

1. The paper *Comprehensive Data Compilation on the Mechanical Properties of Refractory High-Entropy Alloys* provides an abstract on how this data article presents the compilation of mechanical properties for 122 refractory high-entropy alloys (RHEAs) and refractory complex concentrated alloys (RCCAs) reported in the period from 2010 to the end of January 2018. The datasheet gives alloy composition, type of microstructures, and the metallurgical states in which the properties are measured. Data such as the computed alloy mass density, the type of mechanical loadings to which they are subjected, and the corresponding macroscopic mechanical properties, such as the yield stress, are made available as a function of the testing temperature. For practical use, the data are tabulated, and some are also graphically presented, allowing a tag glance to access relevant information for this attractive category of RHEAs and RCCAs.
2. The paper *Development and Exploration of Refractory High Entropy Alloys—A Review* provides an abstract on how open literature publications, in the period from 2010 to the end of January 2018, on refractory high-entropy alloys (RHEAs) and refractory complex concentrated alloys (RCCAs) are reviewed. While RHEAs, by original definition, are alloys consisting of five or more principal elements with the concentration of each of these elements between 5 and 35 at.%, RCCAs can contain three or more principal elements, and the element concentration can be greater than 35%. The 151 reported RHEAs/RCCAs are analyzed based on their composition, processing methods, microstructures, and phases. Mechanical properties, strengthening and deformation mechanisms, oxidation and corrosion behavior, as well as tribology, of RHEAs/RCCAs are summarized. Unique properties of some of these alloys make them promising candidates for high-temperature applications beyond Ni-based superalloys and/or conventional refractory alloys. Methods of development and exploration, future directions of research and development, and potential applications of RHEAs are discussed.
3. The paper *Mapping the World of Complex Concentrated Alloys* provides an abstract on how this work explores the mechanical properties of high entropy alloys (HEAs) and complex concentrated alloys (CCAs) by comparing them with commercially available engineering alloys, including industry-standard aerospace alloys. To reach this goal, we have developed a materials database covering the main mechanical properties of HEAs and CCAs from the published literature. The database is used to represent various property spaces enabling an assessment of their performance for lightweight structures and high-temperature structural applications. In addition, we illustrate the effects of alloying and specific elements on the room temperature mechanical properties of HEAs and CCAs. With densities between titanium alloys and steels or nickel alloys, the best CCAs exceed commercial alloys in uniaxial loading and beam bending at room temperature. Where use temperature or cost excludes commercial alloys based on Mg, Al, or Ti, the best CCAs also offer attractive specific yield strength in panel bending and specific stiffness for all loading conditions at room temperature. Many CCAs have superior structural properties at elevated temperatures. And for Conclusion, in this work, we conducted an alloy network analysis of five different families of CCAs: 3d

transition metal CCAs, refractory metal CCAs, light metal CCAs, CCA brasses and bronzes, and lanthanide CCAs. The potential of the CCAs as structural materials is evaluated graphically using alloy properties maps and performance indices. 3d transition metal CCAs and some of the refractory metal CCAs uniquely fill the gap between commercial titanium alloys and steels or nickel alloys, while light metal CCAs fill the gap between Mg alloys and Ti alloys, providing new material options for structural applications. In terms of the room temperature specific yield strength, the best 3d transition metal CCAs exceed all commercial alloys (including steels, stainless steels, Ti, Al, Mg, Ni, and refractory alloys) in uniaxial loading and perform as well as the best Mg alloys in beam bending. Where the maximum use temperature eliminates conventional Mg-based and Al-based alloys, and where cost excludes Ti-based alloys, 3d transition metal CCAs emerge as the most attractive option in uniaxial loading, beam bending, and panel bending. The room temperature specific stiffness of the best 3d transition metal CCAs is equivalent to the best commercial alloys in uniaxial loading, is better than steels and commercial Ni and refractory alloys in beam and panel bending, but is poorer than Mg, Al, and Ti alloys in bending modes. The room temperature specific yield strength and stiffness of refractory CCAs do not compete with commercial alloys for any of the three loading conditions considered here. However, temperature-dependent yield strength–density charts show that refractory CCAs outperform commercial Ni alloys and 3d transition metal CCAs at 800 °C and 1000 °C, highlighting their potential interest. The effect of Al on the mechanical properties and phases of 3d transition metal CCAs is illustrated using composition trajectories. Increasing Al increases strength while decreasing density and ductility while transforming single-phase FCC microstructures to duplex FCC + BCC or FCC + B2 microstructures. The influence of other elements (Mo, Nb, Si, Ti, V) is also illustrated. The best CCAs have microstructures that are likely to contain significant amounts of one or more intermetallic phases. The graphical approach used here shows that the conventional alloying strategy of small elemental additions to a base element improves the room temperature specific yield strength by increasing strength at a relatively constant density. However, increasing the number of principal elements,  $N$ , has a different effect on the room temperature specific yield strength of CCAs. The overall yield strength increases with increasing  $N$ , while the density range shrinks from a broad span of roughly 500–20000 kg m<sup>-3</sup> at  $N = 1$  to a relatively narrow range of 6000–9000 kg m<sup>-3</sup> at  $N \geq 6$ . The present work gives a visual approach that identifies the most attractive alloys for structural applications, and these results are recommended as an aid to focus future studies on the most promising alloys.

4. The paper *Microstructures and Crackling Noise of Al<sub>x</sub>NbTiMoV High Entropy Alloys* provides an abstract on how a series of high entropy alloys (HEAs), Al<sub>x</sub>NbTiMoV, was produced by a vacuum arc-melting method. Their microstructures and compressive mechanical behavior at room temperature were investigated. It has been found that a single solid-solution phase with a body-centered cubic (BCC) crystal structure forms in these alloys. Among these alloys, Al<sub>0.5</sub>NbTiMoV reaches the highest yield strength (1,625 MPa), which should be attributed to the considerable solid-solution strengthening behavior. Furthermore, serration and crackling noises near the yielding point were observed in the NbTiMoV alloy, which represents the first such reported phenomenon at room temperature in HEAs. And In Conclusion, a refractory HEAs system, Al<sub>x</sub>NbTiMoV, is designed and fabricated by arc melting. It is found that single

solid-solution phases with simple BCC structures and typical dendrite form can be observed in these alloys. These alloys have high compression yield strengths, attributed to solid-solution strengthening. In addition, a serration behavior and crackling noise were found in the stress-strain curves of the NbTiMoV alloys at room temperature, which is reported for the first time in HEAs. Further studies need to be done to investigate this kind of serration behavior and crackling noises in these refractory HEAs.

5. The paper *Microstructure and Compressive Properties of NbTiVTaAlx High Entropy Alloys* provides an abstract on how the novel refractory high entropy alloys with the compositions of NbTiVTaAlx were prepared under a high-purity argon atmosphere, and their microstructure and compressive properties at room temperature were investigated. Despite containing many constituents, all alloys had a single solid solution phase with body-centered cubic (BCC) structure, and possessed high compressive yield strength and ductility, which should be attributed to solid solution strengthening. And In Conclusion, a new series of NbTiVTaAlx high entropy alloys have been successfully prepared, which all have simple phase structures and exhibit obvious dendrite structures. The phase formation rule of them has been discussed, based on the parameters of  $\delta$ ,  $i$  and VEC. It is concluded that these alloys possess excellent BCC solid-solution formation ability. All alloys have high compressive yield strength and ductility (no fracture under 50% strains), which should be attributed to solid solution strengthening.
  
6. The paper *Compositional Variation Effects on the Microstructure and Properties of a Refractory High-Entropy Superalloy AlMo0.5NbTa0.5TiZr* provides an abstract on how an AlMo0.5NbTa0.5TiZr baseline alloy was previously found to have good high-temperature strength but poor ductility below 600 °C due to coarse intermetallic grain boundary particles and a continuous ordered B2 matrix phase. Systematic composition changes were explored in this study to remove the deleterious microstructural features and improve mechanical properties. The baseline alloy and the new alloys studied here, AlMo0.5NbTa0.5TiZr0.5, AlNbTa0.5TiZr0.5, Al0.5Mo0.5NbTa0.5TiZr, and Al0.25NbTaTiZr, all exhibited an ordered B2 matrix crystal structure. Additionally, coherent BCC nanoscale precipitates were present at a high volume fraction inside the B2 matrix grains in AlMo0.5NbTa0.5TiZr, Al0.5Mo0.5NbTa0.5TiZr, and Al0.25NbTaTiZr, and/or coarse grain-boundary particles existed in AlMo0.5NbTa0.5TiZr and AlMo0.5NbTa0.5TiZr0.5. The mechanical properties were assessed using microhardness and compression testing at 25 °C and 1000 °C. Al0.5Mo0.5NbTa0.5TiZr showed the highest hardness ( $H_v = 6.4$  GPa) and strength ( $\sigma_{0.2} = 2350$  MPa) at 25 °C and modest strength ( $\sigma_{0.2} = 579$  MPa) at 1000 °C. AlMo0.5NbTa0.5TiZr0.5 demonstrated the highest strength ( $\sigma_{0.2} = 935$  MPa) at 1000 °C but was brittle at 25 °C. High-temperature deformation resulted in a desirable microstructure in Al0.5Mo0.5NbTa0.5TiZr and Al0.25NbTaTiZr alloys, consisting of a continuous BCC phase and discontinuous B2 nano-precipitates. The relationships between composition, microstructure, and properties were identified and discussed. And In Conclusion, compositional adjustments of the base AlMo0.5NbTa0.5TiZr refractory high-entropy superalloy were made to improve mechanical properties by modifying the phase content and microstructure. Four new alloys were produced by

