

[Back to all Symposium Sessions »](#)

Symposium SF09—High Entropy Materials II—From Fundamentals to Potential Applications

2022-05-09

2022-05-10

2022-05-11

2022-05-24

2022-05-25

2022-05-10 Hide All Abstracts

Times shown in HST (GMT-10:00)

Symposium Organizers

Symposium Support

Bronze

Army Research Office

SF09.02 Refractory High Entropy Alloy

Session Chairs

Daniel Gianola
Matthew Kramer

Tuesday AM, May 10, 2022
Hawai'i Convention Center, Level 3, 325B

9:00 AM - *SF09.02.02

Pathways for Plastic Deformation in Refractory Multi-Principal Element Alloys

[Daniel Gianola](#)¹

University of California, Santa Barbara¹

Hide Abstract

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

9:30 AM - SF09.02.03

Superior High-Temperature Strength in a Supersaturated Refractory High-Entropy Alloy

Rui Feng¹, Bojun Feng², Michael Gao³, Chuan Zhang⁴, Joerg Neumeier¹, Jonathan Poplawsky¹, Yang Ren⁵, Ke An¹, Michael Widom², Peter Liaw⁶

Oak Ridge National Laboratory¹, Carnegie Mellon University², National Energy Technology Laboratory³, Computherm, LLC⁴, Argonne National Laboratory⁵, The University of Tennessee, Knoxville⁶

Hide Abstract

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

9:45 AM - SF09.02.04

Investigation of Microstructure and Mechanical Properties of Selected Phase by Nature on Multi-Component Refractory High Entropy Alloys

Jaekwon Kim¹, Sang Jun Kim¹, Il Hwan Kim¹, Taeyeop Kim², Dongwoo Lee², Eun Soo Park¹

Seoul National University¹, Sungkyunkwan University²

 Hide Abstract

High-entropy alloys composed of a large number of major elements in a similar fraction that cannot select a specific major element does forms BCC or FCC single solid solution phases without intermetallic compounds due to the effect of high configuration entropy. In particular, it is reported that BCC refractory high entropy alloys made of Group 4-6 refractory transition metals have superior high-temperature strength and structural stability than commercial superalloys such as Inconel. However, the number of reported single-phase BCC refractory high entropy is very limited, and it is very difficult to predict an alloy system with a large solid solution region experimentally. Moreover, even a successfully designed single-phase BCC refractory high entropy alloy has limitations in the development of the alloy due to the trade-off relationship between room temperature ductility and high-temperature strength. In this present study, we try to solve the above two significant limitations via a unique alloy design that BCC single-phase selected by nature during solidification of multi-component refractory high entropy alloys. A multi-component refractory high entropy alloy system was selected by Machine Learning predicted model and experimental data. In the case of an alloy selected by nature, it is composed of dilute fractions of minor elements as well as major elements in different fractions. The developed alloy in the study has superior high-temperature phase stability and mechanical properties compared to conventional equiatomic composition refractory high entropy alloys. To understand the intrinsic correlation between alloy constituent elements, micro (Real-time deformation behavior analysis, etc) ~ nanoscale (Lattice distortion analysis, etc) analysis techniques were performed. Based on this, we would like to present a new paradigm of refractory high entropy alloys design.

10:00 AM - SF09.02

BREAK

10:30 AM - *SF09.02.05

Theory-Guided Combinatorial Synthesis and Characterization of Refractory Multi-Principal Element Alloys

Matthew Kramer^{1,2}, Gaoyuan Ouyang¹, Prashant Singh¹, Duane Johnson^{1,2}, Jun Cui^{2,1}

