AWARD

Haruyuki Inui, May 2019, The 16th Honda Frontier Award, The Honda Memorial Foundation.

Haruyuki Inui, September 2019, Materia Japan for Education, The Japan Institute of Metals.

Hidemi Kato and Takeshi Wada, June 2019, JSPM Award for Innovatory Research, Japan Society of Powder and Powder Metallurgy.

Hiroyuki Muto, May 2019, IEEJ Distinguished Paper Award, The Institute of Electrical Engineers of Japan.

Tsuru Tomohito, May 2019, Young Researcher's Award, The Society of Materials Science, Japan.

Tadashi Furuhara, March 2020, Scientific Achievement Merit Prize, The Iron and Steel Institute of Japan

Hiroshi Ohtani, December 2019, Best Paper Award, Japan Copper and Brass Association.

Akihiko Chiba, November 2019, Best Review Paper Award, Smart Processing Society for Materials, Environment & Energy.

Nobuhiro Tsuji, 2019, One of the top 100 read materials science papers for Scientific Reports in 2018.

Nobuhiro Tsuji, August 2019, Best Poster Award of Rex&GG 2019, 7th International Conference on Recrystallization and Grain Growth (Rex&GG 2019)

PRESS

1. Kyoto University Academic Day 2019, 15 September 2019, "New Advanced Materials Design: High-Entropy Alloys", Haruyuki Inui.
2. Japan Meal Bulletin, 17 October 2019, "High-Entropy Shape Memory Alloys", Koichi Tsuchiya.
3. Japan Metal Daily, 17 October 2019, "High-Entropy Shape Memory Alloys", Koichi Tsuchiya.
4. Japan Chemical Daily, 17 October 2019, "High-Entropy Shape Memory Alloys", Koichi Tsuchiya.
5. Press Release (Tohoku University), 19 December 2019, "Successful Synthesis of Nano-porous High-Entropy alloys", Hidemi Kato.
6. Nikkan Kogyo Newspaper, 29 January 2020, "Development of New Implant Materials", Kei Ameyama, Takeshi Nagase.

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/fall-meetings-exhibits/2020-mrs-fall-meeting
- Third International Conference on High Entropy Materials(ICHEM2020), September 27 - October 1, 2020, Berlin, Germany.
  https://www.ichem2020.uni-bayreuth.de/en/index.html
- THERMEC'2021, 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

- The Japan Institute of Metal (JIM) Symposium "Materials Science of High-Entropy Alloys", March 17-19, 2020, Tokyo, Japan. [Canceled due to Coronavirus (Covid-19)]
  https://jim.or.jp/MEETINGS/2020_spr/news/notice_02.html
- 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

HEAs
High Entropy Alloys
Science of New Class of Materials Based on Elemental Multiplicity and Heterogeneity

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Ministry of Education, Culture, Sports, Science and Technology Grant-in-Aid
"Scientific Research on Innovative Areas" for FY2018-22

NEWSLETTER Vol. 2
2020 MAY

HEAs
High Entropy Alloys
Science of New Class of Materials Based on Elemental Multiplicity and Heterogeneity

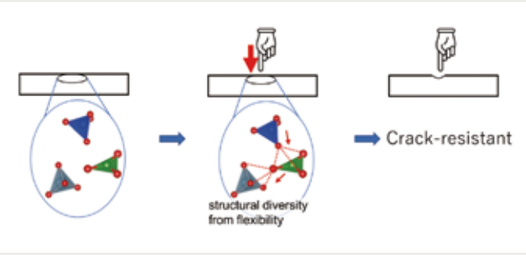
New Research Teams Accelerate HEA Project

Let's Enjoy Materials Design Extended with Elemental Multiplicity and Heterogeneity!