reducing the amounts of Zr, Al, and/or Mo:  $\text{AlMo}_{0.5}\text{NbTa}_{0.5}\text{TiZr}_{0.5}$ ,  $\text{AlNbTa}_{0.5}\text{TiZr}_{0.5}$ ,  $\text{Al}_{0.5}\text{Mo}_{0.5}\text{NbTa}_{0.5}\text{TiZr}$ , and  $\text{Al}_{0.25}\text{NbTaTiZr}$ . The microstructure of the base alloy comprises equiaxed grains of an ordered B2 matrix phase, coherent nanometer-sized precipitates of a disordered BCC phase (~60% by volume) inside the grains, and coarse particles (~10%) of an ordered hexagonal phase at grain boundaries. The alloy possesses  $H_v = 5.8$  GPa,  $\sigma_{0.2} = 2197$  MPa,  $\epsilon_f = 4\%$  at 25 °C, and  $\sigma_{0.2} = 735$  MPa,  $\epsilon_f > 55\%$  at 1000 °C. Reducing Zr eliminates the BCC phase in  $\text{AlMo}_{0.5}\text{NbTa}_{0.5}\text{TiZr}_{0.5}$ , while additional removal of Mo also eliminates the ordered hexagonal phase in  $\text{AlNbTa}_{0.5}\text{TiZr}_{0.5}$ , making it a single-phase B2 structure. Both alloys are brittle ( $\epsilon_f < 1.5\%$ ) at 25 °C but ductile ( $\epsilon_f > 55\%$ ) at 1000 °C.  $\text{AlMo}_{0.5}\text{NbTa}_{0.5}\text{TiZr}_{0.5}$  demonstrates exceptionally high strength ( $\sigma_{0.2} = 935$  MPa) at 1000 °C, whereas removing Mo reduces the strength by 400 MPa ( $\sigma_{0.2} = 535$  MPa) in  $\text{AlNbTa}_{0.5}\text{TiZr}_{0.5}$ . Decreasing Al results in a two-phase  $\text{Al}_{0.5}\text{Mo}_{0.5}\text{NbTa}_{0.5}\text{TiZr}$  alloy with an ordered B2 matrix and coherent nanometer-sized spherical BCC precipitates. A further decrease in Al and replacement of Mo with Ta retains the two-phase structure in  $\text{Al}_{0.25}\text{NbTaTiZr}$  but with cuboidal-shaped coherent BCC precipitates.  $\text{Al}_{0.5}\text{Mo}_{0.5}\text{NbTa}_{0.5}\text{TiZr}$  exhibits  $\sigma_{0.2} = 2350$  MPa,  $\epsilon_f = 3.2\%$  at 25 °C, and  $\sigma_{0.2} = 579$  MPa,  $\epsilon_f > 55\%$  at 1000 °C, while replacing Mo with Ta decreases strength significantly, resulting in  $\text{Al}_{0.25}\text{NbTaTiZr}$  having  $\sigma_{0.2} = 1745$  MPa,  $\epsilon_f = 3.8\%$  at 25 °C, and  $\sigma_{0.2} = 366$  MPa,  $\epsilon_f > 55\%$  at 1000 °C. During high-temperature deformation, these alloys undergo microstructural transformations, resulting in a continuous BCC matrix and ordered B2 phase transforming into discrete particles within the BCC matrix. This transformation contributes to enhanced compressive ductility and a progressive drop in flow stress. The analysis of available phase diagrams suggests that Nb, Ta, and Zr contribute to the decomposition of a high-temperature BCC phase into two BCC phases due to a miscibility gap. Reducing Zr moves the alloy composition outside the miscibility gap, preventing phase separation. The interaction of Al with Zr, Nb, and Ta is likely responsible for BCC  $\rightarrow$  B2 ordering in Zr-rich phases. The ordered intermetallic B2 phase is strong in the presence of Mo but brittle at room temperature, leading to low ductility. In two-phase BCC/B2 alloys, the disordered BCC phase becomes continuous during deformation at 1000 °C, accompanied by enhanced ductility and a decrease in flow stress. It is suggested that a transformed microstructure comprising a disordered BCC matrix with ordered B2 nanometer-sized precipitates could achieve room-temperature ductility suitable for engineering applications. Further work is recommended to develop two-phase BCC/B2 microstructures balancing room-temperature tensile ductility and high-temperature strength.

7. The paper *Microstructure and Mechanical Properties of VTaTiMoAl<sub>x</sub> Refractory High Entropy Alloys* provides abstract on a series of refractory high-entropy alloys VTaTiMoAl<sub>x</sub> with  $x=0, 0.2, 0.6$ , and  $1.0$ , which were designed and produced by vacuum arc melting. The effect of added Al elements on the microstructure and mechanical properties of refractory high-entropy alloys was investigated. The X-ray diffraction results showed that all the high-entropy alloys consist of simple BCC solid solution. SEM indicated that the microstructure of VTaTiMoAl<sub>x</sub> changes from an equiaxial dendritic-like structure to a typical dendrite structure with the addition of Al element. The composition of different regions in the alloys was obtained by energy dispersive spectroscopy and showed that Ta and Mo elements are enriched in the

dendrite areas, and Al, Ti, and V are enriched in inter-dendrite areas. The yield strength and compress strain reach a maximum ( $\sigma_{0.2}=1221\text{MPa}$ ,  $\varepsilon=9.91\%$ ) at  $x=0$  and decrease with the addition of Al element at room temperature. The Vickers hardness of the alloys improves with the addition of Al.

8. The paper *Effect of Al Addition on Mechanical Properties and Microstructure of Refractory  $\text{Al}_x\text{HfNbTaTiZr}$  Alloys* developed a series of refractory  $\text{Al}_x\text{HfNbTaTiZr}$  high-entropy alloys (HEAs) with the aim to improve strength and reduce density of the very ductile base alloy  $\text{HfNbTaTiZr}$ . Despite the diversity of crystal structures among the constituent elements, all the HEAs are single solid solution phase with a body-centered cubic (BCC) structure. The addition of Al significantly improves the strength but reduces the ductility due to large solution hardening. The linear relation between yield strength and atomic percentage of Al suggests that the strengthening effect of a certain element in a single-phase HEA alloy can be explained based on the quasi-binary alloy concept. Crack formations in deformed  $\text{AlHfNbTaTiZr}$  alloy with the lowest fracture strain are mainly along the boundaries between dendrite and interdendrite. This agrees with its large deviation of Al content and thus strength between dendrite and interdendrite.
  
9. The paper *Microstructure and Properties of Aluminum-Containing Refractory High-Entropy Alloys* provides an abstract on the exploration of new composition and phase spaces in the development of new refractory alloys with reduced densities and improved properties using high-entropy alloying (HEA). Six new refractory HEAs were produced by combining Mo, Ta, and Hf with low-density refractory elements (Nb, V, and Zr), along with Ti and Al. These alloys exhibit densities ranging from  $6.9\text{ g/cm}^3$  to  $9.1\text{ g/cm}^3$ . Three of the alloys have single-phase disordered body-centered cubic (bcc) crystal structures, and the other three contain two bcc nanophases with very close lattice parameters. The alloys show high hardness, with values ranging from  $H_v = 4.0\text{ GPa}$  to  $5.8\text{ GPa}$ , and compression yield strength,  $\sigma_{0.2} = 1280\text{ MPa}$  to  $2035\text{ MPa}$ , depending on the composition. Some of these refractory HEAs exhibit significantly improved high-temperature strengths compared to advanced Ni-based superalloys. The compressive ductility of all the alloys is limited at room temperature but improves considerably at  $800^\circ\text{C}$  and  $1000^\circ\text{C}$ . For the conclusion, the phase composition, microstructure, and properties of six new refractory high-entropy alloys are discussed. In addition to the refractory elements, the alloys contain Al and Ti, which reduce the alloy density. Three alloys— $\text{AlMo}_{0.5}\text{NbTa}_{0.5}\text{TiZr}$  (A1),  $\text{Al}_{0.3}\text{NbTaTi}_{1.4}\text{Zr}_{1.3}$  (A4), and  $\text{Al}_{0.5}\text{NbTa}_{0.8}\text{Ti}_{1.5}\text{V}_{0.2}\text{Zr}$  (A6)—contain two bcc phases with very similar lattice parameters. Both phases are present in the form of interpenetrating nanolamellae, creating a basket-weave nanostructure inside grains. One phase is enriched with Nb, while the other is enriched with Zr. The densities of these alloys are  $7.4\text{ g/cm}^3$  (A1),  $8.2\text{ g/cm}^3$  (A4), and  $7.4\text{ g/cm}^3$  (A6), and their Vickers hardness is  $5.8\text{ GPa}$ ,  $4.8\text{ GPa}$ , and  $5.2\text{ GPa}$ , respectively. The remaining three alloys— $\text{AlNb}_{1.5}\text{Ta}_{0.5}\text{Ti}_{1.5}\text{Zr}_{0.5}$  (A2),  $\text{Al}_{0.4}\text{Hf}_{0.6}\text{NbTaTiZr}$  (A3), and  $\text{Al}_{0.3}\text{NbTa}_{0.8}\text{Ti}_{1.4}\text{V}_{0.2}\text{Zr}_{1.3}$  (A5)—are essentially single-phase bcc alloys. However, nanometer-sized secondary phases are present at grain boundaries. The densities of these alloys are  $6.9\text{ g/cm}^3$  (A2),  $9.0\text{ g/cm}^3$  (A3), and  $7.8\text{ g/cm}^3$  (A5), with their Vickers hardness being  $4.0\text{ GPa}$ ,  $4.9\text{ GPa}$ , and  $4.9\text{ GPa}$ ,

respectively. Compression tests reveal very high strength for some of these alloys in the temperature range from 23°C to 1000°C, superior to the tensile strengths of Ni-based superalloys, such as Inconel 718 and Mar-M247. The compressive ductility is limited at 23°C, suggesting that little or no tensile ductility may be present at this temperature.

10. The paper *Effect of Aluminum on the Microstructure and Properties of Two Refractory High-Entropy Alloys* provides an abstract describing the microstructure, phase composition, and mechanical properties of two Al-containing refractory high-entropy alloys (HEAs), AlMo0.5NbTa0.5TiZr and Al0.4Hf0.6NbTaTiZr. The AlMo0.5NbTa0.5TiZr alloy consists of two body-centered cubic (bcc) phases with very close lattice parameters,  $a_1 = 326.8$  pm and  $a_2 = 332.4$  pm. One phase is enriched with Mo, Nb, and Ta, while the other phase is enriched with Al and Zr. The phases form a nano-lamellae modulated structure inside equiaxed grains. The alloy has a density of  $\rho = 7.40$  g/cm<sup>3</sup>, Vickers hardness  $H_v = 5.8$  GPa, a yield strength of 2000 MPa at 298 K, and 745 MPa at 1273 K. The Al0.4Hf0.6NbTaTiZr alloy has a single-phase bcc structure with a lattice parameter  $a = 336.7$  pm. It has a density  $\rho = 9.05$  g/cm<sup>3</sup>, Vickers microhardness  $H_v = 4.9$  GPa, with a yield strength of 1841 MPa at 298 K and 298 MPa at 1273 K. The paper also compares the properties of these Al-containing alloys with the properties of their parent alloys, CrMo0.5NbTa0.5TiZr and HfNbTaTiZr, outlining the beneficial effects of Al additions on the microstructure and properties. Additionally, a thermodynamic calculation of the solidification and equilibrium phase diagrams was conducted, and the results were compared with experimental data. In the conclusion, the compositions of two earlier reported refractory alloys, HfNbTaTiZr and CrMo0.5NbTa0.5TiZr, were modified to produce Al0.4Hf0.6NbTaTiZr and AlMo0.5NbTa0.5TiZr alloys, and the effect of alloying with Al on their microstructure, composition, and mechanical properties was examined. Several beneficial effects from the Al additions were observed. Complete substitution of Cr with Al in the CrMo0.5NbTa0.5TiZr alloy reduced the alloy density by 10.1%, increased room temperature hardness and yield strength by approximately 12%, and notably improved room temperature ductility. Furthermore, the high-temperature strength was improved by more than 50% in the temperature range from 1073 K to 1473 K. These improvements in the mechanical properties were linked to significant changes in the phase composition and microstructure. While the CrMo0.5NbTa0.5TiZr alloy contained three relatively coarse phases (bcc1, bcc2, and Laves), the AlMo0.5NbTa0.5TiZr alloy only contained two disordered bcc phases, mainly in the form of a spinodal-like nano-lamellar structure, with no intermetallic phases present. Partial substitution of Hf with Al in the HfNbTaTiZr alloy reduced the alloy density by approximately 9%, and increased room temperature hardness and yield strength by 29% and 98%, respectively. However, the difference in yield strength between the HfNbTaTiZr and Al0.4Hf0.6NbTaTiZr alloys disappears with increasing temperature, and both alloys had the same properties at 1273 K and 1473 K. Both alloys had a single-phase bcc structure with an average grain size of approximately 140  $\mu$ m. Solidification and phase equilibrium conditions were calculated using the PanTi<sup>TM</sup> thermodynamic database. Although satisfactory agreement between experimentally observed phases and phases predicted after NE solidification was observed, the calculated equilibrium phase diagrams of the three alloys (AlMo0.5NbTa0.5TiZr, Al0.4Hf0.6NbTaTiZr, and CrMo0.5NbTa0.5TiZr) showed noticeable discrepancies with the experimentally