Ames Laboratory¹, Iowa State University²

 Hide Abstract

Refractory Multi-Principal Element Alloys (RMPEA) exhibit a higher specific strength at elevated temperatures and double the melting point compared to conventional nickel-based superalloys, offering great promise for the next-generation superalloys. Unlocking the potential of the high-entropy concept beyond equiatomic compositions, requires a rapid-screening methodology that incorporates an efficient, yet accurate density functional theory (DFT) for estimating phase stability, elastic modulus, and ductility. Coupling theory-guided design to a reliable but straightforward experimental exploration methodology facilitated unlocking the vast potential of RMPEA's by incorporating theory-guided down-selection of systems worth full-scale testing. Recent work [npj comput. mat. 4(1) (2018) 1-8] predicted superior RMPEAs properties in a Mo-rich region of the quinary Mo-W-Ta-Ti-Zr with improved stability and enhanced moduli over near-equiatomic alloys. These promising compositions were synthesized using high-throughput methods specifically developed for this study. Petite bulk samples (1.5g each) were prepared using a combinatorial arc melting system capable of making 32 samples per batch. These samples were rapidly scanned with a handheld XRF for compositions and an ultrasound probe for elastic modulus. Samples with promising moduli underwent room-temperature compression testing. Samples with compressive strengths in excess of 700 MPa and ductility greater than 8% strain were further investigated. To speed up high-temperature property assessment, we developed four small punch-test rigs capable of 800 MPa loading at 1350°C. Exploiting these, unique RMPEAs were discovered and experimentally validated with promising combinations of room-temperature ductility (up to 10% compression strain), high-temperature tensile yield-strength (up to 240 MPa at 1300°C), and excellent creep resistant up to 1300°C ($8.3 \times 10^{-9} \text{ s}^{-1}$ at 100MPa). DFT-estimated elastic parameters as a function of temperature compared well that measured. In less than one-year of effort, we found a composition capable of a tensile yield strength of 250MPa at 1300°C, 9% elongation at room temperature, and a robust high-temperature creep resistance at 1300°C, showing a 16X lower minimum creep rate than typical nickel-based superalloys at 1000°C. Our results demonstrated the effectiveness of theory-guided, high-throughput synthesis and characterization in developing RMPEAs for ultrahigh-temperature structural applications.

11:00 AM - SF09.02.06

Exploring Strength-Ductility Synergy for bcc Refractory HEAs Through Integration of First-Principles Calculations, Statistical Learning and CALPHAD

Yong-Jie Hu¹, Chris Tandoc¹, Liang Qi², Peter Liaw³

Drexel University¹, University of Michigan², The University of Tennessee, Knoxville³

Hide Abstract

Optimizing chemistries of bcc refractory multicomponent alloys to achieve a synergy of high strength and low-temperature ductility requires reliable predictions of the correlated alloy properties across a vast compositional space. In this work, first-principles calculations were performed for ~200 individual bcc refractory alloys to predict several strength/ductility-related fundamental alloy properties, including lattice parameter, lattice distortions, unstable stacking fault energies, and surface energies. With the descriptors based on electronic structures of interatomic bonding, surrogate models were developed using statistical learning algorithms to efficiently and accurately predict these defect energies and magnitudes of lattice distortions according to alloying compositions. A combination of the surrogate models and CALPHAD-based phase stability prediction

further enabled systematic search of potential alloy candidates that are stable as single solution phase, intrinsically ductile, and with high yield strengths across high-order multicomponent systems.

11:15 AM - SF09.02.07

A Fast and Robust Method for Predicting the Phase Stability of Refractory Complex Concentrated Alloys Using Pairwise Mixing Enthalpy

