

LATEST INFORMATION

International Meeting

- International Conference on Processing & Manufacturing of Advanced Materials (Thermec'2021), May 10-14, 2021 - Virtual Conference. <https://www.tugraz.at/events/thermec-2020/home/>
- International Conference on Advances in High-Entropy Alloys (ICAHEA 2021:15), June 3-4, 2021 in New York, USA. <https://waset.org/advances-in-high-entropy-alloys-conference-in-june-2021-in-new-york>
- International Conference on High-Entropy Alloy Design (ICHEAD 2021: 15), September 16-17, 2021 in Amsterdam, Netherlands. <https://waset.org/high-entropy-alloy-design-conference-in-september-2021-in-amsterdam>
- The Materials Science & Technology (MS&T) technical meeting and exhibition, October 17-21, 2021, Columbus, Ohio, USA. <https://www.matscitech.org/mst21>
- 6th World Congress on Integrated Computational Materials Engineering (ICME 2021), November 14-18, 2021, Lake Tahoe, Nevada, USA. <https://www.tms.org/icme2021>
- 2021 MRS Fall Meeting & Exhibit, November 28 - December 2, 2021, Boston, Massachusetts, USA. <https://www.mrs.org/meetings-events/fall-meetings-exhibits/2021-mrs-fall-meeting>
- The 2nd World Congress on High Entropy Alloys (HEA 2021), December 5-8, 2021, Charlotte, North Carolina, USA. https://www.tms.org/portal/MEETINGS___EVENTS/TMS_Meetings___Events/Upcoming_TMS_Meetings/HEA2021/portal/Meetings___Events/2021/HEA2021/default.aspx?hkey=51531264-7d36-4089-aa6f-ac3f591e2681
- Materials Research Meeting 2021 (MRM 2021), December 13-17, 2021, Pacifico Yokohama, Japan. <https://mrm2021.jmru.org/>
- TMS 2022 151st Annual Meeting & Exhibition, February 27-March 3, 2022, Anaheim, California, USA. <https://www.tms.org/tms2022>
- International Conference on Advances in High-Entropy Alloys (ICAHEA 2022:16), March 15-16, 2022 in London, UK. <https://waset.org/advances-in-high-entropy-alloys-conference-in-march-2022-in-london>

Domestic Meeting

- 2021 Startup Meeting of All Research Groups, May 20-21, 2021, Kyoto, Japan. <https://highentropy.mtl.kyoto-u.ac.jp/members>
- The Ceramic Society of Japan, The 34th Fall Meeting, September 1-3, 2021, Online Meeting, Japan. <https://fall34.ceramic.or.jp/>
- The Japan Institute of Metal (JIM) Symposium "Materials Science of High-Entropy Alloys", September 14-17, 2021, Online Meeting, Japan. https://jim.or.jp/MEETINGS/me_index.html



High Entropy Alloys

Science of New Class of Materials Based on Elemental Multiplicity and Heterogeneity

NEWSLETTER
Vol. 3
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Notable Achievements

The Latest Research Results Elucidated in the HEA Project!

A01(b)

Discovery of High-Entropy Alloy Nanoparticles and Exploration of Their 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 in solids. 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 developed a continuous solvothermal flow reactor to synthesize novel solid-solution alloy NPs and high-entropy alloy NPs consisting of immiscible constituents in bulk state (Fig. 1)^[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.

We have also succeeded in developing PdRuIr ternary alloy NPs which exhibit highly stable and active three-way catalytic (TWC) property (Fig. 2)^[2]. The binary PdRu shows higher TWC activity than the most expensive but essential Rh which is known as the best NO_x reduction catalyst. However, their activity significantly deteriorates due to the phase separation during the reaction since Pd and Ru are immiscible in bulk. We performed DFT calculations to elucidate the origin of the stabilization effect in PdRuIr ternary catalyst and found that the solid-solution phase in PdRuIr NPs was extremely stabilized by the combination of enthalpy of mixing and the large configurational entropy by alloying the third element.

Besides, we had succeeded in synthesizing platinum-group metal HEA (PGM-HEA) NPs in the last year. This year we found that all the 6-elements PGM-HEA (RuRhPdOsIrPt) NPs show a record-high ethanol oxidation electrocatalytic activity with a 12-electron process.^[3] We expect that the HEA NPs would be promising catalysts for complex reactions because HEA NPs intrinsically possess various active sites and

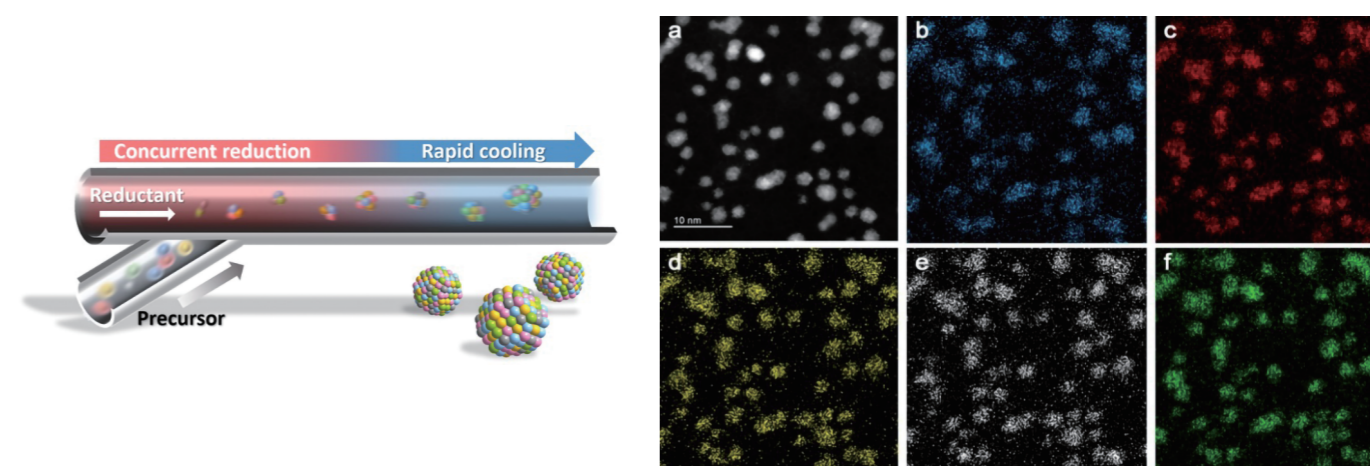


Fig. 1: Schematic of the continuous solvothermal flow reactor ((a) HAADF-STEM image and (b-f) EDS maps of RuRhPdIrPt HEA NP synthesized by a continuous flow reactor ((b) Pd-L, (c) Ru-L, (d) Ir-L, (e) Pt-L, and (f) Rh-L)



