}Ni_{10.8}Ti_{15.9}$ which provides attractive mechanical properties and a density of 5.6 g/cm^3, which is lower compared to well-investigated alloys of the Al-Co-Cr-Fe-Ni-Ti-Cu family. This novel material has a bcc matrix phase and is reinforced by finely dispersed intermetallic particles, which are stable up to about 1100 °C. Hardness measurements and compressive tests in a temperature range between room temperature and 1100 °C show the advanced mechanical performance of this novel CCA compared to competitive high entropy alloys (HEAs). These first results demonstrate the high potential of this alloy as structural engineering material for high temperature applications.
During oxidation tests at 900 °C the material shows a slight mass gain which is due to the formation of an alumina layer at the surface. This layer has a thickness of ~ 1 µm after 100 h of thermal treatment, which again grows during further thermal cycling. Cyclic oxidation experiments at 1000 °C and 1100 °C resulted in spallation of this oxide layer, which leads to a mass loss of the samples. An approach to overcome this problem by the addition of a sixth alloy component will be discussed.

SESSION PM04.12: Thin Films and Micromechanical Behavior
Session Chair: Manja Krueger
Wednesday Afternoon, November 28, 2018
Hynes, Level 1, Room 105

1:30 PM PM04.12.01
Applying Combinatorial and High-Throughput Methods to Develop Compositionally Complex Alloys Alfred Ludwig[1, 2], Alan Savan[1], Janine Pfetzing-Micklich[2], Jan Alsters[1] and Sigurd Thienhaus[1]; [1]Institute for Materials, Ruhr-University Bochum, Bochum, Germany; [2]ZGH, Ruhr-Universität Bochum, Bochum, Germany.

Compositionally complex alloys (CCAs) offer an almost unlimited composition space for new materials, which cannot be explored efficiently by conventional methods. Therefore, the combinatorial fabrication of CCA thin-film materials libraries and their high-throughput characterization is discussed. Materials libraries consist of well-defined composition spreads fabricated by co-deposition from up to five magnetron sputter sources. Chemical (composition), structural (phase, microstructure), electrical (resistivity) and mechanical properties (Young's modulus, hardness) are measured using high-throughput characterization systems. The aims are to find the compositional limits of the single-phase solid solution existence range and to identify the multiphase constitution beyond these limits. Results for different CCA systems (transition metals, refractory metals) are shown and the visualization of multidimensional datasets is discussed.

1:45 PM OPEN DISCUSSION

2:00 PM PM04.12.02
Atomistic Deformation Mechanisms in Single-Crystalline and Biphase HEA Nanowires at Cryogenic Temperatures Zachary H. Aitken[1], Adenike M. Giwa[2], Julia R. Greer[2] and Yongwei Zhang[1]; [1]Institute of High Performance Computing, Singapore, Singapore; [2]California Institute of Technology, Pasadena, California, United States.

High entropy alloys (HEAs) are a class of alloys that contain multiple principle elements and display interesting mechanical properties such as increasing ductility with decreasing temperature and resistance to softening at elevated temperatures. Details of the dominant atomistic deformation mechanisms as a function of temperature are key to understanding these unique mechanical trends. Small-scale mechanical testing is well-suited to investigate deformation mechanisms and isolated microstructural features such as grain or phase boundaries. Here we present molecular dynamics simulations of compression of single-crystalline FCC and BCC HEA nanowires and HEA nanowires that contain a single FCC/BCC axially-aligned phase boundary. In single-crystalline HEAs, we identify dominant deformation mechanisms from 50 K to room temperature and investigate the role of heterogeneity in defected crystal structures. In phase boundary-containing nanowires, we also discuss dislocation-boundary interactions and the role of the FCC/BCC interface as a source, barrier, or sink for dislocations. We supplement these results with calculations of stacking fault energy and also compare observed deformation mechanisms to experimental results of compression of single-crystalline and FCC/BCC phase boundary containing HEA nano-pillars.

2:15 PM PM04.12.03
Laser Processing as a High-Throughput Method to Investigate Microstructure-Processing Relationships in a High Entropy Alloy Mu Li and Katharine Flores; Washington University in St. Louis, Saint Louis, Missouri, United States.