A01(a) Crack-resistant Property Induced by Simultaneous Modification of Coordination Environment Around Various Cations in High-Entropy Hard Oxide Glasses

Atsunobu Masuno (Hirosaki University)

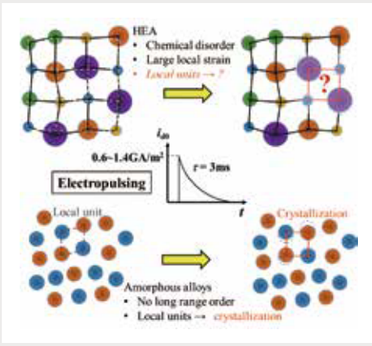
Glasses that combine high hardness with tolerance to surface damage are of great importance for the fabrication of glass products such as cover glasses in electronic devices and window glasses for transportation and construction. The increase of hardness of glasses requires a high atomic packing density and high bonding energy of components, which is realized in Al_2O_3-based glasses. The crack-resistant property is enhanced in glasses with low atomic packing density because the stress applied can be released without cracking by atom displacement in the low-packed glasses. Therefore, hardness and crack-resistance are usually competing attributes in conventional oxide glasses. The materials design concept to obtain glasses with both hardness and crack-resistance is proposed in this project. Some oxide components in glasses are known to modify easily their oxygen coordination number around cations when the stress is applied. The modification without large atom displacement can be realized even in high-packed and hard glasses. Here, we try to fabricate multicomponent glasses including various components such as Al_2O_3, B_2O_3, GeO_2, TiO_2, and Nb_2O_5. The chemical composition is designed so that the components are included in the equivalent molar ratio to enhance configurational disorder and induce the cocktail effect on mechanical properties.



A01(a) Local Structure unit and its Stability in High-Entropy Alloys Investigated by Electropulsing

Hisanori Tanimoto (University of Tsukuba), Ryo Hozumi (University of Tsukuba), Mari Kawamura (University of Tsukuba)

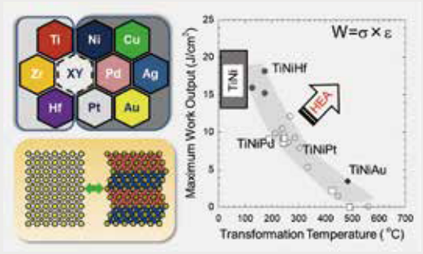
More than 40% decrease in the resistivity of amorphous (a-) ZrCu alloys is induced by applying an electric pulse current which exponentially decays with the time constant of ~3 ms from the initial current density of ~0.6 GA/m² (electropulsing). The diffraction measurements reveal that formation of nanocrystallites is responsible for the large decrease in the resistivity. These observations suggest that crystalline-like local structure units in a-ZrCu are transformed to thermodynamically stable crystallites through collective motions of the local units excited by electropulsing. High-entropy alloys (HEAs) are crystalline but the chemical atomic arrangement is disordered in principle and large local strains are existed. The retarded atomic diffusion of HEAs may reflect existence of some chemically ordered local units which assist the stability of HEAs. The local structure unit and its stability in CrMnFeCoNi HEA are investigated from the changes in the resistivity and microstructure by electropulsing.



A01(a) Elucidation of Martensitic Transformation of High Entropy Type Alloys and Development of Novel High Temperature Shape Memory Alloys

Hee Young Kim (University of Tsukuba)

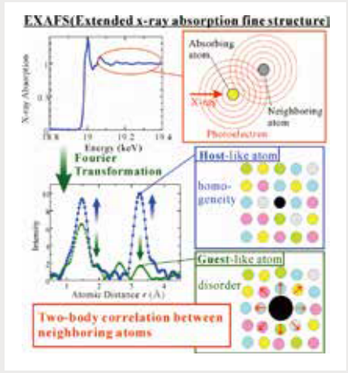
Shape memory alloys have attractive attention not only for basic research but also for practical applications due to their unique functional properties such as shape memory effect and superelasticity. Such unique properties originate from the crystallographically reversible martensitic transformation 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 XY 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.



A01(a) Local Structural Analysis in High-Entropy Alloys

Noriaki Hanasaki (Osaka University)

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.



A01(a) Monocrystalline elastic constants for CrMnFeCoNi high entropy alloys

Katsushi Tanaka (Kobe University), Takeshi Teramoto (Kobe University)

The temperature dependences of monocrystalline 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 monocrystal 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 C_{12} is smaller than that of C_{44} 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 monocrystalline elastic constants, a relatively strong directional interatomic bonding has to be introduced.

