LATEST INFORMATION

International Meeting
- High-Entropy and Compositionally Complex Alloys (MRS 2020 Fall Meeting), November 29 - December 4, 2020, Boston, MA, USA. [https://www.mrs.org/meetings-events/field-meetings-exhibits/2020-mrs-fall-meeting]
- THERMEC2021, May 9 - 14, 2021, Vienna, Austria. [https://www.tugraz.at/events/thermec-2020/home]
- The 8th International Conference on Solid → Solid Phase Transformations in Inorganic Materials (PTM2021), June 28 - July 2, 2021, Xi’an, China. [https://www.medmeeting.org/7691/en]

Domestic Meeting
- 2020 Startup Meeting of All Research Groups, May 26, 2020, Kyoto, Japan. [Canceled due to Coronavirus (Covid-19)] [https://highentropy.mtl.kyoto-u.ac.jp/members]
- The Japan Institute of Metal (JIM) Symposium "Materials Science of High-Entropy Alloys", September 16-18, 2020, Toyama, Japan. [https://jim.or.jp/MEETINGS/me_index.html]

PRESS

3. Hidemi Kato and Takeshi Wada, June 2019, JSPM Award for Innovatory Institute of Metals.
5. Hiroshi Ohtani, December 2019, Best Paper Award, Japan Copper and Brass Association.
10. Hiroshi Ohtani, December 2019, Best Paper Award, Japan Copper and Brass Association.
14. Hiroshi Ohtani, December 2019, Best Paper Award, Japan Copper and Brass Association.
Shape memory alloys have attractive attention not only for basic research but also for practical applications due to their unique functional properties such as shape memory effect and superelasticity. Such unique properties originate from the crystallographically reversible martensitic transformation between the parent phase and the martensite phase. In recent years, there have been significant efforts to develop high temperature shape memory alloys. However, their actual use in an application has not been realized due to several problems; one of the critical issues is the degradation of shape memory properties with increasing the working temperature range due to the plastic deformation. The aim of this research is to elucidate the phase stability and martensitic transformation behavior of multi-principal element alloys, designed based on the concept of HEA, which have the X Y type B2 structure composed of group 4 elements in X site and groups 10 and 11 elements in Y site. The effects of alloying elements on crystal structure, transformation temperature and shape memory properties are investigated to explore possibilities of designing and developing novel high temperature shape memory alloys.

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The high-entropy alloys (HEAs) are promising materials for the high strength. In usual alloys, the host-guest concept helps the development of the materials. However, since the HEA contains many kinds of element in the same ratio, usual host-guest concept cannot be applied. Recently, it is suggested theoretically that some specific elements have large atomic displacement and their displacements have relation with the strength of the HEAs. In order to clarify the element’s character and the local structure in HEAs experimentally, we observe the EXAFS (Extended x-ray absorption fine structure). The example of the EXAFS is shown in the figure. By performing the Fourier transformation of the EXAFS function, we obtain the two-body correlation function with the atoms absorbing the x-ray. By comparing the EXAFS function in each element, we will reveal the character of the element (for example, disorder and atomic displacement), and the origin of the strength in the HEAs.

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The temperature dependences of monocristalline elastic constants of CrMnFeCoNi high entropy alloy with the face-centered cubic (fcc) structure have been experimentally determined using resonance ultrasound spectroscopy from liquid helium temperature to 1173 K. A monocristal of the alloy was grown successfully in an alumina crucible using a modified Bridgeman method at the growth rate of 80 mm/h. Figure 1 shows the temperature dependence of the elastic stiffness constants and fitted curves using the Varshni equation. The value of C11 is smaller than that of C44 below 500 K; this leads negative Cauchy pressures. The negative Cauchy pressure implies us the alloy has low ductility at low temperatures. Since the prediction does not agree with the experimental results, the temperature dependence of ductility of this alloy cannot be discussed by the Cauchy pressure. In order to represent the monocristalline elastic constants, a relatively strong directional interatomic bonding has to be introduced.