High Entropy Alloys

Science of New Class of Materials Based on Elemental Multiplicity and Heterogeneity

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high stability. Furthermore, 5-elements PGM-HEA (RuRhPd IrPt) NPs exhibited a very high hydrogen evolution reaction (HER) electrocatalytic activity in both acid and alkaline solutions.^[4] Although the HER activity is often discussed by *d*-band center theory, this HEA catalyst did not follow the tendency of *d*-band center theory and marked very high activity. Therefore, this result implies that HEA catalysts need a new descriptor to predict their activity. We are further investigating this mechanism.

[1] K. Kusada, et al., "Nonequilibrium Flow-Synthesis of Solid-Solution Alloy Nanoparticles: From Immiscible Binary to High-Entropy Alloys", *Journal of Physical Chemistry C*, 125, 458-463 (2021).

[2] K. Kusada, et al., "Highly Stable and Active Solid-Solution-Alloy Three-Way Catalyst by Utilizing Configurational-Entropy Effect", *Advanced Materials*, 33, 2005206 (2021).

[3] D. Wu, et al., "Platinum-Group-Metal High-Entropy-Alloy Nanoparticles", *Journal of the American Chemical Society*, 142, 13833-13838 (2020).

[4] D. Wu, et al., "On the Electronic Structure and Hydrogen Evolution Reaction Activity of Platinum Group Metal-Based High-Entropy-Alloy Nanoparticles", *Chemical Science*, 11, 12731 - 12736 (2020).

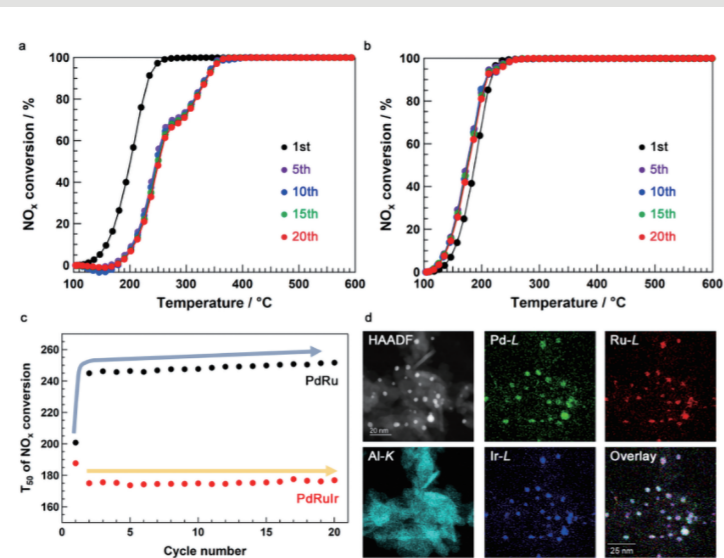


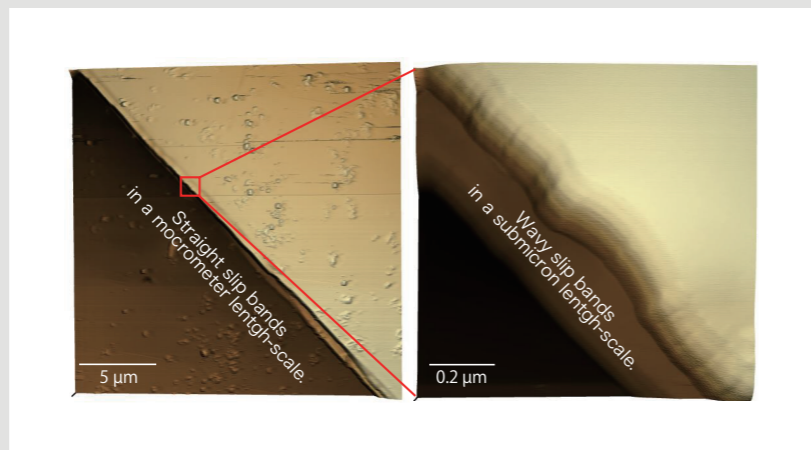
Fig. 2: The endurance test of the PdRu catalyst for the TWC reaction. a, b) The cycle dependence of NO_x conversion on PdRu (Pd:Ru = 1:1) (a) and PdRu (Pd:Ru:Ir = 1:1:1) (b) catalysts, and c) the temperatures corresponding to 50% conversion (T₅₀) of NO_x of (a) and (b). d) HAADF-STEM image and elemental maps of the PdRu catalyst after 20 cycles of the TWC test.

A01(a) Persistent slip in TiZrNbHfTa observed by using an atomic force microscope

Masaki Tanaka (Kyushu University), Shigeto Yamasaki (Kyushu University), Tatsuya Morikawa (Kyushu University)

There are several reports which shows that slip bands in bcc high-entropy alloys are straight and sharp. This phenomenon suggests that cross-slip is restricted in bcc high-entropy alloys. In this study, slip property of TiZrNbHfTa, which has bcc structure, was evaluated by obtaining ψ - χ relationships with bending tests of micro cantilevers, where χ is defined as the angle between the maximum shear stress plane and $(\bar{1}01)$ and ψ is defined as the angle between the apparent slip plane and $(\bar{1}01)$. The ψ - χ relationship indicated that ψ is nearly the same as χ , suggesting that there is no persistent slip. Detailed observations with an atomic force microscope confirm as shown in right figure that cross-slipping is so frequent at a sub-micrometer length-scale that the slip bands appear to be straight and the maximum shear stress plane is observed on a micrometer length-scale. Here, TiZrNbHfTa shows abnormally frequent cross-slipping, which is a novel characteristic of high-entropy body-centered cubic alloys. Although further investigations are necessary to elucidate the reason why TiZrNbHfTa shows such frequent cross-slipping, one possibility is the random atomic arrangement of high-entropy alloys.