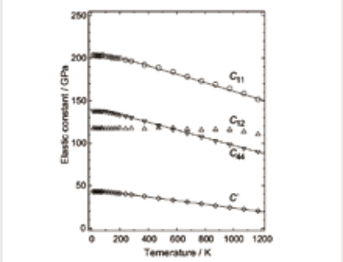


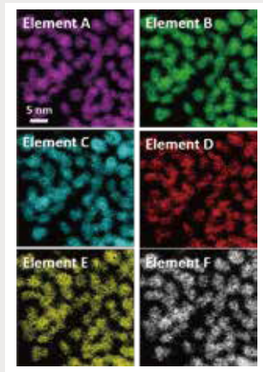
Fig. 1. Monocrystalline elastic constants of CrMnFeCoNi high entropy alloy.

A01(b) Study on the Synthesis of High-Entropy Alloy Nanoparticles and their New Properties

Hiroshi Kitagawa (Kyoto University)

Solid-solution alloys are favorable to tune their properties because the constituent elements of a solid 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 succeeded in synthesizing many types of novel solid-solution alloy NPs and high-entropy alloy NPs consisting of immiscible constituents[1]. 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.

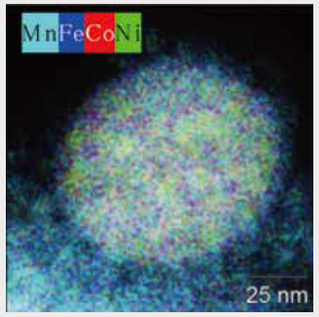
[1] K. Kusada, D. Wu, H. Kitagawa "New Aspects of Platinum Group Metal-Based Solid-Solution Alloy Nanoparticles: Binary to High-Entropy Alloys". *Chem. Euro. J.*, 26, (2020)



A01(b) High Entropy Alloy Nanoparticles Prepared by Plasma-in-Liquid Process

Tetsu Yonezawa (Hokkaido University), Mai Thanh Nguyen (Hokkaido University)

Preparation of nanoparticles of high entropy alloys (HEA) has been carried out by plasma-in-liquid system. We have carefully prepared some HEA ingots by using arc melting method. The elements used in this study were Mn, Fe, Co, and Ni. Mn-Fe-Co-Ni, Fe-Co-Ni, and Fe-Ni alloy ingots were prepared by this way. The melting temperatures of the obtained HEA ingots were revealed by DSC which indicated that the obtained ingots have solid-solution structures. At first, we have tried one of the plasma-in-liquid process, laser ablation to prepare HEA nanoparticles. 532-nm Nd-YAG pulse laser was irradiated to the ingot targets which were put on the bottom of water. By irradiation of laser, the color of the dispersion changed to brown which indicated the formation of metal nanoparticles. We have checked the detailed structure by STEM-HAADF and STEM-EDX, but unfortunately, the particles were oxidized and some particle-in-particle structure was observed as shown in Figure 1 (STEM-EDX image of Mn-Fe-Co-Ni).



A01(b) In-situ observation of radiation damage in FeCrNiMnxCo high entropy alloys

Naoyuki Hashimoto (Hokkaido University), Tatsuya Fukushi (Hokkaido University), Wei-Ying Chen (Argonne National Laboratory), Jien-Wei Yeh (National Tsing Hua University)

The single-phase FCC type high entropy alloys: FeCrNiMn*x*Co (*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-annealed FeCrNiMn*x*Co 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 unfaulted 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.

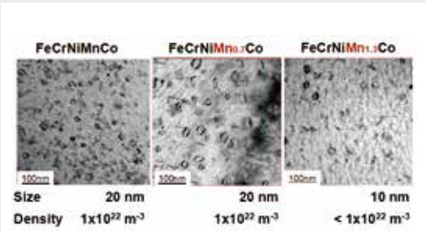


Fig. 1 Irradiation-induced Frank loops formed in FeCrNiMnxCo HEA alloys

A01(b) High-Entropy Hydrogen Absorbing Alloys with Tunable Chemical Equilibrium

Etsuo Akiba (Kyushu University)

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 the exactly 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"; $\ln(P_{H_2}) = \Delta H^0/RT - \Delta S^0/R$. ΔS^0 of formation of solid-state hydride from alloy is almost zero, which means the term of $\Delta S^0/R$ is independent to chemical species. If you would use high entropy alloy for hydride formation, much larger $|\Delta S^0|$ is expected. It increases freedom of material design. Another expectation for high entropy alloy for hydrogen storage is increase of hydrogen capacity. As shown the Figure, we have already reported equimolar five-element high entropy alloy TiZrNbHfTa absorbs hydrogen to metal ratio (H/M) of 2.2 at 300˚C.