observed phase compositions. It was concluded that the current PanTi™ database, developed for Ti-rich alloys, cannot be directly applied to multi-principal-alloy compositions. A thermodynamic database that covers the full composition range for the Al–Cr–Hf–Mo–Nb–Ta–Ti–Zr system needs to be developed to accurately predict phase equilibria and guide the design of refractory HEAs based on this system.

11. The paper *Precipitation-Strengthened Refractory Al<sub>0.5</sub>CrNbTi<sub>2</sub>V<sub>0.5</sub> High Entropy Alloy* provides an abstract detailing the structure and mechanical properties of the Al<sub>0.5</sub>CrNbTi<sub>2</sub>V<sub>0.5</sub> high entropy alloy in both as-cast and annealed conditions (annealed at 1200°C for 24 hours). In the as-cast condition, the alloy has a single body-centered cubic (bcc) phase structure. After annealing, relatively fine and homogeneously distributed particles of Laves phase form in the bcc matrix. The precipitation of the second-phase particles results in an increase in yield strength but a decrease in ductility, as determined in compression at room temperature. When the testing temperature is increased to 1000°C, the alloy's strength decreases and ductility increases. The experimental phase composition of the alloy is compared with predicted equilibrium phases, and possible ways to tailor the structure of the alloy to further enhance its mechanical properties are discussed. In the conclusion, the structure and mechanical properties of the Al<sub>0.5</sub>CrNbTi<sub>2</sub>V<sub>0.5</sub> high entropy alloy were examined. In its initially as-cast condition, the alloy has a single bcc phase, and after annealing at 1200°C for 24 hours, relatively fine and homogeneously distributed C14 Laves phase particles precipitate. The precipitation of the Laves phase particles increases the room temperature compression yield strength of the alloy from 1240 MPa to 1340 MPa but reduces ductility. The yield strength of the annealed alloy decreases with an increase in testing temperature: 910 MPa at 600°C, 445 MPa at 800°C, and 90 MPa at 1000°C. A reasonable correlation between the experimental phase composition of the alloy and the predicted equilibrium phase diagram was established.
12. The paper *Structure and Mechanical Properties of the AlCr<sub>x</sub>NbTiV (x = 0, 0.5, 1, 1.5) High Entropy Alloys* provides an abstract detailing the production of AlCr<sub>x</sub>NbTiV alloys through vacuum arc melting and their structural, microstructural, density, and compression mechanical properties at temperatures ranging from 22°C to 1000°C, after homogenization annealing at 1200°C for 24 hours. Following homogenization, the AlNbTiV and AlCr<sub>0.5</sub>NbTiV alloys consist of a single bcc solid solution phase, while the AlCrNbTiV and AlCr<sub>1.5</sub>NbTiV alloys contain both bcc and hexagonal (C14) Laves phase, with respective amounts of 13% and 35%. The density of the alloys increases with Cr content, ranging from 5590 kg/m<sup>3</sup> for AlNbTiV to 5900 kg/m<sup>3</sup> for AlCr<sub>1.5</sub>NbTiV. The strength of the alloys increases with Cr concentration, with the yield strength of AlNbTiV and AlCr<sub>1.5</sub>NbTiV being 1000 MPa and 1700 MPa at room temperature, respectively, and 560 MPa and 970 MPa at 800°C. However, the strengthening effect is accompanied by a decrease in ductility. Deformation at 800°C and 1000°C results in the precipitation of second-phase particles, which are predominantly Nb<sub>2</sub>Al-type in the AlNbTiV and AlCr<sub>0.5</sub>NbTiV alloys, while the AlCrNbTiV and AlCr<sub>1.5</sub>NbTiV alloys exhibit additional Laves phase precipitates. The paper also compares the experimentally observed phase compositions with thermodynamic modeling of equilibrium phases in the alloys. In the conclusion, the

crystal structure, microstructure, density, and compression mechanical properties of the  $\text{AlCr}_x\text{NbTiV}$  ( $x = 0, 0.5, 1, 1.5$ ) alloys after homogenization annealing at  $1200^\circ\text{C}$  for 24 hours are examined. Several key points are highlighted: - The  $\text{AlNbTiV}$  and  $\text{AlCr0.5NbTiV}$  alloys are single-phase bcc solid solutions, while  $\text{AlCrNbTiV}$  and  $\text{AlCr1.5NbTiV}$  alloys contain 13% and 35% of hexagonal C14 Laves phase in the bcc matrix. - The density of the alloys increases with Cr concentration, with the measured densities being  $5590 \text{ kg/m}^3$ ,  $5710 \text{ kg/m}^3$ ,  $5820 \text{ kg/m}^3$ , and  $5900 \text{ kg/m}^3$  for  $\text{AlNbTiV}$ ,  $\text{AlCr0.5NbTiV}$ ,  $\text{AlCrNbTiV}$ , and  $\text{AlCr1.5NbTiV}$ , respectively. - The alloys show high compression strength up to  $800^\circ\text{C}$ , with yield strength increasing with Cr content. The compression yield strength of  $\text{AlNbTiV}$  and  $\text{AlCr1.5NbTiV}$  at room temperature is  $1000 \text{ MPa}$  and  $1700 \text{ MPa}$ , respectively, and at  $800^\circ\text{C}$ , they are  $560 \text{ MPa}$  and  $970 \text{ MPa}$ . - The ductility of the alloys decreases with increased Cr content at room temperature and  $600^\circ\text{C}$ . For example, the fracture strain of  $\text{AlNbTiV}$  and  $\text{AlCr1.5NbTiV}$  alloys at room temperature is 5.2% and 0%, respectively. - At  $800^\circ\text{C}$  and  $1000^\circ\text{C}$ , the alloys can be compressed to 50% strain without fracture. - After compression deformation at  $800^\circ\text{C}$  and  $1000^\circ\text{C}$ , second-phase precipitation is observed. In the  $\text{AlNbTiV}$  and  $\text{AlCr0.5NbTiV}$  alloys,  $\text{Nb}_2\text{Al}$ -type phases enriched with Nb and Al precipitate mostly on grain boundaries. In the  $\text{AlCrNbTiV}$  and  $\text{AlCr1.5NbTiV}$  alloys, hexagonal C14 Laves phase precipitates, with a higher volume fraction and particle sizes observed at  $1000^\circ\text{C}$ . - Thermodynamic modeling of equilibrium phases indicates the formation of a single-phase bcc structure after solidification. At lower temperatures, the formation of intermetallic phases is predicted, with aluminide phases in  $\text{AlNbTiV}$ , Laves phase in  $\text{AlCrNbTiV}$  and  $\text{AlCr1.5NbTiV}$  alloys, and both aluminide and Laves phases in  $\text{AlCrNbTiV}$ . The comparison with experimental data confirms correct trends but reveals inaccuracies in the prediction of crystal structures, chemical compositions, and volume fractions of phases.

13. The paper *Microstructure and Mechanical Properties at Elevated Temperatures of a New Al-Containing Refractory High-Entropy Alloy Nb-Mo-Cr-Ti-Al* provides an abstract detailing the casting, homogenization, and deformation behavior of the new Al-containing refractory high-entropy alloy Nb-Mo-Cr-Ti-Al. The alloy shows a dendritic microstructure after arc melting, which completely dissolves after a heat treatment at  $1300^\circ\text{C}$  for 20 hours. X-ray diffraction (XRD) and electron backscatter diffraction (EBSD) confirm a major phase in the form of a solid solution with a W prototype structure, while additional phases of small volume fraction appear within the grains and at the grain boundaries. Quasistatic compression tests, performed between room temperature and  $1200^\circ\text{C}$ , reveal sustained high yield strength up to  $800^\circ\text{C}$  and increasing ductility with increasing temperature. The dominant deformation mechanism for quasistatic compression between  $800^\circ\text{C}$  and  $1200^\circ\text{C}$  is the  $\langle 111 \rangle$  pencil glide of dislocations within the solid solution, as proven by the fiber texture components evolving during deformation. The conclusion of the study provides the following main results regarding the microstructure and deformation behavior at elevated temperatures of the Nb-Mo-Cr-Ti-Al high-entropy alloy. The analysis of the microstructure of arc-melted Nb-Mo-Cr-Ti-Al, after homogenization treatments, reveals that the dendritic-like as-cast microstructure transforms into an equiaxed microstructure with minor secondary phases upon annealing at  $1300^\circ\text{C}$  under an argon atmosphere for 20 hours. The formation of the hexagonal modification of the  $\text{Cr}_2\text{Nb}$  Laves phase is suppressed by a homogenization temperature of  $1300^\circ\text{C}$  and above.



Compression tests show a maximum strength of  $\approx 1$  GPa and increasing ductility up to a plastic strain of 24% as the test temperature increases to 1200°C. During compression testing at 1000°C and 1200°C, secondary phases form and coarsen, respectively. The analysis of fiber texture components after uniaxial compression testing at elevated temperatures suggests that Nb-Mo-Cr-Ti-Al deforms by dislocation slip, forming common combined fiber texture components along the compression direction. These components can be explained by the orientation change during slip deformation on slip systems with a common slip direction.