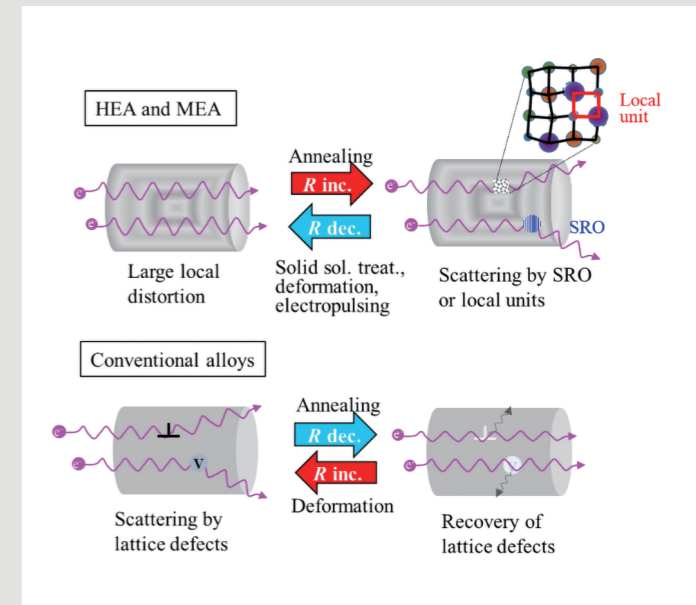
[1] M. Tanaka, S. Okajo, S. Yamasaki, T. Morikawa, "Persistent slip observed in TiZrNbHfTa: A body-centered high-entropy cubic alloy", *Scripta Materialia*, 200, (2021), 113895.



A01(a) Electrical Resistivity and Local Structures of High Entropy Alloys

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

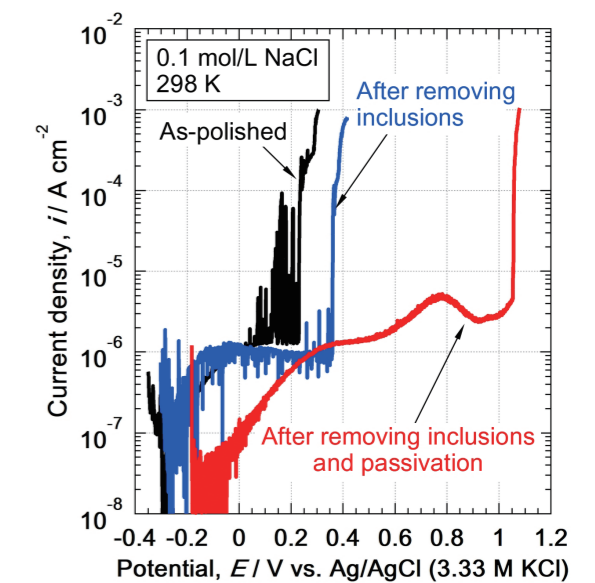
Metallic solid solutions composed of five or more elements in equimolar ratios are called high-entropy alloys (HEAs). HEAs are crystalline but the chemical atomic arrangement is disordered in principle and the lattice is locally strained. It was reported that locally-ordered atomic clusters are existed in chemically and topologically disordered amorphous alloys. The retarded atomic diffusion in HEAs suggests the formation of chemical short-range-orders (SROs) or local units. The electrical resistivity is a macroscopic property but quite sensitive for changes in atomic configurations. The local structures and their stabilities in CrMnFeCoNi HEA have been surveyed from the electrical resistivity measurement. By isothermal annealing below 1073K, the resistivity of CrMnFeCoNi HEA showed a gradual increase from the initial value after the solid solution treatment. The increased resistivity by annealing showed a slight decrease by passing electric pulse current (electropulsing). It was reported that the resistivity of CrMnFeCoNi HEA decreased by cold working. The resistivity of conventional alloys shows increases due to lattice defects and precipitates and the increased resistivity shows the recovery by annealing. The changes in the resistivity observed for HEAs indicate that SROs or the local units are formed by annealing and some of them are dissolved to the original random state by electroplusing or deformation.



A01(b) Electrochemical Passivation for Improving Pitting Corrosion Resistance of Equiatomic CoCrFeMnNi High-Entropy Alloy

Li Pao (Tohoku University), Izumi Muto (Tohoku University), Yu Sugawara (Tohoku University)

The pitting corrosion behavior of arc-melted equimolar CoCrFeMnNi alloy was investigated by macro-scale and micro-scale potentiodynamic polarization. It was found that Cr-Mn-O inclusions with S-containing parts were the pit initiation sites for pitting in chloride solutions at near-neutral pH. During polarization, *in situ* observations on the alloy surface were performed, and the selective dissolution of the S-containing parts was found to occur under open-circuit and anodic potentials. It was concluded that the S-containing parts of the inclusions were the first to dissolved, followed by the initiation of pitting. The S-containing parts of the inclusions were removed by potentiostatic polarization and immersion in H₂SO₄, but the pitting corrosion resistance after these treatments did not improve apparently. In contrast, by potentiodynamic polarization in H₂SO₄, the S-containing parts of the inclusions were removed and the passive film on the alloy-matrix became Cr enriched, resulting in significant improvement in the pitting corrosion resistance. As a result, the pitting potential in 0.1 mol/L NaCl increased to above 1 V. To elucidate the protective ability of the passivated alloy surface, the measurements of depassivation-pH were conducted. In the case of as-polished surface, the depassivation pH was approx. 2.0, but it decreased to 0.0 after the electrochemical passivation.