We are working to develop alloys light weighted and working at room temperature.

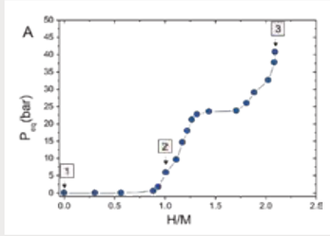


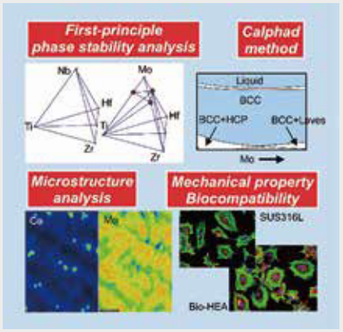
Fig. Hydrogen absorption by TiZrNbHfTa high entropy alloy at 300˚C [1]

[1] C. Zlotea et al., " Hydrogen sorption in TiZrNbHfTa High Entropy Alloy". *J. Alloys Comp.*, **775** (2019) 667-674.

A01(b) Development of High-Entropy Alloys for Metallic Biomaterials

Takeshi Nagase (Osaka University), Yuuka Iijima (Osaka University), Aira Matsugaki (Osaka University), Kei Ameyama (Ritsumeikan University), Takayoshi Nakano (Osaka University)

Ti-Zr-Hf-Cr-Mo and Ti-Zr-Hf-Co-Cr-Mo high-entropy alloys for metallic biomaterials (bio-HEAs) were designed using the empirical alloy parameters of HEAs, Materials Project as an open-web-based predicted and known-structure database including the state-of-the-art electronic structure methods, and CALculation of PHAse Diagrams (CALPHAD) using the FactSage and Scientific Group Thermodata Europe (SGTE) databases. The BCC phase formation during the solidification process was predicted by CALPHAD, and the BCC phase formation in arc-melted ingots was experimentally confirmed by microstructure analysis using XRD and electron microscopy. The Ti-Zr-Hf-Cr-Mo and Ti-Zr-Hf-Co-Cr-Mo bio-HEAs showed superior biocompatibility comparable with CP-Ti and much higher hardness than CP-Ti and conventional Ti alloys.

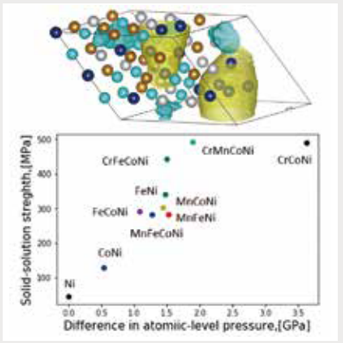


[1] T. Nagase, Y. Iijima, A. Matsugaki, K. Ameyama, T. Nakano: Design and fabrication of Ti-Zr-Hf-Cr-Mo and Ti-Zr-Hf-Co-Cr-Mo high-entropy alloys as metallic biomaterials, Materials Science and Engineering C, 107, (2020), 110322.

A02(c) Atomic stress state inside high-entropy alloys: first-principles local stress calculation

Yoshinori Shiihara (Toyota Technological Institute)

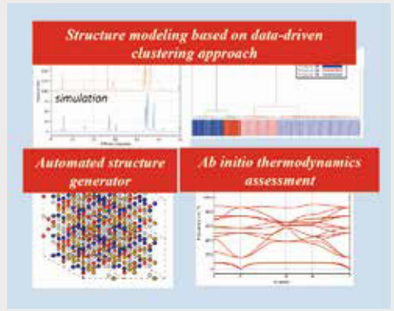
Outstanding mechanical properties of high-entropy alloys probably originates from solid-solution strengthening due to elastic disturbance inside crystals; However, the details are not clear. While solid-solution strengthening is caused by the interaction between lattice defects such as dislocations, stacking faults, etc., and stress field around the solute atoms, stress field inside high-entropy alloys are inhomogeneous because there exist five or more elements with different sizes. Hence, existing theories on the strengthening mechanism were not able to be applied straightforwardly. Several geometric quantities of the crystals are proposed to the elastic disturbance called lattice distortion. They do not directly tell lattice distortion inside the crystals; moreover, there is no way to discuss the effectiveness of the methods appropriately. The purpose of this study is to clarify the atomic-level stress field inside high-entropy alloys directly from the first-principles local stress calculation method developed by the author.