The compositional complexity of multiprincipal element alloys, consisting of 4 or more elements without a dominant solvent, presents a challenge for studying their microstructural development and stability. In the present work, we apply a direct laser deposition processing method to construct compositional and microstructural libraries in an efficient and high-throughput manner. Phase formation in an $Al_xCoCrFeNi$ high entropy alloy was first examined over a wide composition range. As the Al content increased from x = 0.15-1.32, the crystal structure was observed to transition from FCC to BCC/B2. While the onset of BCC/B2 formation was consistent with previously reported results based on cast materials, the FCC structure was observed at larger Al contents in the laser-processed materials, resulting in a wider two-phase regime. In addition to the presence of the expected phases, the laser-processed microstructure was surprisingly consistent with that produced by casting. The 2-3 orders of magnitudes faster cooling rates inherent to laser processing resulted in feature sizes 2-3 times smaller than cast materials, however the morphology of the phases was similar. At low-to-intermediate Al contents, the two-phase alloy exhibited a cellular structure, while at higher Al content, the FCC structure was isolated and confined to the BCC/B2 grain boundaries. The BCC/B2 morphology was also similar to that observed in cast materials. Ongoing work continues to investigate the sensitivity of the microstructure to the laser processing conditions, and will be discussed. This study suggests that the high-throughput laser processing method is an ideal method for rapidly and efficiently evaluating multiprincipal element alloys.

2:30 PM BREAK

SESSION PM04.13: Novel Synthesis and Mechanical Properties
Session Chair: Alfred Ludwig
Wednesday Afternoon, November 28, 2018
Hynes, Level 1, Room 105

3:30 PM PM04.13.01
Solid State Manufacture of High Entropy Alloys via the Metalysis Process Ian Mellor, Lyndsey Benson, Mike Ellis and Nader Khan; Metalysis Ltd, Rotherham, United Kingdom.

Historically Metalysis have produced tantalum, titanium and titanium alloy powders for high performance applications using their solid state electrochemical process. The route for alloy production involves initial preparation of a mixed metal oxide feedstock, followed by electro-deoxidation, to generate an intimately mixed alloy on a microscopic scale. This low energy intensive and environmentally friendly technology, has been used to demonstrate a number of High Entropy Alloys (HEA's), with complex compositions and microstructures.

In most conventional cases, the manufacture of HEA's involves high temperature melting, which puts all of the alloying elements into the liquid phase. This can lead to numerous problems and restrict the number of combinations, which can be reliably made. In particularly those where one needs to combine low melting and/or boiling point with refractory elements, and also where there are significant liquid density differences between the constituents causing melt segregation.

The aim is to present the preliminary work carried out by Metalysis, and to show how the solid state process, based on molten salt electrolysis, lends itself to the manufacture of the next generation of HEA's. This study will focus on some examples whose constituent elements have large differences in both their melting points and liquid densities, for example, but not limited to, chromium, niobium, tantalum, titanium and aluminium.

3:45 PM PM04.13.02
Growth and Mechanical Characterisation of Single-Phase Single-Crystalline FCC and BCC High-Entropy Alloys Tim Lienig, Michael Feuerbacher and Carsten Thomas; Forschungszentrum Jülich GmbH, Jülich, Germany.

High-entropy alloys (HEAs) represent a novel class of metallic materials. Composed of at least five elements in equiatomic or near-equiatomic proportion they show crystalline long-range order while maintaining chemical disorder throughout their lattice. The simultaneous presence of topological order and chemical disorder is unique in metals and poses fundamental questions in basic materials science. Various alloy systems have been reported to form HEAs, crystallising in face-centred cubic, body-centred cubic, and hexagonal structure.

In-depth investigation of structure-property relations of HEAs requires high-quality single-phase, preferably single-crystalline samples. Single-crystalline samples allow the determination of intrinsic materials properties without the influence of secondary phases or grain boundaries.

We report on the mechanical characterisation of single-crystalline equiatomic fcc CrMnFeCoNi and our advancements in the production of single-crystalline bcc TiVZrNbHf HEAs. Single-crystals are grown by means of the Bridgman technique from master-alloys synthesised from high-purity elements by arc-melting and in an inductively-coupled levitation crucible. Mechanical characterisation was performed on a modified Zwick Z050 compression deformation rig.