A01(b) Suppression of Frank loop growth in CoCrFeNiMn_x by the control of stacking fault energy

Naoyuki Hashimoto (Hokkaido University), Eyo Wada (Hokkaido University), Tatsuya Fukushi (Hokkaido University), Hiroshi Oka (Hokkaido University), Shigehito Isobe (Hokkaido University)

It has been reported that HEAs have unique properties such as a high radiation resistance and corrosion resistance at elevated temperatures compared with conventional nuclear component materials. This attractive property could make HEAs candidates for high temperature nuclear reactor components. However, the studies on their microstructural evolution and mechanical property change under irradiation, especially at elevated temperatures, is very limited. In this study, the single-phase FCC type high entropy alloys: CoCrFeNiMn_x ($x: 0.7\sim 1.3$) were prepared and analyzed to understand the Mn effect on the growth of Frank loops under irradiation. TEM observation of deformed HEAs indicated that the stacking fault energy would have a positive dependence on Mn content (Fig. 1(a)). Furthermore, the irradiation experiments revealed the suppression of Frank loop growth with increasing stacking fault energy (Fig. 1(b)).

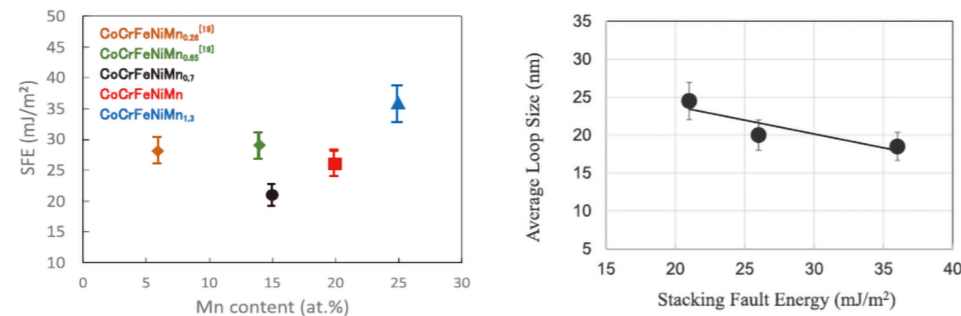


Fig. 1 (a) Mn content dependence on stacking fault energy of HEAs, (b) the average Frank loop size as a function of stacking fault energy

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

Etsuo Akiba and Rika Hayashi (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 was to explore at the middle of phase diagrams not at the corners nor edges. This is the exactly same concept of high-entropy alloy development. We extend our concept for four, five and six element alloy systems under this program.

We developed four element alloys by adding the fourth elements to the Ti-V-Cr equimolar alloy. Among them, Nb and Mo added alloys are pure BCC and readily absorb and desorb hydrogen. We selected Nb and Mo to form five element high entropy Ti-V-Cr-Nb-Mo alloys and they were successfully prepared. Both equimolar and $\text{Ti}_{0.1}\text{V}_{0.3}\text{Cr}_{0.2}\text{Nb}_{0.1}\text{Mo}_{0.3}$ are BCC and desorb and absorb hydrogen at room temperature. They are the first high entropy pure BCC alloys show hydrogen absorption/desorption at room temperature.

Fig shows the PCT isotherms of TiVCrNbMo at 30°C. The green line was the first hydrogen absorption/desorption and the red and orange lines were the second and the third cycle, respectively. It clearly shows room temperature hydrogen absorption and good cyclability.

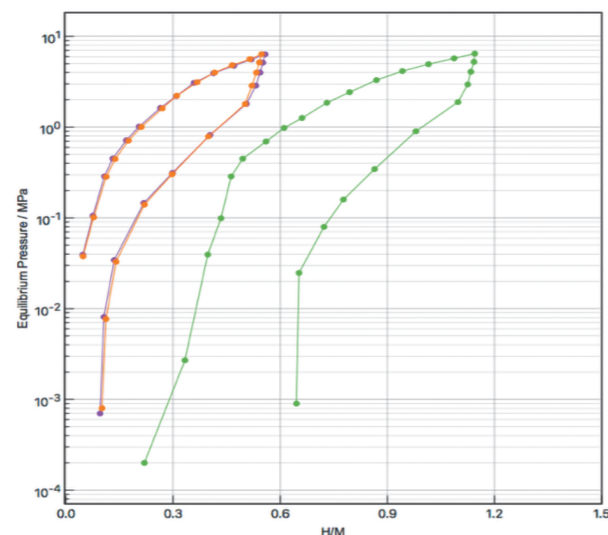


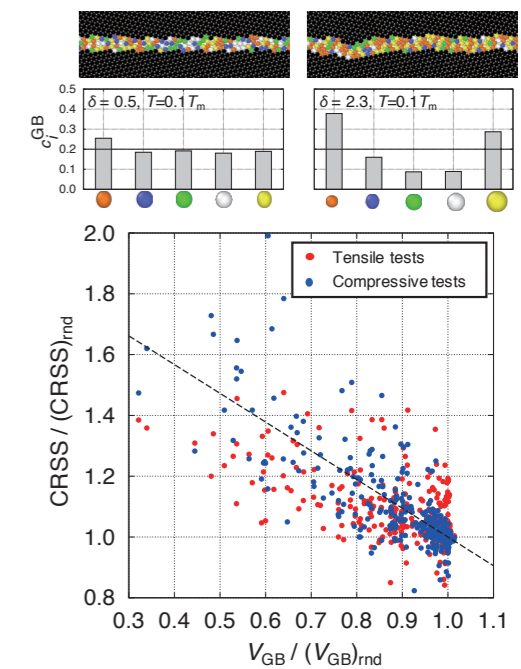
Fig. Hydrogen absorption by TiVCrNbMo high entropy alloy at 30°C

A02(c) A Strengthening Mechanism by Grain-Boundary Segregation in High Entropy Alloys through Atomic Simulations

Tomotsugu Shimokawa, Kohei Shiotani, Tomoaki Niiyama (Kanazawa University)