14. The paper *Contribution of Lattice Distortion to Solid Solution Strengthening in a Series of Refractory High Entropy Alloys* provides an abstract which presents an experimental approach for revealing the impact of lattice distortion on solid solution strengthening in a series of body-centered-cubic (bcc) Al-containing, refractory high entropy alloys (HEAs) from the Nb-Mo-Cr-Ti-Al system. By systematically varying the Nb and Cr content, a wide range of atomic size difference, a common measure for lattice distortion, was obtained. Single-phase, bcc solid solutions were achieved by arc melting and homogenization, which were verified using scanning electron microscopy and X-ray diffraction. The atomic radii of the alloying elements for determining atomic size difference were recalculated based on the mean atomic radii and chemical compositions of the solid solutions. Microhardness ( $\mu\text{H}$ ) at room temperature correlated well with the deduced atomic size difference. Nevertheless, the mechanisms of microscopic slip lead to a pronounced temperature dependence of mechanical strength. To account for this feature, a combined approach using  $\mu\text{H}$ , nanoindentation, and compression tests was presented. The athermal proportion to the yield stress of the investigated equimolar alloys was revealed. These parameters support the universality of this correlation. Therefore, the pertinence of lattice distortion for solid solution strengthening in bcc HEAs is proven. The conclusion of the study provides the following results: with almost single-phase microstructure, dislocation-mediated plasticity with Burgers vectors, and varying atomic size differences between 3.25 and 5.15 pct, NbMoCrTiAl and its derivatives are well suited for investigating the impact of lattice distortion on solid solution strengthening in concentrated bcc alloys. A correlation between the atomic size difference  $\delta$  and RT microhardness  $\mu\text{HRT}$ , namely,  $\mu\text{HRT} = 1.52 \text{ GPa} + 101.56 \text{ GPa} \cdot \delta$ , was found for a series of Nb-Mo-Cr-Ti-Al alloys, including two quaternary and one quinary, equimolar composition. The following conclusions can be drawn: Bcc solid solutions were stabilized by appropriate heat treatments in all investigated alloys, and competing phases were suppressed when gradually reducing the concentration of Nb and Cr. Individual atomic radii of the alloying elements were determined by evaluating the experimentally observed mean atomic radii of all the investigated alloys. Although  $\mu\text{HRT}$  reasonably correlates with the atomic size difference  $\delta$ , the magnitude of  $\mu\text{HRT}$  is altered by the well-known feature of thermally activated dislocation slip in bcc metals and solid solutions. Thus, combined temperature-dependent mechanical characterization through both nanoindentation and compression tests was used to exemplarily assess the athermal strength of the equimolar alloys. Both  $y_{\text{plateau}}$  and  $n\text{H}_{\text{plateau}}$  further support the correlation with  $\delta$  found for  $\mu\text{HRT}$ . The variation of shear moduli remains small within the composition range of the investigated alloys and cannot account for the observed dependence of the hardness of the alloys.

15. The paper *Development of a Refractory High Entropy Superalloy* provides abstract on the microstructure, phase composition, and mechanical properties of a refractory high entropy superalloy, AlMo0.5NbTa0.5TiZr. The alloy consists of a nano-scale mixture of two phases produced by the decomposition from a high-temperature body-centered cubic (BCC) phase. The first phase is present in the form of cuboidal-shaped nano-precipitates aligned in rows along  $\langle 100 \rangle$ -type directions, has a disordered BCC crystal structure with the lattice parameter  $a_1 = 326.9 \pm 0.5$  pm, and is rich in Mo, Nb, and Ta. The second phase is present in the form of channels between the cuboidal nano-precipitates, has an ordered B2 crystal structure with the lattice parameter  $a_2 = 330.4 \pm 0.5$  pm, and is rich in Al, Ti, and Zr. Both phases are coherent and have the same crystallographic orientation within the former grains. The formation of this modulated nano-phase structure is discussed in the framework of nucleation-and-growth and spinodal decomposition mechanisms. The yield strength of this refractory high entropy superalloy is superior to the yield strength of Ni-based superalloys in the temperature range of 20 °C to 1200 °C. The conclusion of the study states that the microstructure and mechanical properties of the refractory high entropy superalloy, AlMo0.5NbTa0.5TiZr, are reported. After annealing at 1400 °C and slow cooling to room temperature, the superalloy microstructure consists of cuboidal nano-precipitates with a disordered BCC crystal structure and two types of thin and large channels or gaps of an ordered B2 phase between these precipitates. The average edge length and volume fraction of the cuboidal precipitates are  $\sim 30$  nm and  $62 \pm 5\%$ , respectively, and the average thickness of the thin channels is  $\sim 7$  nm. The disordered BCC precipitates are rich in Mo, Nb, and Ta, and its lattice parameter is  $a_1 = 326.9$  pm. The ordered B2 phase is rich in Al, Ti, and Zr, and its lattice parameter is  $a_2 = 330.4$  pm. Both phases are coherent and have the same crystallographic orientation inside former grains of a high-temperature phase. The small lattice mismatch (1.07%) between the phases is likely responsible for the specific morphology and high thermal stability of this nano-phase structure. The superalloy has exceptionally high yield strength, which is superior to the strength of Ni superalloys in the temperature range of 20 °C to 1200 °C. It is suggested that the two-phase, BCC/B2 nano-structure is responsible for the high strength and hardness of the AlMo0.5NbTa0.5TiZr superalloy.
16. The paper *Structure and Mechanical Properties of a Light-Weight AlNbTiV High Entropy Alloy* examines the crystal structure, microstructure, density, microhardness, and mechanical properties of a new AlNbTiV high entropy alloy. The alloy had a coarse-grained single bcc phase structure with a density of 5.59 g cm<sup>-3</sup> and hardness ranging from 4315 to 4394 MPa. The compressive yield strength of the alloy gradually decreased from 1020 MPa at room temperature to 685 MPa at 800 °C, and then dropped to 158 MPa at 1000 °C. The specific yield strength of the alloy was found to be comparable with the strength of multiphase refractory high entropy alloys. The effect of chemical composition on mechanical properties and potential ways to optimize the composition are discussed. The conclusion of the study states that the structure, density, and mechanical properties of the novel AlNbTiV high entropy alloy were examined. The alloy had a single bcc phase coarse-grained structure and low density of 5.59 g cm<sup>-3</sup> after homogenization. The compressive yield strength of the alloy gradually decreased from 1020 MPa at room temperature to 685 MPa at 800 °C, and then dropped

to 158 MPa at 1000 °C. A comparison between the specific strengths of the AlNbTiV alloy and previously reported multiphase refractory HEAs has demonstrated no significant difference. The high compressive strength was attributed to the effect of Al. Potential ways to optimize the composition of the alloy are proposed.

17. The paper *Structure and Mechanical Properties of a B2 Ordered Refractory AlNbTiVZrx (x = 0–1.5) High-Entropy Alloys* investigates the structure and mechanical properties of AlNbTiVZrx alloys after arc melting and annealing at 1200 °C for 24 hours. The AlNbTiV alloy had a B2 ordered single-phase structure. Alloying with Zr resulted in (i) a change in the degree of order of the B2 phase, and (ii) the precipitation of Zr<sub>5</sub>Al<sub>3</sub> and C14 Laves ZrAlV phases. The density of the AlNbTiVZrx alloys varied from 5590 kg m<sup>-3</sup> for the AlNbTiV alloy to 5870 kg m<sup>-3</sup> for the AlNbTiVZr1.5 alloy. The compression yield strength at 22 °C increased with an increase in the Zr content from 1000 MPa for the AlNbTiV alloy to 1535 MPa for the AlNbTiVZr1.5 alloy. The plasticity raised from 6% for the AlNbTiV alloy to >50% for the AlNbTiVZr0.5 alloy and then dropped to 0.4% for the AlNbTiVZr1.5 alloy. At 600 °C, the strongest alloy was also the AlNbTiVZr1.5, while at 800 °C, the AlNbTiVZr0.1 alloy demonstrated the maximum strength. The plasticity of the AlNbTiV alloy at 600 °C increased up to 14.3%, while the Zr-containing alloys had lower plasticity. At 800 °C, all the AlNbTiVZrx alloys could be plastically deformed up to 50% of strain without fracture. The ordering in the alloys and the reasons for the complicated dependence of the mechanical properties of the AlNbTiVZrx alloys on the Zr content and temperature were discussed. The conclusion of the study states that the structure and mechanical properties of the AlNbTiVZrx (x = 0; 0.1; 0.25; 0.5; 1; 1.5) refractory high-entropy alloys after annealing at 1200 °C for 24 hours were examined. The AlNbTiV alloy possessed the single-phase ordered B2 structure. The AlNbTiVZrx (x = 0.1; 0.25) alloys were composed of the B2 and hexagonal Zr<sub>5</sub>Al<sub>3</sub>-type phases. The phase composition of the AlNbTiVZrx (x = 0.5; 1; 1.5) alloys was presented by the B2 phase, Zr<sub>5</sub>Al<sub>3</sub>-type phase, and hexagonal C14 Laves phase of ZrAlV-type. The volume fraction of the second phases increased with an increase in the Zr content from <1% for the AlNbTiVZr0.1 alloy to 50% for the AlNbTiVZr1.5 alloy. The long-range order parameter (LROP) of the B2 phase was found to depend on the Zr content. The LROP reduced with an increase in the Zr content from 0.71 for the AlNbTiV alloy to 0.37 for the AlNbTiVZr1.5 alloy. Zr resulted in a gradual increase in the density of the alloys from 5590 kg m<sup>-3</sup> for the AlNbTiV alloy to 5870 kg m<sup>-3</sup> for the AlNbTiVZr1.5 alloy. The strength of the AlNbTiVZrx alloys changed significantly with an increase in the Zr content. The values of the yield strength at 22 °C raised rapidly from 1000 MPa for the AlNbTiV alloy to 1485 MPa for the AlNbTiVZr0.5 alloy, and from 780 MPa to 1135 MPa for the respective alloys at 600 °C. The strength increment at 22 and 600 °C was associated with solid solution strengthening (SSS). Further increase in the Zr content did not result in a pronounced enhancement of strength: the yield strength of the AlNbTiVZr1.5 alloy was 1535 MPa at 22 °C and 1195 MPa at 600 °C, respectively. At 800 °C, the maximum strength was demonstrated by the AlNbTiVZr0.1 alloy, whereas the AlNbTiVZr1.5 alloy was the softest. A decrease in strength of the AlNbTiVZrx alloys at 800 °C with an increase in the Zr content was associated with a lowering of the LROP of the B2 phase and a large fraction of the soft second phase particles. The plasticity of the AlNbTiVZrx alloys had a complex dependence on the Zr content. At 22 °C, the plasticity increased from 6% for the AlNbTiV alloy to >50% for the

AlNbTiVZr0.5 alloy. The plasticity enhancement was associated with a reduction of the LROP of the B2 phase. The plasticity then dropped to 0.4% for the AlNbTiVZr1.5 alloy, supposedly due to the presence of a large volume fraction of the intermetallic second phases. At 600 °C, the plasticity of the AlNbTiV alloy increased up to 14.3%, while the Zr-containing alloys had lower plasticity. At 800 °C, all the AlNbTiVZrx alloys were plastically deformed up to 50% of strain without fracture. After compression tests of the AlNbTiVZr0.5 alloy at 22 °C to 50% of height reduction, the initial B2 ordered matrix phase was found to be transformed into disordered bcc, i.e., plastic deformation of the alloy results in the B2-to-bcc transition.