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Solid-solution alloys are favorable to tune their properties because the constituent elements of a solution are randomly and homogeneously distributed. However, the majority of the bulk alloys are phase-separated under ambient conditions, where the constituent elements are immiscible with each other. To overcome the challenge of the bulk-phase metallurgical aspects, we have focused on the nano-size effect. Metal nanoparticles (NPs) are known to show different chemical and physical properties from bulk metals because of their high surface-to-volume ratios and the quantum size effect. We have succeed ed in synthesising many types of novel solid-solution alloy NPs and high-entropy alloy NPs consisting of immiscible constituents. In addition to the configurational entropy, it is expected that surface and vibrational entropies would have more impact on the thermodynamics of metal NPs rather than bulk metals due to the nanosized effect. The purpose of this group is to synthesize new high-entropy alloy NPs and to investigate their properties including the difference in the high entropy effect in NPs and bulk metals.

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The single-phase FCC type high entropy alloys: FeCrNiMnxCo (x: 0.7–1.3), were prepared and the Kr+ ion irradiation was performed to the alloys in order to understand the effect of Mn content on the change in microstructure and mechanical property under irradiation. There was no difference of grain size and dislocation density between as-irradiated FeCrNiMnxCo alloys, and the yield strength and the elongation seemed to be independent with Mn contents. Microstructural analysis on Kr+ ion irradiated HEAs revealed that three types of irradiation-induced secondary defects such as SFT, faulted loop (Frank Loop) and unfaulfted loop (perfect loop) were formed. Formation of SFTs and Frank loops in FCC is strongly affected by the stacking fault energy (SFE) as shown in Figure 1. The size and the number density of irradiation-induced dislocation loops (Frank loops) was decreased and increased with increasing Mn contents, respectively, meaning that Mn could have a positive effect on the change in the stacking fault energy of the HEAs.
Laves phase related BCC solid solution alloys for hydrogen storage have been developed in 1990's by the author. The concept of development of these alloys was to explore at the middle of phase diagrams not at the corners nor edges. This is exactly the same to the concept of high-entropy alloy development. We extend our concept for four, five and six element alloy systems, now. One of the roadblocks for further development of hydrogen storage materials is the limitation of "van’t Hoff equation": \( \ln(P) = \Delta S/RT - \Delta H/R \). \( \Delta S \) of formation of solid-state hydrate from alloy is almost zero, which means the term of \( \Delta S/RT \) is independent to chemical species. If you would use high entropy alloy for hydrate formation, much larger \( |\Delta S| \) is expected. It increases freedom of material design. Another expectation for high entropy alloy for hydrogen storage is increase of hydrogen capability and corrosion resistance of stainless steels, possibly by Cr enrichment at the surface [2]. UFG formation may even decrease the critical potential. Whether it is attributed to an intrinsic nature of HEAs or chemical inhomogeneity due to inappropriate processing is not clear yet. It has been reported by numerous researcher that grain refinement to ultrafine grain (UFG) size or nanostructure enhance passivating capability and corrosion resistance of stainless steels. However, its quantitative microstructure-property relationship has yet to be elucidated, which is due to the fact that methodologies of structural characterizations are not well developed for HEAs. The aim of this study is to address this issue by developing a data-driven approach to structural modeling followed by ab initio thermodynamics assessment for computational thermodynamics simulations: (i) a clustering technique is developed to identify a phase and its components from the X-ray diffraction patterns, (ii) according to the information, all the possible structures are automatically generated as inputs for the next step, and (iii) high-throughput first-principles electronic and phonon simulations based on all the inputs are performed on our high-performance computing facilities to obtain thermodynamic parameters for Calphad simulations. Our approach is expected to shed light on the better understanding of structure-property relationship in HEAs.