In conventional alloys, smaller excess free volume at grain boundaries (GBs) is known to increase the stress required for dislocation emission, e.g., twin boundary. In high-entropy alloys (HEAs) consisting of various elements with different atomic sizes, smaller GB free volume can be achieved even in large misorientation angles if GB segregation occurs due to large (small) atoms occupying large (small) atomic sites. We investigate the possibility of the strengthening mechanism by GB segregation in HEAs through a simple two-dimensional atomic simulation. Virtual equiatomic quinary HEA models with 5 types of atomic size difference δ ranging from 0 to 2.28 are expressed by a tunable two-body atomic potential [1]. Thermally equilibrium atomic configurations of 18 types of bicrystal models at different temperatures ($0.01 T_m, 0.1 T_m, 0.3 T_m, 0.5 T_m, 0.7 T_m, T_m = 960 \text{ K}$) obtained by hybrid MD and MC analyses show that stronger GB segregation of the maximum and the minimum size atoms, which decreases GB free volume, occurs as the temperature becomes lower (see the right upper figure. Both grain boundaries have the same misorientation angle of 21.8 degrees but different δ and the larger δ enhances the GB segregation.). Uniaxial tensile and compressive deformation tests are performed to all cases of bicrystal models at 1K and reveal the suppression of dislocation emission from segregated GBs with small free volumes. As results, GB segregation could be a strengthening mechanism in HEAs.

[1] K. Shiotani, T. Niiyama, T. Shimokawa, "Dislocation Emission from Grain Boundaries in High-Entropy Alloys: Influence of Atomic Composition at Grain Boundaries". Materials Transactions., 61(7), (2020), 1272-1279.



A02(c) Geometric Study on Microscopic Structures in Thermodynamic Equilibrium for High-Entropy Alloys

Koretaka Yuge (Kyoto University)

Whereas microscopic structures (Q) in high-entropy alloys (HEAs) in thermodynamic equilibrium, including short-range ordering (SRO), can be reasonably predicted for given potential energy surface (U) through statistical mechanics, nonlinear Q-U correspondence is far from well-understood due to its complexity, especially enhanced for multicomponent systems. We here tackle this fundamental problem based on a variety of geometry, leading us clear and systematic insight into how nonlinear character is essentially governed by underlying lattice. Our recent, main results are: (i) We find that SRO tendency near transition temperature can be well-characterized by a set of a few specially-selected configurations without requiring any thermodynamic information, i.e., they are common for any combination of constituents[1]. (ii) We apply tropical geometry to evolution of the nonlinearity, finding that asymmetric linear character around random state is mainly bounded by the number of non-crossing, closed path on the lattice, corresponding to spatial constraint on constituents[2]. (iii) Based on Riemannian manifold with dual-orthogonal foliation, we reveal that the nonlinearity can always be geometrically decomposed into the sum of three contributions of deviation from Gaussian in individual structural degree of freedom (SDF), entanglement in SDF and nonadditivity in the entanglement (Fig. 1)[3]. Particularly, the nonadditivity is specific and enhanced for multicomponent systems, which should play essential role for cocktail effect in HEAs on the Q-U correspondence nonlinearity.

References: [1] K. Yuge, R. Miyake, S. Ohta, J. Phys. Soc. Jpn. **89**, 094803 (2020). [2] K. Yuge and S. Ohta, J. Phys. Soc. Jpn. **89**, 084802 (2020). [3] K. Yuge, arXiv:1811.09612 [cond-mat.stat-mech].

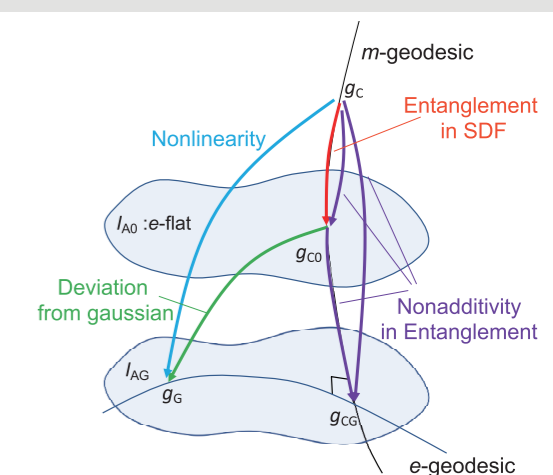
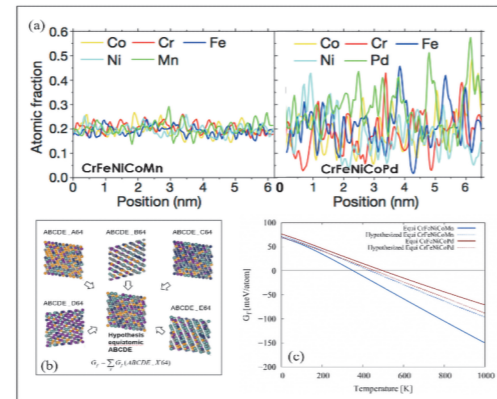


FIG. 1: Geometric interpretation of nonlinearity on α -connected dually flat Riemannian manifold.

A02(d) First-principles Investigation on Effect of Inhomogeneous in High-Entropy Alloys: CrFeNiCoMn vs. CrFeNiCoPd, Equiatomic vs. Non-equiatomic Compositions

Tran Nguyen Dung and Ying Chen (Tohoku University)

Cantor alloy CrFeNiCoMn is a well-known HEA which consists of five 3d elements with similar properties. CrFeNiCoPd has been newly synthesized with intentionally substituting Mn in Cantor alloy by Pd which has a markedly different atomic size and electronegativity from the other constituent elements, and has been achieved in experiments the better mechanical properties than Cantor alloy, while manifests rather bigger fluctuation of atomic composition (Nature, 2019, 574, 223). Comprehensive DFT-based calculations for both zero K and finite temperature have been conducted on these two quinary systems using the special quasirandom structures (SQSs) in order to investigate the effect of Pd-to-Mn substitution. It has been found that substituting Mn with Pd in Cantor alloy introduces the inhomogeneous feature so that increases the average atomic local displacement of the CrFeNiCoPd to a moderate amount, consequently enhances the mechanical properties of the new HEA. We constructed a model of hypothesized equiatomic composition as a mixture of several non-equiatomic compositions to simulate the local inhomogeneous environment in CrFeNiCoPd, and found that for CrFeNiCoPd, the hypothesized equiatomic composition is more stable than its equiatomic composition, showing an opposite trend in CrFeNiCoMn. This explained the experimental observation and gave a hint to design new HEAs with compromising inhomogeneous and stability.