Rohan Mishra¹, Zhaohan Zhang¹, Mu Li¹, John Cavin¹, Katharine Flores¹

Washington University in St. Louis¹

Hide Abstract

The ability to predict the composition- and temperature-dependent stability of refractory complex concentrated alloys (RCCAs) is vital to the design and discovery of high-temperature structural alloys. Here, we present a model based on first-principles calculations to predict the thermodynamic stability of multicomponent solid solutions in a high-throughput manner and apply it to screen over 20,000 compositions. We develop a database that contains pairwise mixing enthalpy of 17 refractory metals using density-functional-theory (DFT)-based total energy calculations. To these, we fit thermodynamic solution models that can accurately capture the mixing enthalpy of multicomponent BCC solid solutions. By comparing their energy with DFT-calculated intermetallic enthalpies obtained from the Materials Project database and using convex hull analyses, we identify the ground state phase for any multi-component alloy composition as a function of temperature. The predicted phase diagrams for NbTiZr-V- (Mo, Ta, Cr) systems agree well with prior experimental observations. We apply our model to predict the phase evolution in NbVZr-Ti_x ($0 < x < 1$), which are confirmed using laser-based alloy library deposition. With this method, we provide a fast and accurate way to estimate the microstructure of new RCCAs system and expedite experimental discovery. This method can also be adapted for multi-cation high entropy compounds.

11:30 AM - SF09.02.08

ULtrahigh TEmperture Refractory Alloys (ULTERA) Database

Adam Krajewski¹, Shuang Lin¹, Marcia Ahn¹, Hui Sun¹, Arindam Debnath¹, Allison Beese¹, Wesley Reinhart¹, Zi-Kui Liu¹

The Pennsylvania State University¹

Hide Abstract

ULTERA database, developed under the ARPA-E's ULTIMATE program, is aimed at collecting literature data on high entropy alloys (HEAs) to facilitate rapid discovery of new ones using forward and inverse design, with the primary focus on creep

behavior, yield stress, ductility, and hardness.

As of January 2022, ULTERA contains over 5,900 property-datapoints, corresponding to 1,900 unique HEAs, collected from 442 source DOIs. All data is available through a high-performance API, following FAIR principles, while statistics on it can be found at our phaseslab.com/ultera web page.

The database architecture is designed to automatically integrate starting literature data in real-time with methods such as experiments, generative modeling, predictive modeling, and validations.

11:45 AM - SF09.02.09

Hydrogen Accommodation in the TiZrNbHfTa High Entropy Alloy.

Christopher Moore^{1,2,3}, Jack Wilson^{1,4}, Michael Rushton¹, William Lee^{1,5,3}, Jack Astbury³, Simon Middleburgh^{1,6}

Bangor University¹, Royal Society of Chemistry², Tokamak Energy³, National Nuclear Laboratory⁴, Royal Academy of Engineering⁵, Institute of Materials, Minerals and Mining⁶

Hide Abstract

The body-centred cubic high entropy alloy (HEA) TiZrNbHfTa has been of particular interest as a hydrogen storage medium as it offers a maximum storage capacity that could feasibly replace compounds that contain rare earth elements. We report that the TiZrNbHfTa structure and its hydrides (TiZrNbHfTa)H_{0.4-2.0}, as well as the BCC to BCT to FCC phase transformation that results from increased hydrogen concentration, have successfully been modelled as special quasi-random structures (SQS) with density functional theory calculations employed to analyse key thermodynamic processes such as vacancy formation and hydrogen solution energies. Local environments, the nearest neighbour lattice atoms surrounding an interstitial, were observed to effect the hydrogen solution energy of a given site and resulted in a wide distribution of energies throughout the structures. By considering the diverse hydrogen solution energies for the various environments in the HEA and the temperature dependence of configurational and vibrational entropy terms, a model predicting the decomposition of the hydrides has been produced. Accounting for interstitials bound to vacancies in the structure, the formation of which were found to be promoted by the presence of hydrogen interstitials – which lowered the energy barrier of vacancy formation by 0.16 eV, identified a second major decomposition peak at an elevated temperature, in agreement with recent findings. The introduction of vacancies in the local environment was found to result in interstitials adopting octahedral positions upon relaxation, in contrast to systems where vacancies were not present and tetrahedral sites were favourably occupied. This observation, and the hydride decomposition model, provides a mechanistic basis for experimentally observed behaviour and provides a comprehensive understanding of hydrogen absorption and desorption in the TiZrNbHfTa HEA.