18. The paper *Microstructure and Mechanical Properties of In-Situ MC-Carbide Particulates-Reinforced Refractory High-Entropy Mo0.5NbHf0.5ZrTi Matrix Alloy Composite* investigates the preparation and properties of the Mo0.5NbHf0.5ZrTi alloy matrix composite, reinforced with MC-carbide particulates, using arc melting. The Mo0.5NbHf0.5ZrTiC0.1 and Mo0.5NbHf0.5ZrTiC0.3 alloys consist of one disordered body-centered cubic (BCC) solid solution phase as the matrix phase and MC carbide phase. The MC carbide is enriched with Zr and Hf due to the higher binding strength and contains no Mo. Noticeable strengthening from the carbide is not observed for C0.1 and C0.3 alloys, although the compressive plasticity is slightly improved due to the decrease of solution strengthening for the matrix BCC disordered solid solution phase. In summary, carbon elements with molar ratios of 0.1 and 0.3 are added into the refractory high-entropy alloy Mo0.5NbHf0.5ZrTi to prepare the in-situ MC-carbide ceramic particulates-reinforced Mo0.5NbHf0.5ZrTi matrix composite by arc melting successfully. The Mo0.5NbHf0.5ZrTiC0.1 and Mo0.5NbHf0.5ZrTiC0.3 alloys are composed of a BCC solid solution phase and a particulates-reinforced phase, MC-carbide. The MC carbide, with an FCC crystal structure, is enriched with Zr and Hf, containing a small amount of Nb and Ti. Both the compressive strength and plasticity of Mo0.5NbHf0.5ZrTiC0.1 and Mo0.5NbHf0.5ZrTiC0.3 alloys are improved compared to the master alloy Mo0.5NbHf0.5ZrTi.
  
19. The paper *Microstructure and Mechanical Properties of a Refractory CoCrMoNbTi High-Entropy Alloy* investigates a new refractory high-entropy alloy in the Co-Cr-Mo-Nb-Ti system as a candidate material for high-temperature structural applications. CoCrMoNbTi x (x values in terms of molar ratios, x = 0, 0.2, 0.4, 0.5, and 1.0) alloys were prepared by vacuum arc melting. The effects of variations in the Ti content on the phase constituents, microstructure, and mechanical properties of the alloys were examined using x-ray diffractometry, scanning electron microscopy equipped with energy-dispersive x-ray spectroscopy, and compressive testing. The results showed that the CoCrMoNbTi0.4 alloy possessed a typical cast dendritic microstructure consisting of a single body-centered cubic (BCC) solid solution. Laves phases (Cr2Nb and Co2Ti) were formed in other alloys with different Ti contents. The results were discussed in terms of the mixing enthalpy, atomic size difference, electronegativity difference, and valence electron concentrations among the elements within the alloys. The alloy hardness exhibited a slightly decreasing trend as the Ti content increased, resulting from the coarser microstructure and reduced amount of Laves phases. Augmented Ti content increased the compressive strength but decreased the ductility. Particularly, for the

CoCrMoNbTi0.2 alloy, the hardness, compressive strength, and fracture strain were as high as 916.46 HV0.5, 1906 MPa, and 5.07%, respectively. The solid solution strengthening of the BCC matrix and the formation of hard Laves phases were the two main factors contributing to alloy strengthening. In this study, by applying the strategy of equiatomic ratios and high entropies of mixing, Ti content additions into the Co-Cr-Mo-Nb-Ti alloys are proposed as a family of candidate materials for high-temperature structural applications. The CoCrMoNb-Ti  $x$  alloy series ( $x$  values in terms of the molar ratio,  $x = 0, 0.2, 0.4, 0.5$ , and  $1.0$ ) exhibited a relatively simple microstructure and promising properties. (1) The microstructures of all studied alloys, with the exception of the CoCrMoNbTi0.4 alloy, exhibited a typical dendritic structure, corresponding to the majority BCC solid solution and other Laves phases (Cr<sub>2</sub>Nb and/or Co<sub>2</sub>Ti). The Ti0.4 alloy is composed of only a single BCC phase. (2) Mo and Nb were enriched in the coarse dendritic regions, whereas Co and Cr were distributed in the inter-dendritic regions, and Ti was uniformly distributed throughout both regions. (3) The hardnesses of the alloys decreased slightly as the Ti content increased. The Ti0 alloys exhibited the highest hardnesses up to 959.62 HV0.5. This feature is ascribed to the coarser microstructure and reduced amount of Laves phase. (4) Augmented Ti content increased the compressive strength but decreased the ductility. The Ti0.2 alloy exhibited a compressive strength of 1906 MPa and a fracture strain of 5.07%. The solid solution strengthening of the BCC matrix and the formation of hard Laves phases are the two main factors contributing to alloy strengthening. (5) This work provides some guidance for the further development of current ideas to obtain refractory high-temperature structural materials. Further studies are being carried out to investigate the phase stability and high-temperature mechanical properties of the alloy.

20. The paper *Experimental and Theoretical Study of Ti<sub>20</sub>Zr<sub>20</sub>Hf<sub>20</sub>Nb<sub>20</sub>X<sub>20</sub> (X = V or Cr) Refractory High-Entropy Alloys* investigates the microstructure and mechanical properties of Ti<sub>20</sub>Zr<sub>20</sub>Hf<sub>20</sub>Nb<sub>20</sub>X<sub>20</sub> (X = V or Cr) high-entropy alloys (HEA), produced by induction melting and casting in an inert atmosphere. The structures of these alloys were studied via X-ray diffractometry and scanning electron microscopy. Results show that Ti<sub>20</sub>Zr<sub>20</sub>Hf<sub>20</sub>Nb<sub>20</sub>V<sub>20</sub> has mainly the body-centered cubic (BCC) structure, whereas the BCC matrix of Ti<sub>20</sub>Zr<sub>20</sub>Hf<sub>20</sub>Nb<sub>20</sub>Cr<sub>20</sub> contains a small amount of Cr<sub>2</sub>Nb and Cr<sub>2</sub>Hf intermetallic compounds. Ti<sub>20</sub>Zr<sub>20</sub>Hf<sub>20</sub>Nb<sub>20</sub>V<sub>20</sub> alloy shows high strength and homogeneous deformation under compression at room temperature. The strength and hardness of Ti<sub>20</sub>Zr<sub>20</sub>Hf<sub>20</sub>Nb<sub>20</sub>Cr<sub>20</sub> alloy are further enhanced by the Cr-containing Laves phases segregated during casting. The structural and mechanical properties remained almost unchanged after a short time (10 min) heat treatment at 573, 773, 973, and 1173 K, indicating resistance to working temperature peaks for these two alloys. Ab initio calculations predict ductile behavior for these and similar refractory HEAs. The theoretically calculated Young's modulus  $E$  is in good agreement with the experimental ones. The conclusion stated Two new refractory high-entropy alloys, Ti<sub>20</sub>Zr<sub>20</sub>Hf<sub>20</sub>Nb<sub>20</sub>V<sub>20</sub> and Ti<sub>20</sub>Zr<sub>20</sub>Hf<sub>20</sub>Nb<sub>20</sub>Cr<sub>20</sub>, were produced by induction melting and casting. The Ti<sub>20</sub>Zr<sub>20</sub>Hf<sub>20</sub>Nb<sub>20</sub>V<sub>20</sub> has a BCC + unknown intermetallic phase structure, while the Ti<sub>20</sub>Zr<sub>20</sub>Hf<sub>20</sub>Nb<sub>20</sub>Cr<sub>20</sub> alloy forms the Cr<sub>2</sub>Nb and Cr<sub>2</sub>Hf intermetallic compounds between the BCC phase particles. A single BCC phase was formed in the Ti<sub>20</sub>Zr<sub>20</sub>Hf<sub>20</sub>Nb<sub>20</sub>V<sub>20</sub> alloy as a result of annealing at 573, 773, and 973 K, whereas a V<sub>2</sub>Hf phase precipitated from the BCC phase at 1173 K. For both alloys, almost no changes were observed in the Vickers microhardness before

and after annealing. The Ti<sub>20</sub>Zr<sub>20</sub>Hf<sub>20</sub>Nb<sub>20</sub>V<sub>20</sub> and Ti<sub>20</sub>Zr<sub>20</sub>Hf<sub>20</sub>Nb<sub>20</sub>Cr<sub>20</sub> as-cast alloys have high compression yield strength  $\sigma_y$  values of 1170 and 1375 MPa, respectively, at room temperature. The Ti<sub>20</sub>Zr<sub>20</sub>Hf<sub>20</sub>Nb<sub>20</sub>V<sub>20</sub> alloy shows considerable strengthening and homogeneous deformation. Replacement of V with Cr produced strengthening of the alloy due to Laves phase precipitation in the BCC matrix. Our experiments and ab initio calculations indicate that these alloys are relatively ductile. The Ti<sub>20</sub>Zr<sub>20</sub>Hf<sub>20</sub>Nb<sub>20</sub>X<sub>20</sub> (X = V or Cr) alloys show a large elastic and plastic strain limits while the BCC phase is stable against heating for 600 s up to 1173 K.