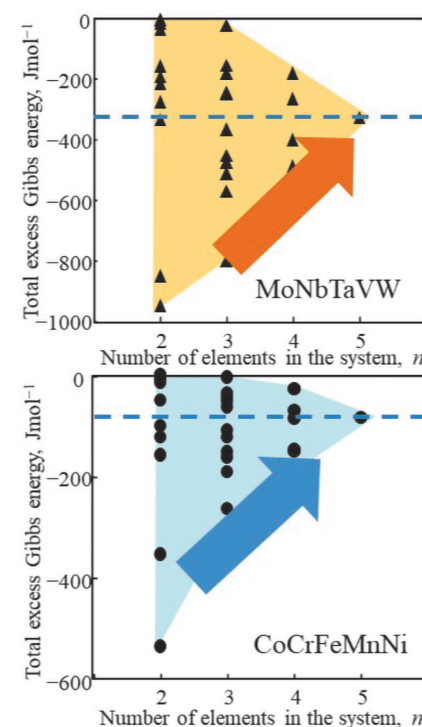
(a) The fluctuation of atomic compositions in CrFeNiCoMn and CrFeNiCoPd ((Nature, 2019, 574, 223)). (b) Hypothesized equiatomic composition model. (c) Gibbs formation energies as the function of temperature for the hypothesized (dashed lines) and real equiatomic modeled (solid lines) equiatomic CrFeNiCoMn (blue) and CrFeNiCoPd (red).

A02(d) CALPHAD modeling of Effect of Short-Range Ordering in High-Entropy Alloys

Taichi Abe (NIMS), Ikuo Ohnuma (NIMS), Kwangsik Han (NIMS)

In the framework of the CALPHAD (Calculation of phase diagrams) the description of the short-range ordering (SRO) for binary systems was expanded to multi-component systems [1]. The effect of SRO in high entropy alloys (HEAs) were estimated based on the Gibbs energy functions from the CALPHAD-type thermodynamic assessments. It was applied to the BCC-based HEA (MoNbTaVW) and FCC-based HEA (CoCrFeMnNi). In the present calculation, the total contribution of the SRO to the Gibbs energy was approximately -1 kJmol^{-1} and -0.2 kJmol^{-1} in the BCC- and FCC-based HEAs at 1000 K, respectively. The variations in the excess Gibbs energy (presented in the right figure) and excess entropy due to SRO in lower-order systems can be averaged in the HEAs because of the mixing of multiple elements, as formally suggested in the previous work [2] for the excess Gibbs energy in Cantor alloy. It suggested that if the high-entropy effect on the mechanical properties were originated from SRO, it might not be related directly to integral quantities but local atomic arrangements.

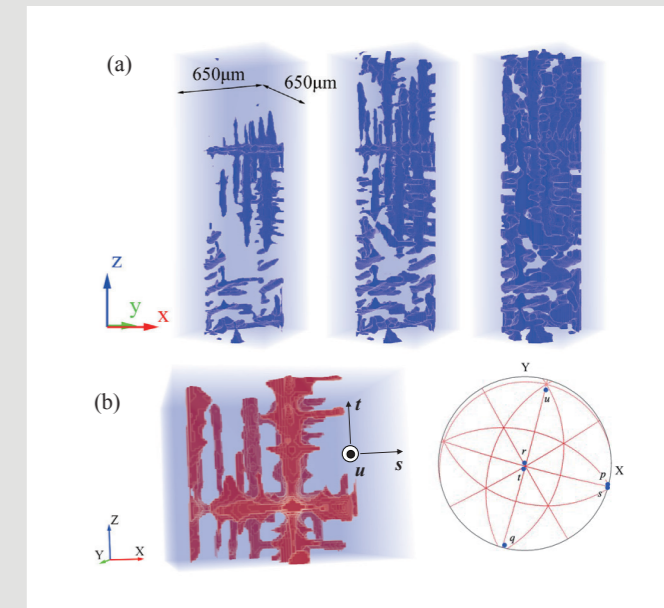
- [1] T. Abe, "Effect of Short-Range Ordering in High-Entropy Alloys", Mater. Trans., 62[6], (2021), 711-718.
 [2] T. Abe, "Thermal Vacancies in High-Entropy Alloys", Mater. Trans., 61[4], (2020), 610-615.



A03(e) Characterization of dendritic growth in an equimolar CrMnFeCoNi high entropy alloy

Hideyuki Yasuda (Kyoto University), Keita Nakano (Kyoto University), Taka Narumi (Kyoto University), Kohei Morishita (Kyoto University, Now at Kyushu University)

Dendrite arms generally grow along a preferred growth direction which is intrinsically determined by anisotropy of solid – liquid interface energy. Although most of conventional FCC alloys grow in the $\langle 100 \rangle$ directions, some of FCC alloys such as Al-Zn alloys grow in the $\langle 110 \rangle$ directions [1]. Solidification structure and microsegregation in the interdendritic region are significantly influenced by the dendritic growth. Thus, it is of interest to characterize the dendritic growth of high entropy alloys. We have developed a time-resolved *in-situ* tomography (4D-CT) and X-ray diffraction (XRD). This technique allows to observe growing dendrites and to determine crystallographic orientation *in-situ*. Typical time resolution and spatial resolution for the observation in SPring-8 are 0.5 - 8 s and 1 - 7 μm . Figure shows time evolution of dendrites during cooling at 0.083 K/s in the CrMnFeCoNi alloy [2]. Three-dimensional images were reconstructed from 200 projection images and the images were improved by an image filter using a phase field model. The crystallographic orientations measured during cooling is also shown in the figure. The observations proved that the dendrite arms strictly grew along the $\langle 100 \rangle$ directions. The specific solid-liquid interfacial area, which was normalized by the total volume, was also evaluated as a function of solid fraction. The interfacial area was compatible with the reported values of conventional alloys such as Al and Mg alloys. The secondary arm spacing was on the same order of magnitude as the spacing of conventional alloys. Overall, the solidification in this high-entropy alloy can be analyzed by models for pseudo-binary alloys.