Session Chairs

Hyejung Chang
Eun Soo Park

Tuesday PM, May 10, 2022
Hawai'i Convention Center, Level 1, Kamehameha Exhibit Hall 2 & 3

5:00 PM - SF09.04.01

Asymmetry of Element-Specific Lattice Distortion in 3D Transition Metal-Based Complex Concentrated Alloys

Hyunseok Oh^{1,2}, Khorgolkhuu Odbadrakh^{3,4}, Yuji Ikeda^{5,6}, Sai Mu⁴, Fritz Koermann^{5,7}, Chengjun Sun⁸, Hye Sang Ahn¹, Kooknoh Yoon¹, Duancheng Ma⁹, Cem Tasan², Takeshi Egami^{4,3}, Eun Soo Park¹

Seoul National University¹, Massachusetts Institute of Technology², The University of Tennessee, Knoxville³, Oak Ridge National Laboratory⁴, Max-Planck-Institut für Eisenforschung⁵, University of Stuttgart⁶, Delft University of Technology⁷, Argonne National Laboratory⁸, Friedrich-Alexander-Universität Erlangen-Nürnberg⁹

Hide Abstract

Lattice distortion has been regarded as one of the four core effects of complex concentrated and high entropy alloys. Recently, it was shown that atomic-level pressure (or the misfit volume) in 3d transition metal element (V, Cr, Mn, Fe, Co, Ni)-based complex concentrated alloys (3d CCAs) with face-centered cubic structure originates from charge transfer between neighboring atoms, which suggests the electronic origin of lattice distortion, rather than a classical mechanical view mainly based on atomic size arguments. Here we show that the magnitude of the local lattice distortion of a specific element is strongly affected by its electronegativity. The trend is only a little affected in the presence of short-range order. This study provides an important link between atomistic properties (electronegativity) and physical properties in 3d CCA and rationalizes the proposed relation between lattice distortion and complexity-induced properties in 3d CCAs.

5:00 PM - SF09.04.02

Atomic-Scale Measurement of Chemical Short-Range Order (C-SRO) in CrMnFeCoNi High Entropy Alloys and Its Effect on the Deformation Behaviors

Kooknoh Yoon¹, Hyunseok Oh², Baptiste Gault^{3,4}, Dierk Raabe³, Eun Soo Park¹

Seoul National University¹, Massachusetts Institute of Technology², Max-Planck-Institut für Eisenforschung³, Imperial College London⁴

[-] Hide Abstract

Since high entropy alloy (HEA) is constituted with multi-principal elements, it can be understood in a very severe condition of solid solution strengthening (SSS). In particular, the short-range order (SRO), sub-nano scale atomic structure, can be easily formed in HEAs. Understandably, the SRO can drive HEAs to extreme conditions of SSS.

The SRO can be classified into two different ones: topological (T) and chemical (C) SRO. Since the T-SRO has a different crystallographic property with the matrix, it can be easily measured. However, it is far more difficult to measure the C-SRO, because it is the only cluster of a few atoms having preferential bonding among specific elements with thermodynamic stability. In the present study, we systematically evaluate the influence of C-SRO formation on the degree of SSS in various CrMnFeCoNi HEAs. The SRO formation was carefully controlled by solidification history intensive structural analysis, including APT, EXAFS, and so on. Finally, this work will establish a tuning recipe for SSS in HEAs, which uses the sub-nano scale structural information.

5:00 PM - SF09.04.03

Short Range Order Correlated with Hardening and Softening Behavior of High Entropy Brasses and Bronzes

Anna Soper¹, Jonas Kaufman², Aurora Pribram-Jones³, Lori Bassman¹, Kevin Laws⁴

Harvey Mudd College¹, University of California, Santa Barbara², University of California, Merced³, University of New South Wales⁴