The introduction of high-entropy oxides (HEOs), i.e. compounds containing oxygen and five or more cations in their crystal structure, has led to interesting functionalities in recent years in a recent study [3]. The first high-entropy photocatalyst with a full electronic configuration is synthesized by high-pressure torsion process followed by high-temperature oxidation. The synthesized oxide with an overall composition of TiHfZrNbTaO\(_3\) contains 60 mol% of monoclinic phase and 40 mol% of orthorhombic phase. This two-phase oxide with an orange color shows an appreciable light absorbance in the visible-light region (corresponding to simple oxide) with a bandgap of 2.9 eV and conductivity of 10 \( \mu \)S cm\(^{-1}\) with conductions bands for water splitting. The material successfully produces hydrogen by photocatalytic water splitting, suggesting the potential of HEOs as new low-bandgap photocatalysts. [1] P. Edalati, Q. Wang, H. Razavi-Khosroshahi, M. Fujii, T. Ishihara, K. Edalati, “Photocatalytic hydrogen evolution on a high-entropy oxide”, Journal of Materials Chemistry A, 8(7), (2020), 3814-3821.

Corrosion resistance is an important property for load-carrying structural materials. The role of solute elements on corrosion properties of the conventional binary and ternary alloys has been established. However, effect of chemical composition on corrosion properties of high-entropy alloys with equimolar composition is far less understood. A typical example is seen in HEAs with Cr, which is the passivation former in the conventional Fe-Cr alloys. Cr-containing HEAs represented by Cantor alloys with 20at\%Cr can be expected to exhibit higher corrosion resistance than or comparable to the conventional stainless steels such as SUS304. However, the result for the pitting potential reported in several papers are rather disappointing [1]. Whether it is attributed to an intrinsic nature of HEAs or chemical inhomogeneity due to inappropriate processing is not clear yet. It has been reported by numerous researcher that grain refinement to ultrafine grain (UFG) size or nanostructure enhance passivating capability and corrosion resistance of stainless steels, possibly by Cr enrichment at the surface [2]. UFG formation may even decrease the critical Cr for passivation threshold. In the present research, severe plastic deformation (SPD) is employed for UFG formation of HEAs because it can be applied to the broad range of composition and can shuffle or redistribute chemical inhomogeneity, which is detrimental to corrosion resistance.

\[ \frac{Q}{Y} = K F_e Z_i Z_f U_i \]

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The high-temperature properties of high-entropy alloys have various grain sizes are important to provide feedback to material creation design, and provide guidance for practical application by understanding the mechanism of property development and microstructure formation. However, the underlying mechanism controlling the high temperature properties remains unknown due to the compositional complexity of the system and the interactions among the elements. This system and the interactions are further complicated when some phases are present due to the phase instability at higher temperatures. Using measurements by in-situ neutron diffraction under high-temperature and external stress environments, to elucidate the fundamental mechanism for controlling high-temperature properties.

High entropy alloys (HEAs) has superior mechanical properties compared with conventional alloys [1, 2]. Recently, microstructure control of HEAs by thermomechanical process has been reported [3]. The electrical properties of HEAs was reported between crystalline and amorphous materials since the chemical composition of HEAs is near-equimolar, and furthermore, Kondo effect like behavior was reported which normal-ly seen in dilute alloys [4]. Such abnormal electrical properties of HEAs is associated with the cocktail effect which is the interaction between composing elements. It is known that the electrical resistivity of pure metals increases with increasing the density of lattice defects introduced by plastic deformation, since lattice defects work as scattering centers of free electrons in metals [5]. Fig. 1 is the electrical resistivity of Al depending on the severe plastic deformation (taken from the literature as an example [5]). In the present study, various types or microstructure of HEAs will be produced by either sputtering or conventional thermomechanical process. Then, it will be studied whether the electrical resistivity of HEAs affected by changing the density of lattice defects or not.

To investigate the fundamental mechanism of how the local electronic properties generated by the local atomic structure are expressed as a cocktail effect in the high-entropy alloy (HEA) systems, first-principle simulations have been carried out in terms of relatively small supercellics of HEAs. As a typical body-centered cubic (BCC) HEA, TaZrNiHfTa alloy local models have been devised using a lot of 54-atom BCC superlattices. The average atomic displacement from the ideal positions for each element has been analyzed with the Seebeck coefficient for each model was evaluated in terms of the density of state for carriers, and the relations with the molar entropy of mixing and the average atomic displacement were discussed. The absolute values of the Seebeck coefficients in the HEA region are generally larger than those in the medium-entropy alloy region, and their plus/minus signs are nonlinearly controlled to average valence electron concentration.