21. The paper *Microstructure and Properties of a Refractory NbCrMo<sub>0.5</sub>Ta<sub>0.5</sub>TiZr Alloy* investigates the new refractory alloy, Nb<sub>20</sub>Cr<sub>20</sub>Mo<sub>10</sub>Ta<sub>10</sub>Ti<sub>20</sub>Zr<sub>20</sub>, produced by vacuum arc melting. To close shrinkage porosity, it was hot isostatically pressed (HIPd) at  $T = 1723$  K and  $P = 207$  MPa for 3 hours. In both as-solidified and HIPd conditions, the alloy contained three phases: two body-centered cubic (BCC1 and BCC2) and one face-centered cubic (FCC). The BCC1 phase was enriched with Nb, Mo, and Ta and depleted with Zr and Cr, and its lattice parameter after HIP was  $a = 324.76 \pm 0.16$  pm. The BCC2 phase was enriched with Zr and Ti and considerably depleted with Mo, Cr, and Ta, and its lattice parameter after HIP was estimated to be  $a = 341.0 \pm 1.0$  pm. The FCC phase was highly enriched with Cr, and it was identified as a Laves C15 phase, (Zr,Ta)(Cr,Mo,Nb)<sub>2</sub>, with the lattice parameter  $a = 733.38 \pm 0.18$  pm. The volume fractions of the BCC1, BCC2, and FCC phases were 67%, 16%, and 17%, respectively. The alloy density and Vickers microhardness were  $\rho = 8.23 \pm 0.01$  g/cm<sup>3</sup> and  $H_v = 5288 \pm 71$  MPa. The alloy had compression yield strength of 1595 MPa at 296 K, 983 MPa at 1073 K, 546 MPa at 1273 K, and 171 MPa at 1473 K. During deformation at 296 K and 1073 K, the alloy showed a mixture of ductile and brittle fracture after plastic compression strain of ~5–6%. No macroscopic fracture was observed after 50% compression strain at 1273 K and 1473 K. Phase transformations and particle coarsening considerably accelerated by the plastic deformation occurred in the temperature range of 1073–1473 K. In conclusion a new refractory alloy, NbCrMo<sub>0.5</sub>Ta<sub>0.5</sub>Ti<sub>20</sub>Zr<sub>20</sub>, was produced and its crystal structure, microstructure, density, hardness, and compression properties were determined in the as-solidified and HIPd condition. The alloy consisted of two disordered BCC1 and BCC2 phases and one ordered FCC (Laves C15) phase. After HIP at 1723 K, 207 MPa for 3 hours, the BCC1 phase was present in the form of large individual particles, which were surrounded by the BCC2 phase. Smaller particles of the Laves phase were present inside the BCC2 phase. The volume fractions of the BCC1, BCC2, and FCC phases were 67%, 16%, and 17%, respectively. The HIPd alloy density was  $\rho = 8.23$  g/cm<sup>3</sup> and the Vickers microhardness was  $H_v = 5.29$  GPa. The alloy showed high yield strengths of  $\sigma_{0.2} = 1595$  MPa, 983 MPa, 546 MPa, and 170 MPa at 293 K, 1073 K, 1273 K, and 1473 K, respectively. Ductile-type fracture occurred after ~5–6% compression strain at 293 K and 1073 K. Brittle Laves particles were responsible for the fracture at these temperatures. No fracture occurred during compression testing at 1273 K and 1473 K.

22. The paper *Mechanical Properties of Low-Density, Refractory Multi-Principal Element Alloys of the Cr–Nb–Ti–V–Zr System* reports on the room temperature and elevated temperature mechanical properties of four multi-principal element alloys, NbTiVZr, NbTiV2Zr, CrNbTiZr, and CrNbTiVZr. The alloys were prepared by vacuum arc melting followed by hot isostatic pressing and homogenization. Disordered BCC solid solution phases are the major phases in these alloys. The Cr-containing alloys additionally contain an ordered FCC Laves phase. The NbTiVZr and NbTiV2Zr alloys showed good compressive ductility at all studied temperatures, while the Cr-containing alloys showed brittle-to-ductile transition occurring somewhere between 298 and 873 K. Strong work hardening was observed in the NbTiVZr and NbTiV2Zr alloys during deformation at room temperature. The alloys had yield strengths of 1105 MPa and 918 MPa, respectively, and their strength continuously increased, exceeding 2000 MPa after ~40% compression strain. The CrNbTiZr and CrNbTiVZr alloys showed high yield strength (1260 MPa and 1298 MPa, respectively) but low ductility (6% and 3% compression strain) at room temperature. Strain softening and steady-state flow were typical during compression deformation of these alloys at temperatures above 873 K. In these conditions, the alloys survived 50% compression strain without fracture, and their yield strength continuously decreased with an increase in temperature. During deformation at 1273 K, the NbTiVZr, NbTiV2Zr, CrNbTiZr, and CrNbTiVZr alloys showed yield strengths of 58 MPa, 72 MPa, 115 MPa, and 259 MPa, respectively. It discusses a new alloy development strategy based on stabilizing the solid solution of four or more principal elements has been used to produce four new alloys. Properties of these materials were measured using compression tests in order to assess which alloys warrant further study. New refractory multi-principal element alloys, NbTiVZr, NbTiV2Zr, CrNbTiZr, and CrNbTiVZr, have densities of 6.52, 6.34, 6.67, and 6.57 g/cm<sup>3</sup>, respectively. After homogenization at 1473 K for 24 hours and slow cooling at a rate of 10 K/min, the NbTiVZr is essentially a single-phase BCC crystal structure with small amounts of submicron-sized particles precipitated at grain boundaries and dislocations. The composition of the BCC phase is close to the composition of the alloy. The NbTiV2Zr contains three disordered BCC phases, one of which has the composition close to the composition of the alloy, another is enriched with Zr, and the third is enriched with V. The CrNbTiZr and CrNbTiVZr alloys consist of a disordered BCC phase and an ordered Laves phase, with the volume fraction of the latter being 35% and 61%, respectively. The Laves phase is rich in Cr in CrNbTiZr and with Cr and V in CrNbTiVZr, while the BCC phase is enriched with Nb and Ti in both Cr-containing alloys. The compression properties of the NbTiVZr, NbTiV2Zr, CrNbTiZr, and CrNbTiVZr alloys were determined in the temperature range from 298 K to 1273 K. The NbTiVZr and NbTiV2Zr alloys showed good compressive ductility at all studied temperatures, while the Cr-containing alloys showed brittle-to-ductile transition occurring somewhere between RT and 873 K. Strong work hardening was observed in the NbTiVZr and NbTiV2Zr alloys during deformation at room temperature. The alloys had yield strengths of 1105 MPa and 918 MPa, respectively, and their strength continuously increased, exceeding 2000 MPa after ~40% compression strain. The CrNbTiZr and CrNbTiVZr alloys showed high yield strength (1260 MPa and 1298 MPa, respectively) but low ductility (6% and 3% compression strain, respectively, before fracture) at room temperature. Cleavage fracture of Laves phase particles and ductile fracture of the BCC phase was observed in these alloys. The fracture of these alloys was associated with extensive material fragmentation and local heating beyond the melting temperature. Strain softening and steady-state flow were typical during compression deformation of these alloys at temperatures above 873 K. In these

conditions, the alloys survived 50% compression strain without fracture and their yield strength continuously decreased with an increase in temperature. During deformation at 1273 K, the NbTiVZr, NbTiV2Zr, CrNbTiZr, and CrNbTiVZr alloys showed yield strengths of 58 MPa, 72 MPa, 115 MPa, and 259 MPa, respectively. During deformation at 1273 K, the NbTiVZr and NbTiV2Zr alloys had a single-phase BCC structure. After deformation at 1273 K followed by cooling to room temperature, the phase compositions of the NbTiVZr and NbTiV2Zr alloys noticeably changed relative to the respective homogenized conditions. In addition to the matrix phase, two additional BCC phases were observed in NbTiVZr, predominantly inside the deformation bands. In NbTiV2Zr, the volume fraction of one of the three BCC phases observed after homogenization treatment considerably reduced after deformation. It is suggested that the high density of dislocations and subgrain boundaries in the deformed alloys facilitates transformation of the high-temperature BCC phase into the low-temperature BCC phase during cooling after deformation. The results indicate that the phases present in these two alloys at room temperature are likely metastable phases, which are quenched from higher temperatures due to slow diffusion kinetics of the alloying elements. During deformation at 1273 K, the CrNbTiZr and CrNbTiVZr alloys retained their two-phase (BCC plus Laves) structure, and their phase compositions were unaffected by deformation. The high-temperature deformation resulted in the formation of new recrystallized grains inside the BCC phase and deformation twins inside large Laves-phase particles. The CrNbTiVZr alloy showed the most attractive properties, such as considerably improved elevated temperature strength, reduced density, and much higher melting point, as compared to three other high-entropy alloys and referenced Ni superalloys (In718 and Haynes 230). A microstructural approach to improve the limited room temperature ductility is suggested via dissolution and controlled precipitation of the strengthening Laves phase.

23. The paper *The Effect of Ti on the Sintering and Mechanical Properties of Refractory High-Entropy Alloy TixWTaVCr Fabricated via Spark Plasma Sintering for Fusion Plasma-Facing Materials* presents the synthesis and characterization of TixWTaVCr alloys for high-temperature and fusion plasma-facing applications. Specimens of TixWTaVCr containing 0 to 7 at% Ti were prepared via spark plasma sintering of an elemental powder mixture at 1500 °C. Characterization of sintered samples via X-ray diffraction and scanning electron microscopy with energy dispersive spectroscopy revealed increased formation of a BCC solid solution due to the addition of up to 7 at% Ti. Mechanical characterizations of the TixWTaVCr alloys indicate that they are harder and stronger than several reported high-entropy alloys. The alloy that contained 7 at% Ti also exhibited improved oxidation resistance in air at 1000 °C. Its improved strength, hardness, and oxidation resistance suggest future applications for this high-entropy alloy in high-temperature and nuclear applications. It concludes the effect of Ti on the sintering and properties of TixWTaVCr has been explored. Adding 7 at% Ti helped form solid solutions in the majority of the sample via enhanced diffusion. The room temperature and high-temperature compressive yield strengths of the BCC alloy TixWTaVCr (x = 7 at%) were higher than those of pure W and several other refractory, HEAs owing to solid solution strengthening and the effects of Cr and V. Improved oxidation resistance was observed at 1000 °C owing to the formation of thinner non-volatile oxide layers (from ~1.16 mm (0Ti) to ~0.22 mm (7Ti)). The improved



mechanical and oxidation properties of  $\text{Ti}_{10}\text{W}_2\text{Ta}_2\text{V}_2\text{Cr}$  indicate the potential for future use in fusion applications.