[-] Hide Abstract

High entropy brasses and bronzes are emerging as one of the first commercially viable high entropy alloy families with wide applications in plumbing fixtures, household appliances, industrial tooling, and military munitions. While significant work has been done in the experimental development and characterization of these alloys, there is a gap in corresponding computational work, which holds promise to provide insights into the internal energetics and chemical ordering that impact material properties. Short range order a property that, while difficult to probe experimentally, is accessible through computation. Recently, anomalous, composition dependent softening was demonstrated experimentally in several ternary constituents of the Cu-Zn-Mn-Ni-Al system. This computational study correlates short range order with the experimentally observed composition dependent softening. Ternary cluster expansions paired with Monte Carlo simulations are used to extract Warren-Cowley short range order parameters at the annealing temperature. Strong correlations are observed between clustering in these constituent ternaries and composition dependent softening. This work has the potential to provide valuable insight into the chemical ordering that can inform future alloy design.

5:00 PM - SF09.04.04

Multiscale Microstructural Modeling and Simulation of Deformation in AlCoCrCuFeNi High Entropy Alloys via X-Ray Computed Tomography and Homogenization Analysis

Ryo Inoue¹, Kai Kiyomiya¹, Yutato Arai¹

Tokyo University of Science¹

 Hide Abstract

The improvement in heat resistance of alloys reaches the limit. This means that there is a limit to the method of developing conventional alloys by adding small amounts of additive element to large amounts of main element. The concept of high entropy alloy (hereafter denoted as HEA) emerged at the beginning of this century as multi component alloys in which the main elements cannot be specified.

In the present study, Al_xCoCrCuFeNi (x = 0.3, 1.0, 3.0) HEA with different atomic ratios were prepared by arc melting furnace. As-melted samples were machined and their tensile mechanical properties were evaluated. Their microstructures were also characterized, by SEM, TEM, EDS, XRD, and EBSD. Furthermore, microstructural features in three dimensions were also examined by X-ray computed tomography (CT).

The specimen with x=0.3 shows ductile tensile mechanical behavior. This is because it is composed of solid solution with FCC structures and Cu-rich phase. As the increase of Al content, crystal structure changes from FCC to BCC structures. Simultaneously, formation of intermetallic compounds is also confirmed. As a result, the samples tend to fail with brittle fashion at low stress levels. Mechanical properties of as-melted samples have significant scattering because of its heterogeneous microstructures due to the difference of cooling rate during melting.

In this study, 3D microstructures were modeled using binarized tomographic images of each sample. Deformation of the samples is simulated using reconstructed models and finite element method (FEM). The results of simulation using image-based model reflecting actual microstructures is in good agreement with experimental results.

5:00 PM - SF09.04.09

A Study of Ideal Glass State via High Entropy Metallic Glasses

Ji Young Kim¹, Geun Hee Yoo¹, Jung Soo Lee², Jinyeon Kim¹, Hyejung Chang³, Jinwoo Hwang⁴, Eun Soo Park¹

Seoul National University¹, Ulsan National Institute of Science and Technology², Korea Institute of Science and Technology³, The Ohio State University⁴

 Hide Abstract

In the field of metallic glasses, ideal glass state has attracted special attention because it is expected to have the characteristic of high mechanical strength based on its unique atomic structure. The unique structure is characterized by high diversity in local structure, which means that it is not dominated by particular motifs. Even though it is suggested that mixing a large number of elements with different atomic sizes is a way to design ideal glass, there is a lack of research on analyzing the ideal glass experimentally. In this study, we designed high entropy metallic glasses (HE-MGs) with 10 different elements to make the atomic structure close to ideal glass state. Using this HE-MGs, we studied the various characteristics of ideal glasses. The results

contributed us to enhance the insight of ideal glass state in terms of structural characteristics, mechanical property, and abnormal crystallization behavior based on the experimental evidence.