CrMnFeCoNi single-crystals successfully produced by the Bridgman technique have a volume of several cubic centimetres and a maximum diameter of 20 mm, making the high-quality material accessible to most physical-property measurements. X-ray Laue back-scattering images taken across the surface are sharp and mutually consistent. SEM and light microscope images reveal a grain-free microstructure, with EDS measurements confirming the equiatomic composition of the crystal. Macroscopic specimens (2.5x2.5x5 mm^3) prepared from the large single crystals are used to perform mechanical compression testing along different crystallographic directions. By incremental testing, e.g. stress relaxations and strain-rate changes, thermodynamic activation parameters of the plastic deformation mechanism are determined.

A growth route for equiatomic TiVZrNbHf single crystals is currently under development and will be presented additionally. Our previously published results reveal that this material is a homogeneous single-phase HEA with bcc structure that has a significantly lower melting temperature than TiZrNbHfTa bcc HEAs. Therefore single-crystal growth of TiVZrNbHf HEAs can be addressed by means of the Bridgman technique, and we expect to grow crystals of

the same volume as CrMnFeCoNi single-crystals.

4:00 PM PM04.13.03
Microstructure and Phase Transformation in Al-Containing Refractory High Entropy Alloys SangJun Kim, Hyunseok Oh and Eun Soo Park; Seoul National University, Seoul, Korea (the Republic of).

Refractory high entropy alloys with BCC structure composed of group-4 to group-6 refractory elements (Ti, Zr, Hf, V, Nb, Ta, Cr, Mo and W) were reported to exhibit superior mechanical properties at high temperature above 1000 C comparing Ni-based superalloys. Recently, Al-containing refractory high entropy alloys were reported to have unique structure in which disordered BCC phase (A2) are precipitated in ordered BCC matrix (B2). In spite of exceptional high strength at high temperature, however, they showed low ductility due to the ordered matrix and Zr-based precipitates in grain boundaries. Here, we investigated the phase transformation behavior of Al-containing refractory high entropy alloys to control the microstructure for balancing strength at high temperature and ductility at room temperature. Microstructural evolutions of various alloys in (Ti,Zr,Hf)-(Nb,Mo)-Al system during heat treatment were analyzed in terms of phase equilibrium and decomposition of disordered and ordered BCC phase. Through systematic studies of thermal processing condition, refractory high entropy alloy in which ordered B2 phase are precipitated in disordered A2 matrix was developed. This result could provide an effective guideline for tailoring microstructure of Al-containing refractory high entropy alloys, and developing promising HEAs for high temperature structural materials.

4:15 PM PM04.13.04
Two Modes of Screw Dislocation Motion in an Equiatomic Alloy Yuri Osetsky[1], James R. Morris[1, 2] and George M. Pharr[3]; [1]Oak Ridge National Laboratory, Oak Ridge, Tennessee, United States; [2]The University of Tennessee, Knoxville, Knoxville, Tennessee, United States; [3]Texas A&M University, College Station, Texas, United States.

Molecular dynamics simulations show two distinct mechanisms of ½<110>{111} screw dislocation glide in an equiatomic Ni-Fe solid solution face centered cubic crystal structure (fcc). At high stresses (above ~130 MPa), it glides under "typical" friction-controlled conditions. At lower stresses, the dislocation moves in a very rough manner that cannot be described as continuous glide but rather a motion through a set of obstacles. We demonstrate that these obstacles are localized and can produce large pinning, yet the dislocation does not exhibit significant bowing as normally expected for strong, localized pinning. The threshold stress for transition between modes depends on the dislocation segment length and ambient temperature. At 300 K the flow stress saturates at ~130 MPa for length above ~140 $|\boldsymbol{b}|$ ($\boldsymbol{b}$ is the Burgers vector). We demonstrate that the statistical behavior is important, with rare events dominating the behavior. The nature of internal obstacles to dislocation glide is likely due to the low stacking fault energy and composition effects in the core energy: dislocation accommodates its width and shape for its Shockley partials contain more Ni atoms. Energy barriers between minimum energy configurations define the flow stress. The observations are discussed in terms of their potential relevance to the mechanisms of plastic deformation in single-phase high entropy alloys.

This work was supported by the US Department of Energy Office of Science, Basic Energy Sciences, Materials Science and Engineering Division.