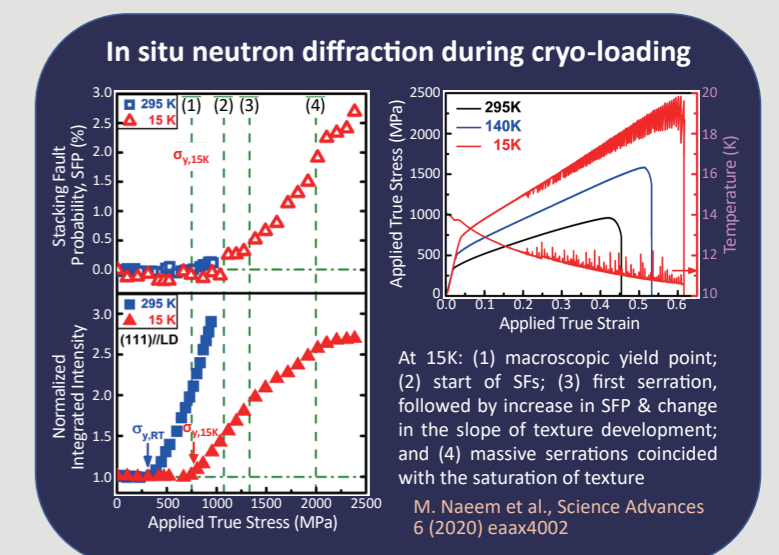


- [1] A. Sémoroz et. al, Acta Mater 49 (2001) 529, [2] K. Nakano et. al, Mater. Trans 61 (2020) 596

A03(e) Multimode Deformation in High-Entropy Alloy at Cryogenic Temperature Revealed by In Situ Neutron Diffraction

Muhammad Naeem (City University of Hongkong), Haiyan He (City University of Hongkong), Fan Zhang (University of Science and Technology Beijing), Stefanus Harjo (Japan Atomic Energy Agency), Takuro Kawasaki (Japan Atomic Energy Agency), Si Lan (Nanjing University of Science and Technology), Xun-Li Wang (City University of Hongkong)

High-entropy alloys exhibit exceptional mechanical properties, high strengths and large elongations accompanied with large work hardening, at cryogenic temperatures. *In situ* neutron diffraction studies during tensile loading at cryogenic temperatures were performed to elucidate the mechanism of such exceptional mechanical properties. The activation of twinning in addition to dislocation slip was observed displaying the coexistence of multiple deformation pathways, and how the individual deformation mechanisms compete or synergize during plastic deformation were discussed based on the evolutions of lattice strains, dislocation densities and textures obtained from neutron diffraction. It was found that the interaction of a rich variety of deformation mechanisms in high-entropy alloys at 15 K, began with dislocation slip, followed by stacking faults and twinning, before transitioning to inhomogeneous deformation by serrations. The cooperation of these different deformation mechanisms led to extreme work hardening. The stable face-centered cubic structure with the low stacking fault energy at cryogenic temperatures, enabled by the high-entropy alloying, played an important role provoking and mutually bridging dislocation slip and serration. Insights from these *in situ* neutron diffraction studies point to the role of entropy in the design of structural materials at cryogenic temperatures with superior properties.



At 15K: (1) macroscopic yield point; (2) start of SFs; (3) first serration, followed by increase in SFP & change in the slope of texture development; and (4) massive serrations coincided with the saturation of texture

M. Naeem et al., Science Advances 6 (2020) eaax4002

A03(f)

Vacancy Formation Enthalpy in Medium-Entropy and High-Entropy Alloys Studied by Positron Lifetime Measurements and First-Principles Calculations

Masataka Mizuno (Osaka University), Kazuki Sugita (Osaka University), Hideki Araki (Osaka University)

To quantitatively evaluate the vacancy formation enthalpy in medium-entropy and high-entropy alloys, we performed in-situ positron lifetime measurement under high-temperature condition and first-principles calculations based on the special quasi-random structure (SQS) approach. Figure 1 shows the temperature dependence of mean positron lifetime in CrFeNi and CoCrFeMnNi alloys. The vacancy formation enthalpy H_f can be determined by the threshold temperature at which the mean positron lifetime sharply increases. We obtained $H_f = 1.80 \pm 0.14$ eV for CrFeNi and $H_f = 1.69 \pm 0.13$ eV for CoCrFeMnNi. These values do not differ much from the vacancy formation enthalpies of constitutional elements of these alloys. Figure 2 shows the average value of calculated vacancy formation enthalpies of each element in CrFeNi, CoCrFeNi and CoCrFeMnNi alloys. The vacancy formation enthalpy slightly increases with increasing number of elements. This trend is partly due to the difference in the energy gain by structural relaxations. The addition of Co and Mn to CrFeNi reduces the energy gain by structural relaxation around a vacancy. The general shape of averaged density of states of each element is quite similar among these three alloys, which indicates that the increase in the number of elements does not affect the chemical bonding.

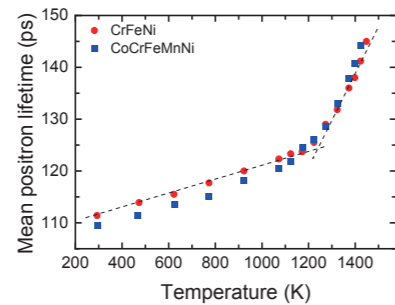


Fig.1 Temperature dependence of mean positron lifetime.