5:00 PM - SF09.04.10

Nanotribology of High Entropy Alloy Thin Films

Gokay Adabasi¹, Koichi Tanaka², Aditya Deshpande², Suneel Kodambaka², Mehmet Baykara¹

University of California, Merced¹, University of California, Los Angeles²

Hide Abstract

High entropy alloys (HEAs), consisting of five or more principal elements in similar equimolar ratios, are gaining rapid attention from the scientific community thanks to their intriguing combination of attractive mechanical properties with high thermal and chemical stability. In thin-film form, HEAs exhibit potential for use as wear-resistant coatings that could endure harsh environmental conditions. Motivated in this fashion, we explore the fundamental tribological properties of HEA thin films ((VNbTaMoW)₂) on the nanoscale by way of atomic force microscopy experiments. In particular, we are able to observe connections between local film morphology and frictional behavior, opening the door to detailed studies of structure-property relationships in the nanotribology of HEA thin films.

5:00 PM - SF09.04.11

Exploring M₃O₄ Spinel High-Entropy Oxide Nanoparticles for Emissions Catalysis

Sreya Paladugu¹, Katharin Page¹

University of Tennessee, Knoxville¹

Hide Abstract

The complete catalytic oxidation of carbon monoxide (CO) and methane (CH₄) has been a long-standing challenge in the field of heterogeneous catalysis. Noble metal nanoparticles (Au, Pt) dispersed on transition metal oxide supports are predominantly used as active catalysts for CO oxidation. While these noble metals display high catalytic performance towards CO oxidation, they are expensive, scarcely found in nature and have a propensity to sinter into larger particles at high temperatures, resulting in loss of surface area and reduction in catalytic activity. These challenges motivate us to design a scalable, low-cost, earth-abundant, sinter-resistant catalyst that can maintain higher surface area and facilitate long-term catalytic operation.

High-entropy oxides (HEOs) are a class of multi-component oxides comprised of five or more cations in an equal or near-equal

atomic ratio on specific crystallographic sub-lattices. In recent years, significant research efforts have been devoted to investigating HEOs for catalytic applications, as the complex systems offer new and exquisitely tunable opportunities to combine desired material properties. In this work, we have successfully synthesized a series of mesoporous M_3O_4 (M=transition metal) spinel HEOs, using an eco-friendly soft-templating approach. The low temperature soft templating synthesis route allows us to incorporate transition metal cations into phase pure entropy stabilized nanostructures with high surface area to volume ratios. By tailoring the composition of the metal cations, we can tune the redox properties of the materials and optimize catalytic activity, selectivity, and resistance to poisoning. We employ neutron scattering, x-ray scattering, electron microscopy and catalytic property measurement techniques to correlate chemical and structural order/disorder with the resulting catalytic performance. Overall, the fundamental structure-property insights gained from this study will lead to a better understanding of how HEO nanostructured catalysts may enable superior low-temperature methane and CO oxidation and outstanding resistance to thermal degradation.

5:00 PM - SF09.04.12

Sol-gel Synthesis of Ceria-Zirconia-Based High-Entropy Oxides as High-Promotion Catalysts for the Synthesis of 1,2-Diketones from Aldehyde

Igor Djerdj¹, Dalibor Tatar¹, Jelena Kojcinovic¹, Aleksandar Miletic², Gabor Varga³

Department of Chemistry, Josip Juraj Strossmayer University of Osijek¹, University of Novi Sad², University of Szeged³

 Hide Abstract

Four ceria–zirconia-based high-entropy catalysts were successfully synthesized. The applied synthetic route, the modified sol-gel citrate route, resulted in phase-pure compounds with a cubic structure, with lattice parameters that differ from pure CeO_2 . This is related to the lattice expansion/contraction due to the incorporation of five cations into a single-cation lattice. The investigation of the physicochemical properties of the newly developed and synthesized catalysts shows that the crystallite size, lattice parameters, surface areas, and pore volumes are similar, while the Lewis acidity differs significantly.