24. The paper *Plastic Deformation Properties of Zr–Nb–Ti–Ta–Hf High-Entropy Alloys* investigates the plastic deformation properties of single-phase Zr–Nb–Ti–Ta–Hf high-entropy alloys from room temperature (RT) up to 300 °C. Uniaxial deformation tests at a constant strain rate of  $10^{-4} \text{ s}^{-1}$  were performed, including incremental tests such as stress relaxations, strain-rate changes, and temperature changes in order to determine the thermodynamic activation parameters of the deformation process. The microstructure of deformed samples was characterized by transmission electron microscopy. The strength of the investigated Zr–Nb–Ti–Ta–Hf phase is not as high as the values frequently reported for high-entropy alloys in other systems. At RT, we measure a flow stress of about 850 MPa. We find an activation enthalpy of about 1 eV and a stress-dependent activation volume between 0.5 and 2 nm<sup>3</sup>. The measurement of the activation parameters at higher temperatures is affected by structural changes evolving in the material during plastic deformation. To the Conclusion a new alloy development strategy based on stabilizing the solid solution of four or more principal elements has been used to produce four new alloys. Properties of these materials were measured using compression tests in order to assess which alloys warrant further study. New refractory multi-principal element alloys, NbTiVZr, NbTiV<sub>2</sub>Zr, CrNbTiZr, and CrNbTiVZr, have densities of 6.52, 6.34, 6.67, and 6.57 g/cm<sup>3</sup>, respectively. After homogenization at 1473 K for 24 h and slow cooling at a rate of 10 K/min, the NbTiVZr is essentially single-phase BCC crystal structure with a small amount of submicron-sized particles precipitated at grain boundaries and dislocations. The composition of the BCC phase is close to the composition of the alloy. The NbTiV<sub>2</sub>Zr contains three disordered BCC phases, one of which has the composition close to the composition of the alloy, another is enriched with Zr, and the third is enriched with V. The CrNbTiZr and CrNbTiVZr alloys consist of a disordered BCC phase and an ordered Laves phase, with the volume fraction of the latter of 35% and 61%, respectively. The Laves phase is rich with Cr in CrNbTiZr and with Cr and V in CrNbTiVZr, while the BCC phase is enriched with Nb and Ti in both Cr-containing alloys. The compression properties of the NbTiVZr, NbTiV<sub>2</sub>Zr, CrNbTiZr, and CrNbTiVZr alloys were determined in the temperature range from 298 K to 1273 K. The NbTiVZr and NbTiV<sub>2</sub>Zr alloys showed good compressive ductility at all studied temperatures, while the Cr-containing alloys showed brittle-to-ductile transition occurring somewhere between RT and 873 K. Strong work hardening was observed in the NbTiVZr and NbTiV<sub>2</sub>Zr alloys during deformation at room temperature. The alloys had yield strengths of 1105 MPa and 918 MPa, respectively, and their strength continuously increased, exceeding 2000 MPa after ~40% compression strain. The CrNbTiZr and CrNbTiVZr alloys showed high yield strength (1260 MPa and 1298 MPa, respectively) but low ductility (6% and 3% compression strain, respectively, before the fracture) at room temperature. Cleavage fracture of Laves phase particles and ductile fracture of the BCC phase was observed in these alloys. The fracture of these alloys was associated with extensive material fragmentation and local heating beyond the melting temperature. Strain softening and steady-state flow were typical during compression deformation of these alloys at temperatures above 873 K. In these conditions, the alloys survived 50% compression strain without fracture, and their yield strength continuously decreased with an increase in temperature. During deformation at 1273 K, the NbTiVZr, NbTiV<sub>2</sub>Zr, CrNbTiZr,

and CrNbTiVZr alloys showed yield strengths of 58 MPa, 72 MPa, 115 MPa, and 259 MPa, respectively. During deformation at 1273 K, the NbTiVZr and NbTiV2Zr alloys had a single-phase BCC structure. After deformation at 1273 K followed by cooling to room temperature, the phase compositions of the NbTiVZr and NbTiV2Zr alloys noticeably changed relative to the respective homogenized conditions. In addition to the matrix phase, two additional BCC phases were observed in NbTiVZr, predominantly inside the deformation bands. In NbTiV2Zr, the volume fraction of one of the three BCC phases observed after homogenization treatment considerably reduced after deformation. It is suggested that the high density of dislocations and subgrain boundaries in the deformed alloys facilitates transformation of the high-temperature BCC phase into the low-temperature BCC phase during cooling after deformation. The results indicate that the phases present in these two alloys at room temperature are likely metastable phases, which are quenched from higher temperatures due to slow diffusion kinetics of the alloying elements. During deformation at 1273 K, the CrNbTiZr and CrNbTiVZr alloys retained their two-phase (BCC plus Laves) structure and their phase compositions were unaffected by deformation. The high-temperature deformation resulted in the formation of new recrystallized grains inside the BCC phase and deformation twins inside large Laves-phase particles. The CrNbTiVZr alloy showed the most attractive properties, such as considerably improved elevated temperature strength, reduced density, and much higher melting point, as compared to three other high-entropy alloys and referenced Ni superalloys (In718 and Haynes 230). A microstructural approach to improve the limited room temperature ductility is suggested via dissolution and controlled precipitation of the strengthening Laves phase.

25. The paper *Microstructure and Mechanical Properties of Refractory High Entropy (Mo<sub>0.5</sub>NbHf<sub>0.5</sub>ZrTi)BCC/M<sub>5</sub>Si<sub>3</sub> In-Situ Compound* investigates the effect of Si on the microstructure and mechanical properties of Mo<sub>0.5</sub>NbHf<sub>0.5</sub>ZrTi alloy. The base alloy has the single body-centered cubic (BCC) phase. After adding Si, the alloy is composed of one BCC phase and the intermetallic M<sub>5</sub>Si<sub>3</sub> phase with a hexagonal close-packed (HCP) crystal structure. The microstructure gradually evolves from the hypoeutectic structure to eutectic structure and finally to hypereutectic structure with the increase of Si concentration. The addition of Si reduces the density and increases the hardness and strength of the base alloy due to the formation of the M<sub>5</sub>Si<sub>3</sub> phase. The plasticity of Si<sub>0.1</sub> alloy is also improved due to grain refinement and the weakening of the solution strengthening for the dominant BCC phase, while the M<sub>5</sub>Si<sub>3</sub> phase is fine. However, the plasticity decreases due to the formation of more brittle M<sub>5</sub>Si<sub>3</sub> phase with a larger size as Si content increases. Coming to the Conclusion in this study, Si is added into Mo<sub>0.5</sub>NbHf<sub>0.5</sub>ZrTi alloy to produce the BCC/M<sub>5</sub>Si<sub>3</sub> in-situ compounds. The microstructure and mechanical properties were characterized and discussed. Based on obtained results and analysis, the conclusions can be drawn as follows. The Si-containing alloys are composed of BCC phase and intermetallic M<sub>5</sub>Si<sub>3</sub> phase, and the volume of M<sub>5</sub>Si<sub>3</sub> phase increases with the increasing Si content. When Si content is lower than  $x = 0.5$ , the microstructure exhibits the hypoeutectic structure, the microstructure is very close to the eutectic structure, and the microstructure is the hypereutectic structure when Si content increases. The chemical compositions of the M<sub>5</sub>Si<sub>3</sub> phase have close relationships with the mixing enthalpy between Mo, Nb, Hf, Zr, Ti, and Si. The content is the highest in the M<sub>5</sub>Si<sub>3</sub> phase due to the most negative enthalpy of Zr with Si. HV and yield strength increase with the addition of Si. The yield

strength and plasticity are improved for Si0.1 alloy. Only the strength increases, while the plasticity decreases with more addition of Si.

26. The paper *Alloy Design for Intrinsically Ductile Refractory High-Entropy Alloys* explores the development of a ductile refractory high-entropy alloy (RHEA). Refractory high-entropy alloys (RHEAs), comprising group IV (Ti, Zr, Hf), V (V, Nb, Ta), and VI (Cr, Mo, W) refractory elements, can be potentially new generation high-temperature materials. However, most existing RHEAs lack room-temperature ductility, similar to conventional refractory metals and alloys. The authors propose an alloy design strategy to intrinsically ductilize RHEAs based on the electron theory and specifically to decrease the number of valence electrons through controlled alloying. A new ductile RHEA, Hf<sub>0.5</sub>Nb<sub>0.5</sub>Ta<sub>0.5</sub>Ti<sub>1.5</sub>Zr, was developed as a proof of concept, with a fracture stress of close to 1 GPa and an elongation of near 20%. The findings shed light on the development of ductile RHEAs for ultrahigh-temperature applications in aerospace and power-generation industries. To conclude, the study developed a new ductile RHEA, Hf<sub>0.5</sub>Nb<sub>0.5</sub>Ta<sub>0.5</sub>Ti<sub>1.5</sub>Zr, with a density of 8.13g/cm<sup>3</sup>, a yield stress of 903MPa, a fracture stress of 990MPa, and an elongation of 18.8%, performing better than previously developed ductile RHEAs. More importantly, the authors proposed the mechanism and route for ductilizing RHEAs comprising groups IV (Ti, Zr, Hf), V (V, Nb, Ta), and VI (Cr, Mo, W) refractory elements, using the electron theory. Intrinsically ductile RHEAs can be developed by alloying elements from group VI or group V, with elements from group V or group IV, or in other words, by decreasing the number of valence electrons (s + d electrons) in single-phase bcc solid solutions.
27. The paper *Mechanical Properties and Thermally Activated Plasticity of the Ti<sub>30</sub>Zr<sub>25</sub>Hf<sub>15</sub>Nb<sub>20</sub>Ta<sub>10</sub> High Entropy Alloy at Temperatures 4.2–350 K* investigates the mechanical properties of the Ti<sub>30</sub>Zr<sub>25</sub>Hf<sub>15</sub>Nb<sub>20</sub>Ta<sub>10</sub> high-entropy bcc alloy over a wide range of low temperatures (4.2–350 K). Values of microhardness and Young's modulus at 300 K, temperature dependencies of the yield strength, deforming stress, and strain rate sensitivity were registered and analyzed within the framework of thermally activated deformation models. Empirical estimates were made of the microscopic parameters of plasticity, such as Peierls stress, activation energy for dislocations, and the level of internal stresses. To conclude the Ti<sub>30</sub>Zr<sub>25</sub>Hf<sub>15</sub>Nb<sub>20</sub>Ta<sub>10</sub> high-entropy alloy demonstrates an exceptional combination of high strength and reasonable plasticity, even at cryogenic temperatures, indicating its good application perspectives as a structural material. Additional improvement of mechanical properties can probably be achieved by decreasing grain sizes. The temperature dependences of the flow stress, strain rate sensitivity, and the activation volume across a wide range of low temperatures indicate thermally activated plasticity of the Ti<sub>30</sub>Zr<sub>25</sub>Hf<sub>15</sub>Nb<sub>20</sub>Ta<sub>10</sub> high-entropy alloy. The thermal activation analysis of experimental data has shown that the process of plastic deformation at low temperatures is controlled by thermally activated motion of dislocations in the Peierls potential relief, which is realized by nucleation and expansion of kink pairs at dislocation lines. The empirical estimates of the microscopic parameters of dislocation interaction with the Peierls barriers (such as activation energy, energy of kink pair nucleation, and height of the Peierls barrier) and estimates of internal stresses are obtained. Similar values of

the activation volume for dislocation motion of Ti<sub>30</sub>Zr<sub>25</sub>Hf<sub>15</sub>Nb<sub>20</sub>Ta<sub>10</sub> high-entropy alloy and the bcc metals, where Peierls barriers control the motion of dislocations, indicate the same deformation mechanism. Differences in activation energy between Ti<sub>30</sub>Zr<sub>25</sub>Hf<sub>15</sub>Nb<sub>20</sub>Ta<sub>10</sub> and the bcc metals are probably due to the distorted crystal lattice of the high-entropy alloy.