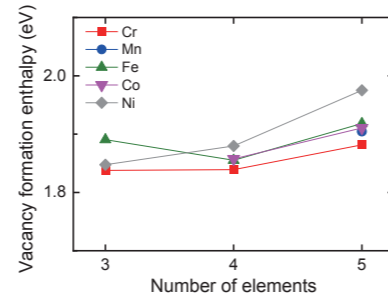


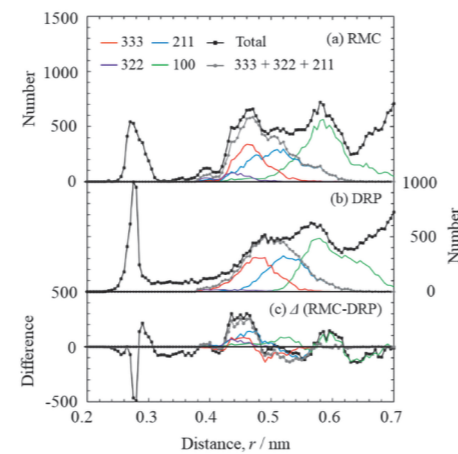
Fig. 2 Vacancy formation enthalpy as a function of the number of elements.

A03(f)

Middle Range Ordering realized in ZrPt Amorphous Alloy

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Atomic ordering in both the short-range region and the middle-range region in amorphous alloys is known to be closely correlated with unique material properties. AXS-RMC technique is one of the powerful techniques to elucidate the interesting short and middle range ordering of an amorphous alloy. AXS-RMC study of $Zr_{80}Pt_{20}$ amorphous alloy reveals a dominant topological short-range ordering of the icosahedral-like cluster. The discussion on such the correlation distance and corresponding coordination number in the short range ordering is very useful for understanding the fundamental structural features. However, it is sometimes necessary to conduct further analysis with respect to the middle range ordering. The present amorphous alloy could be included in this category because the partial pair distribution function of the Pt-Pt pair indicates a significant enlargement at approximately 0.45 nm in the second-nearest neighbor region. The middle range connection specified by the two Pt atoms can be considered as a unit of face-sharing tetrahedra (FST), which lead to one of the dense packing structural units among Bernal polyhedral. And further analysis indicates the strong preference of the chemically featured Pt-Zr3-Pt middle range linkage, by suggesting the strong chemical affinity between Pt and Zr. This is also attributed to the saturation of the quasicrystalline phase found in the annealed $Zr_{80}Pt_{20}$. Present AXS-RM analysis also revealed unique middle-range linkages based on non-Bernal polyhedra, having a higher and lower packing density of atoms with slight preference for Zr and Pt, respectively. Notably, such chemical and density fluctuations identified by using the concepts of the Bernal polyhedral units are expected to be utilized for characterizing the middle range ordering of a variety of amorphous alloy systems.



The middle-range Pt-Pt correlations realized in $Zr_{80}Pt_{20}$ amorphous alloy.

AWARD

Akihiko Chiba, April 2020, Commendation for Science and Technology (Research Division), The Minister of Education, Culture, Sports, Science and Technology, Japan.

Nagase Takeshi, Terayama Akira, Nagaoka Takashi, Fuyama Nobuyuki and Sakamoto Tatsuaki, May 2020, The Best Paper Award, Japan Foundry Engineering Society.

Koichi Tsuchiya, September 2020, The 17th Murakami Memorial Award, The Japan Institute of Metals and Materials.

Akira Takeuchi, Takeshi Wada and Hidemi Kato, September 2020, The 68th Best Paper Award (Materials Processing Category), The Japan Institute of Metals and Materials.

Akira Takeuchi, Takeshi Wada and Hidemi Kato, September 2020, The 68th Best Paper Award (Material Characteristics Category), The Japan Institute of Metals and Materials.

Naohiro Hayashi, Kazuki Nakashima, Masanori Enoki, Hiroshi Ohtani, September 2020, The Best Paper Award for Young Speaker, The Japan Institute of Metals and Materials.

Takaaki Hara, Toshiki Ishida, Katsunari Oikawa, September 2020, The Best Paper Award for Young Speaker, The Japan Institute of Metals and Materials.

Tomohiro Nishimura, Ryota Matsubayashi, Kouhei Morishita, Masato Yoshiya, Tomoya Nagora and Hideyuki Yasuda, March 2021, The Best Paper Award (Sawamura Award), The Iron and Steel Institute of Japan.

Masaki Tanaka, Scientific Achievement Commemorative Prize (Nishiyama Commemorative Prize), The Iron and Steel Institute of Japan.

PRESS

- 1 The Science News, 15 January 2021, "Deformation observation of high Mn steel: Elucidation of serration behavior-, in Kyoto University", Sukyoung Hwang, Myeong-Heom Park, Yu Bai, Akinobu Shibata, Wenqi Mao, Hiroki Adachi, Masugu Sato and Nobuhiro Tsuji.
- 2 Kyoto University HP: Latest research news, 25 December 2020, Elucidation of serration behavior -Approaching the fundamental mechanism of deformation in high Mn steel showing high strength and high ductility", Sukyoung Hwang, Myeong-Heom Park, Yu Bai, Akinobu Shibata, Wenqi Mao, Hiroki Adachi, Masugu Sato and Nobuhiro Tsuji.
- 3 Press Release, 25 August 2020, "Elucidation of cast iron strengthening mechanism by high-intensity neutron beam, -Observation of cast iron microstructure at atomistic scale by in-situ neutron diffraction experiment-", Stefanus Harjo, Takuro Kawasaki, Wu Gong, Satoru Kubota, Si Gao.
- 4 Kyoto Shimbun, Morning edition: 12 August 2020, "Fabrication of a uniform alloy with 6 platinum family elements", Hiroshi Kitagawa.
- 5 Yume Navi Web Lecture No.10234, 24 April 2020, "By controlling "powder" you can freely create new materials", Hiroyuki Muto.
- 6 Press Release, 7 April 2020, "Elucidation of spontaneous fracture of Aluminum, - Investigating the cause of aluminum brittleness with hydrogen and expectations for high-strength alloys from computational materials science", Tomohito Tsuru.
- 7 Press Release, 28 March 2020, "Elucidation of the unique deformation mechanism observed at extremely low temperatures in advanced alloys, -Expectations for the development of high-performance low-temperature structural materials useful for space technology-", Xun-Li Wang, Stefanus Harjo, Takuro Kawasaki, *et al.*