The pinacol-type oxidative coupling reaction of the aldehydes was presented, using HEOs as the actual catalysts, which demonstrated the catalytic abilities and chemoselectivity of the catalysts. The reaction conditions were optimized followed by a comparative study of the HEOs under the same conditions. Upon using high-entropy oxides as the catalysts, the desired diketone product was produced with almost the same selectivity, unlike the activity, which followed the trend of increasing acidity. The remarkable activity of the HEOs was proven in comparison with the pure building block oxides and their physically mixed composites, especially in the case of the $Ce_{0.2}Zr_{0.2}La_{0.2}Pr_{0.2}Y_{0.2}O_2$ (CZLPY) compound. CZLPY oxide proved to be a versatile, reusable, and heterogeneous catalyst, taking into account the results of the recycling and hot filtration test, as well as the scope.

5:00 PM - SF09.04.13

Synthesis of Nanoporous Structure by Selective Phase Dissolution of AlCoCrFeNi High Entropy Alloy and Its Electrochemical Properties as Supercapacitor Electrode

Kim Chamil¹, Kong Kyeong Ho¹, Jae Ik Hyun¹, Kim Yong Joo¹, Kim Won Tae², Do Hyang Kim¹

yonsei university¹, Cheongju University²

Hide Abstract

Fabrication of nanoporous metal core/oxide shell structure using equiatomic AlCoCrFeNi high entropy alloy (HEA) and its electrochemical property as supercapacitor electrode have been investigated in the present study. As-cast AlCoCrFeNi HEA consists of interconnected Al-Ni rich and Cr-Fe rich phases by spinodal phase separation. Nanoporous structure can be obtained by selectively dissolving the Al-Ni rich phase and retaining the remaining Cr-Fe rich phase by passivation in sulfuric acid solution at 313 K. In particular, the scale of nanoporous structure in the present study is predictable since it only depends on the scale of original spinodal-decomposed microstructure in as-cast state. When used as a binder free electrode for supercapacitor, Cr-Fe rich nanoporous structure exhibits high volumetric capacitance of 700 F cm^{-3} and excellent cycling stability of over 3000 cycle. As the microstructural scale in as-cast state becomes finer, the nanoporous structure exhibits better capacitance properties. The present result shows that Cr-Fe rich nanoporous metal core/oxide shell has a good potential for application as supercapacitor electrode.

5:00 PM - SF09.04.14

First Principles Study of Phase Stability, Mechanical Properties, Martensitic Transformation and Phonon Dispersion of $\text{Ni}_{44}\text{Ti}_{35}\text{Zr}_{15}\text{Co}_6$ Alloy System

Tapasendra Adhikary¹

Indian Institute of Technology Kharagpur¹

Hide Abstract

In the present work we explain the effect of Zr and Co addition on the lattice parameters, phase stability, martensitic transformation temperature and electronic properties of binary NiTi alloys has been investigated with first principle density functional theory calculations. The supercell approach in VASP was used to substitute Ti with Zr, Ni with Co on the NiTi structure to evaluate their structural and electronic property for actuators and higher temperature applications. The DFT results suggest that the decrease of formation energy is caused by a stabilization of the monoclinic B19' phase compared to B2 phase. The transformation temperature increased with the addition of Zr and Co. There is evidence of change in density of states (DOS) during the Ti-3d and Zr-3d orbitals as predicted by the geometric nonlinear theory of martensite. The calculated electron-density show the presence of covalent bonding in all the compounds. The calculation of phonon dispersion by direct method, of the cubic austenite and martensitic monoclinic phases of NiTi intermetallic compound have been calculated.

Surface properties are essential to materials research

Discover them using state-of-the-art instrumentation from the world's leading supplier



PHYSICAL ELECTRONICS
A DIVISION OF ULVAC-PHI

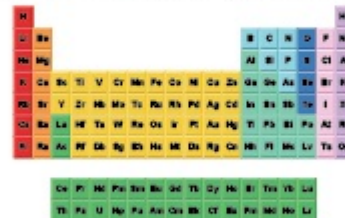
[Learn More →](#)

Stay Connected.

Manage your contact preferences.



 **AMERICAN ELEMENTS**
THE ADVANCED MATERIALS MANUFACTURER®



Now Invent.™

www.americanelements.com