4:30 PM PM04.13.05
Effect of Ti and C Additions on Microstructural Refinement and Mechanical Properties of Cast AlCoCrFeNi Compositionally Complex Alloys Alex Asabre[1], Ulrich F. Volkert[1], Oleg Stryzhyboroda[2], Janine Pfetzing-Micklich[1], Ulrike Hecht[2] and Guillaume Laplanche[1]; [1]Ruhr University Bochum, Bochum, Germany; [2]ACCESS e.V., Aachen, Germany.

Hot forming tools need to exhibit good strength, high hardness and wear resistance at high temperatures, combined with an adequate ductility at high and low temperatures. Currently boron doped steels are used for such applications, however there is a growing demand of new materials with improved properties. In the present study, the influence of Ti and C additions on microstructure and mechanical properties of an as-cast multi-phase $Al_{13}Co_{22}Cr_{22}Fe_{22}Ni_{22}$ (composition in at. %) compositionally complex alloys is investigated. The alloys with various additions were arc melted and subsequently drop cast. The as-cast microstructures were characterized using scanning and transmission electron microscopy. Microstructural analyses revealed a Widmanstätten microstructure in all cast alloys consisting of face-centered-cubic (FCC) plates which formed upon cooling in a disordered body-centered-cubic (BCC) matrix containing ordered B2 precipitates. The additions of Ti and C resulted in microstructural refinement with the presence of titanium carbides at grain boundaries and inside the grains of the high temperature BCC matrix. This result in combination with thermodynamic calculations suggest that titanium carbides formed in the melt and acted as nucleation sites for heterogeneous nucleation during solidification. The volume fraction of the BCC phase slightly increases with increasing Ti and C additions while the Cr-, Fe-, Co-, and Ni-concentrations are decreased accordingly and the Al-content remains constant. The alloying of Ti and C to the $Al_{13}Co_{22}Cr_{22}Fe_{22}Ni_{22}$ alloy increases the Vickers's microhardness by about 10 %. The yield stress and tensile strength at room temperature increases from 400 MPa to 920 MPa and from 950 MPa to 1360 MPa, respectively, with Ti and C additions while the ductility is found to decrease from 21 % to 4 %. These results can be attributed to the slight increase in BCC volume fraction and the microstructural refinement with Ti and C additions.

4:45 PM PM04.13.06
Precipitation Hardenable High Entropy Alloy for Tooling Applications Oleg Stryzhyboroda[1], Ulrike Hecht[1], V. Vitusevych[1], Alex Asabre[2], Guillaume Laplanche[2], Markus Wilms[3], Andreas Weisheit[3], Lorenz Gerke[4], Markus Löcker[5], Christian Mutke[6] and Christoph Escher[6]; [1]ACCESS e.V., Aachen, Germany; [2]Ruhr-Universität Bochum, Bochum, Germany; [3]Fraunhofer Institute for Laser Technology ILT, Aachen, Germany; [4]W.S. Werkstoff Service GmbH, Essen, Germany; [5]Kirchhoff Automotive GmbH, Iserlohn, Germany; [6]Dörrenberg Edelstahl GmbH, Engelskirchen, Germany.

We present a high entropy alloy (HEA) from the system Al-Co-Cr-Fe-Ni-W-Mo-Si-C which was designed to allow for precipitation hardening by annealing in the temperature range from 600 to 900ºC. The alloy development was performed using centrifugally casted specimens and supported by thermodynamic computations using ThermoCalc software and the TCFE9 database. The microstructure of two selected samples in as-cast and annealed conditions was analysed using XRD, SEM, EBSD, EDX and TEM measurements. The as-cast microstructure consists of spinodally decomposed BCC dendrites enveloped by FCC/$M_{23}C_6$ eutectic. Upon annealing at 700ºC for 24h nanoscale intermetalic phase precipitates form within the spinodal BCC as well as from FCC. Furthermore, the $L1_2$ phase precipitates within the FCC phase below 600ºC. Precipitation is exquisitely uniform leading to an increase in microhardness from 415 HV0.5 in the as-cast state to 560 HV0.5 after annealing, making the material suitable for tooling applications. We investigated the stability and coarsening of this microstructure using (i) varying annealing temperatures and (ii) varying time for a constant temperature of 700ºC. We will present the microstructure evolution during coarsening and the corresponding mechanical properties obtained from instrumented indentation experiments.