A02(d) Ab initio Thermodynamics Assessment Based on Data-driven Structure Modelling

Kenta Hongo (JAIST)

Recently, high-entropy alloys (HEAs) have attracted great attention to their mechanical properties. 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.



A03(e) Hydrogen Production on a High-Entropy Photocatalyst

Parisa Edalati (Kyushu University), Qing Wang (Kyushu University), Hadi Razavi-Khosroshahi (Nagoya Institute of Technology), Masayoshi Fuji (Nagoya Institute of Technology), Tatsumi Ishihara (Kyushu University), Kaveh Edalati (Kyushu University)

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 [1], the first high-entropy photocatalyst with a d^0 electronic configuration is synthesized by high-pressure torsion process followed by high-temperature oxidation. The synthesized oxide with an overall composition of $TiHfZrNbTaO_{11}$ 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 (compared to simple oxide) with a bandgap of 2.9 eV and appropriate valance and conduction bands for water splitting. The material successfully produces hydrogen by photocatalytic water splitting, suggesting the potential of HEOs as new low-bandgap photocatalysts.

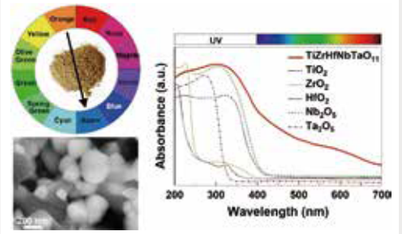


Fig. 1. High-entropy oxide with orange color and appreciable light absorbance in visible-light region for photocatalysis.

[1] P. Edalati, Q. Wang, H. Razavi-Khosroshahi, M. Fuji, T. Ishihara, K. Edalati, "Photocatalytic hydrogen evolution on a high-entropy oxide". Journal of Materials Chemistry A, 8 (7), (2020), 3814-3821.

A03(e) Corrosion behavior of High-Entropy Alloys by Severe Plastic Deformation

Hiroyuki Miyamoto, Shizuka Shimizu, Motohiro Yuasa (Doshisha University)

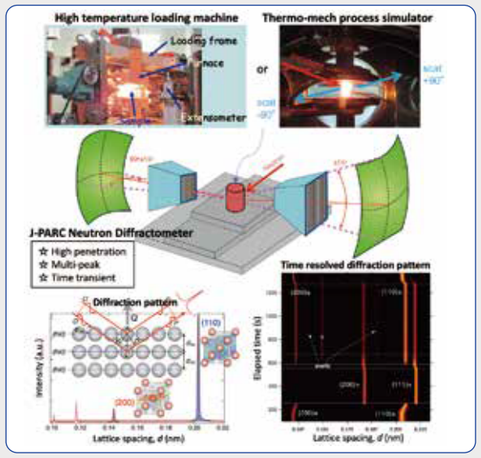
Corrosion resistance is an important property for load-carrying structural materials. The role of solute elements on corrosion properties of the conventional binary and ternary alloys has been established. However, effect of chemical composition on corrosion properties of high-entropy alloys with equimolar 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.

[1] Q. Ye, K. Feng, Z. Li, F. Lu, R. Li, J. Huang, Y. Wu, Applied Surface Science 396 (2017) 1420-1426.
[2] H. Miyamoto, Corrosion of ultrafine grained materials by severe plastic deformation, an overview, Materials Transactions 57 (2016) 559-572.

A03(e) Elucidation of The Fundamental Mechanism for Controlling High-Temperature Properties of High Entropy Alloys using Neutron Diffraction

Stefanus Harjo (Japan Atomic Energy Agency)

The high-temperature properties of high-entropy alloys with 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 the neutron diffraction technique, we can obtain in-situ crystallographic microstructure information in the bulk state of a specimen under external environment such as temperature and load by taking advantage of the large neutron penetration ability and the ability to see how atoms are arranged. In this study, the crystal structures of high-entropy alloys with various grain sizes are measured by in-situ neutron diffraction under high-temperature and external stress environments, to elucidate the fundamental mechanism for controlling high-temperature properties.



A03(e) Electrical Properties of High-Entropy Alloys Fabricated by Sputtering and Thermomechanical process

Yoji Miyajima (Kanazawa University)

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 normally 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.

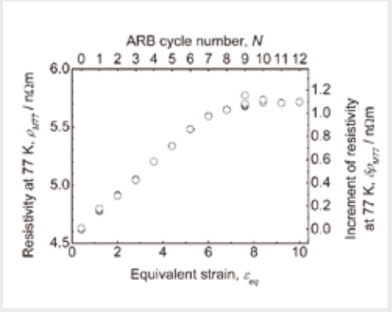


Fig. 1 Electrical resistivity of 2N-Al depending on the severe plastic deformatnio process taken from the litarature [5].

[1] J. W. Yeh *et al., Advanced engineering materials*, **6** (2004) 299-303.
[2] B. Cantor *et al., Materials science and engineering A*, **375-377** (2004) 213-218.
[3] T. Bhattacharjee *et al., Scientific reports*, (2018) doi: 10.1038/s41598-018-21385-y.
[4] Y. F. Kao, *Journal of alloys and compounds*, **509** (2011) 1607-1614.
[5] Y. Miyajima *et al., ", Philosophical Magazine*, **90** (2010) 4475-4488.

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2020 MAY

A03(f) EXAFS Study for Local Structures of Medium-entropy Alloys TCoNi (T=Cr, Mn, Fe)

Yoichi Ikeda (Institute for Materials Research, Tohoku University), Daiju Matsumura (JAEA)

Local structures of medium-entropy alloys TCoNi (T = Cr, Mn and Fe) have been investigated by means of the X-ray absorption edge fine structure (EXAFS) measurement in the fluorescence mode at BL14B1, SPring-8. Polycrystalline samples were prepared with a conventional arc melting method, annealed at 1000˚C for 2 hours, and then quenched into a liquid nitrogen. Figure 1 shows the magnitude of EXAFS function, $|\chi(R)|$, of CrCoNi (blue), MnCoNi (red), and FeCoNi (green) at room temperature. The entire shape of EXAFS functions can be explained with an FCC-structure model; this result is consistent with the result of x-ray diffraction. The slight differences in the EXAFS functions suggest that the local bond lengths between the absorption atom and the surrounding atoms may be different among Cr, Mn, and Fe alloys.

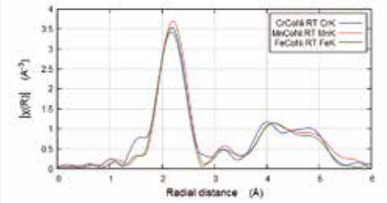

Fig. 1. EXAFS functions in real space of medium entropy alloys measured around *K*-edge of the T elements (Cr, Mn, and Fe) at room temperature.

A03(f) High Throughput Survey on the Existence Range of the CrMnFeCoNi High Entropy Alloys.

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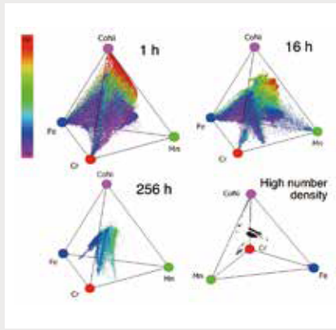
High entropy alloys exhibit various unique characteristics, understanding of which will lead to significant developments in materials science. Existence range of alloys is related to their thermodynamic properties and is necessary for basic understanding of the alloy system. High entropy alloys inherently contain five or more constituent elements and hence their phase diagrams are drawn in five or more dimensional spaces. To explore such a vast compositional space, conventional experiments such as annealing followed by observations with compositional analysis will take too much time and efforts. Our research group has developed an experimental technique to efficiently examine the range of existence and phase equilibria of alloys with multiple constituent elements. In this study, we apply this technique to survey the CrMnFeCoNi high entropy alloys. As a result, the compositional region with high number density (right, below in the figure) has been determined, which might be related to the existence range of the alloys. The other figures show the distribution of compositional points in multiple diffusion samples after annealing for respective time periods shown in the figures.



A03(f) Simulation of the Cocktail Effect in Electronic Properties of High-Entropy Alloys Based on Electronic-State Calculations

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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 superlattices of HEAs. As a typical body-centered cubic (BCC) HEA, TiZrNbHfTa 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 respect to the combination of the first closest atoms. 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.