28. The paper *Solution Strengthening of Ductile Refractory HfMoxNbTaTiZr High-Entropy Alloys* investigates the crystal structure, microstructure, and mechanical properties of HfMoxNbTaTiZr ( $x \leq 1$ ) alloys using X-ray diffraction, scanning electron microscopy, and compression testing. All the as-solidified HfMoxNbTaTiZr alloys possess a simple body-centered cubic structure. Lattice parameters of the HfMoxNbTaTiZr alloys decrease with an increase in Mo concentration, but the corresponding densities show an opposite trend. The yield strength of the HfMoxNbTaTiZr alloys increases from 1015 MPa to 1512 MPa as  $x$  increases from 0 to 1. The solid solution strengthening is linearly proportional to Mo concentration, suggesting that the strengthening effect from each Mo atom is additive. Except for the HfMoNbTaTiZr alloy, HfMoxNbTaTiZr ( $x < 1$ ) alloys exhibit excellent room-temperature plasticity ( $> 50\%$ ). The material with  $x = 0.75$  is a new ductile refractory high-entropy alloy with promising mechanical properties. The conclusion of the study shows that HfMoxNbTaTiZr alloys ( $x \leq 1$ ) have a simple BCC structure. The lattice parameters of these alloys decrease with an increase in Mo concentration, but their densities show an opposite trend. The microstructures of all studied alloys correspond to a typical dendritic structure, and no other phases were formed in the interdendrite region. The yield strength of the studied alloys increases from 1015 MPa to 1512 MPa with an increase in Mo concentration from zero to 16.7 at%, indicating a significant solid solution strengthening in the HfMoxNbTaTiZr alloys due to Mo addition. The obtained HfMoxNbTaTiZr alloys show excellent room-temperature plasticity. The studied alloys, except for the Mo-1 alloy, underwent a 50% compression strain without any evidence of fracture. The HfMoxNbTaTiZr alloys can be considered as quasi-binary alloys, and a linear correlation between their yield strength and solute atom concentration is established.
  
29. The paper *Microstructure and Mechanical Properties of Refractory HfMo0.5NbTiV0.5Six High-Entropy Composites* reports on the synthesis of HfMo<sub>0.5</sub>NbTiV<sub>0.5</sub>Si<sub>x</sub> ( $x = 0, 0.3, 0.5, 0.7$ ) high-entropy alloys by induction levitation melting, aiming to achieve a balanced combination of excellent strength at elevated temperatures and reasonable ductility at room temperature (RT). The microstructure, phase evolution, and compression mechanical properties of the alloys from 20 °C to 1200 °C are investigated. It is found that the HfMo<sub>0.5</sub>NbTiV<sub>0.5</sub> matrix forms a simple disordered body-centered cubic (BCC) phase. After adding the Si element, multi-component silicide (Hf, Nb, Ti)<sub>5</sub>Si<sub>3</sub> is generated inside the alloys, exhibiting a transition from hypoeutectic structure to eutectic structure and then to hypereutectic structure as the Si content increases. The addition of Si significantly improves the hardness and strength but reduces the ductility. At room temperature, the HfMo<sub>0.5</sub>NbTiV<sub>0.5</sub> and HfMo<sub>0.5</sub>NbTiV<sub>0.5</sub>Si<sub>0.7</sub> alloys show yield strengths of 1260 MPa and 2134 MPa, respectively. The compressive mechanism transitions from ductile deformation to brittle fracture from  $x = 0$  to  $x = 0.7$ . Strain softening and silicide

segmentation are observed during compression deformation of these alloys at elevated temperatures. Under these conditions, the alloys survive at least 35% of engineering compression strain without fracture. During deformation at 1200 °C, the yield strengths of HfMo0.5NbTiV0.5 and HfMo0.5NbTiV0.5Si0.7 alloys are 60 MPa and 235 MPa, respectively. The attractive strength of the Si-containing alloys at elevated temperatures is strongly dependent on the strengthening effect caused by the silicides. The conclusion of the study shows that a refractory high-entropy alloy of HfMo0.5NbTiV0.5Six was synthesized by induction levitation melting. The microstructure and mechanical properties were characterized and discussed. Based on the obtained results and analysis, the following conclusions are summarized: 1. The HfMo0.5NbTiV0.5 matrix was mainly composed of a BCC phase. After adding the Si element, multi-component silicide (Hf, Nb, Ti)5Si3 was generated inside the alloys. When x of Si content was 0.3, the silicide presented a hypoeutectic microstructure. With the increase in Si concentration, the microstructure of silicide exhibited an evolution from hypoeutectic structure to eutectic structure and then to hypereutectic structure. 2. The density of the HfMo0.5NbTiV0.5Six alloys decreased with increasing Si content. The strength greatly increased with the Si content, while the plasticity at room temperature was reduced gradually. For example, the respective yield strength and fracture strain of the HfMo0.5NbTiV0.5 alloy were >35% and 1260 MPa, while the yield strength and fracture strain of the HfMo0.5NbTiV0.5Si0.7 alloy were 9.2% and 2134 MPa, respectively. The fracture surfaces of the Si-containing alloys suggest that the fracture mode was a mixture of plastic fracture of the matrix phase and brittle cleavage fracture of the silicide. 3. The yield strengths of HfMo0.5NbTiV0.5 and HfMo0.5NbTiV0.5Si0.7 alloys were 60 MPa and 235 MPa at 1200 °C, respectively. The attractive strength at elevated temperatures of the Si-containing alloys was strongly dependent on the strengthening effect caused by the silicides.

30. The paper *Enhanced Mechanical Properties of HfMoTaTiZr and HfMoNbTaTiZr Refractory High-Entropy Alloys* investigates the modification of the HfNbTaTiZr alloy to improve its strength at high temperatures while retaining reasonable toughness at room temperature. Although refractory high-entropy alloys (HEAs) generally have exceptional strength at high temperatures, they are often brittle at room temperature. One exception is the HfNbTaTiZr alloy, which has a plasticity of over 50% at room temperature, but its strength at high temperature is insufficient. In this study, two new alloys with simple BCC structure, HfMoTaTiZr and HfMoNbTaTiZr, were designed and synthesized. The results show that the yield strengths of the new alloys are significantly higher than that of HfNbTaTiZr, while a fracture strain of 12% is successfully retained in the HfMoNbTaTiZr alloy at room temperature. The conclusion of the study highlights several findings: both alloys have a simple BCC structure, and the lattice constants and densities of the two alloys are close to the values obtained by rule-of-mixture. However, the hardness of both alloys is about three times higher than the rule-of-mixture values, indicating strong solid-solution strengthening. The compression yield strengths of the HfMoTaTiZr alloy at room temperature (RT), 800, 1000, and 1200 °C are 1600, 1045, 855, and 339 MPa, respectively. The corresponding values for the HfMoNbTaTiZr alloy are 1512, 1007, 814, and 556 MPa, respectively. The fracture strain of the HfMoTaTiZr alloy is 4%, while for the HfMoNbTaTiZr alloy, it is 12% at RT. The fracture surfaces of the two alloys suggest that the fracture mode is a mixture of cleavage and quasi-cleavage, with fewer cleavage fracture features

observed in the HfMoNbTaTiZr alloy. As the temperature increases, the yield strengths of the alloys decrease, while plastic strains increase. The combination of strength and plasticity for the HfMoNbTaTiZr alloy is better than that of HfMoTaTiZr at all test temperatures. During compression at 1000 °C (for HfMoTaTiZr) or 1200 °C (for both alloys), Mo-rich and (Zr, Hf)-rich precipitates form in the interdendrite regions. The crystal structure of the (Zr, Hf)-rich precipitate is FCC, which is different from the prediction of the binary phase diagram. Compared to the base alloy (HfNbTaTiZr), the strengths of the two modified alloys at elevated temperatures are markedly higher. The yield strength of HfMoNbTaTiZr is more than six times that of HfNbTaTiZr at 1200 °C. The yield strength values of the modified alloys are higher than those of Inconel 718 and CMSX-4 at all testing temperatures, except for CMSX-4 at 800 °C. The resistances to thermal softening for both modified alloys are also higher than those of the superalloys. Both new alloys have great potential for high-temperature applications, with the combination of strength and plasticity in HfMoNbTaTiZr being better than in HfMoTaTiZr.

31. The paper *Microstructure and Mechanical Properties of Refractory MoNbHfZrTi High-Entropy Alloy* investigates the microstructure, phase stability, and mechanical properties of a new refractory MoNbHfZrTi high-entropy alloy. MoNbHfZrTi alloy consists of a disordered body-centered cubic (BCC) solid solution phase in as-cast and homogenized states. Homogenization treatment and DSC analysis indicate that there is no any phase transition below 1743 K. At room temperature, the compressive yield strength for the alloy in as-cast and as-homogenized states reaches about 1719 MPa and 1575 MPa, respectively, and the fracture mechanism is brittle quasi-cleavage fracture. At elevated temperatures, this alloy has compression yield strength of 825 MPa at 1073 K, 728 MPa at 1173 K, 635 MPa at 1273 K, 397 MPa at 1373 K, and 187 MPa at 1473 K and some fine grains form at grain boundaries due to partial dynamic recrystallization. In this paper, a new refractory high-entropy alloy, MoNbHfZrTi, was explored and prepared. The microstructure, phase stability, and mechanical properties were studied. Based on the obtained results and analysis, four conclusions can be drawn as follows. MoNbHfZrTi alloy is composed of a single disordered BCC phase in as-cast and as-homogenized states. The observed phase in this alloy can be predicted using the existing criteria. The homogenization and DSC analysis confirm that there is no any phase transition below 1743 K for MoNbHfZrTi alloy with the single BCC phase. The structural stability makes this alloy be a promising candidate for elevated-temperature applications. At room temperature, the alloy has high compressive yield strength of 1719 MPa and 1575 MPa in as-cast and as-homogenized states. The fracture mechanism is quasi-cleavage fracture from the features of cleavage steps, river patterns, and tongue patterns. At elevated temperatures, this alloy still has high compressive yield strength (825 MPa at 1073 K, 728 MPa at 1173 K, 635 MPa at 1273 K, 397 MPa at 1373 K, and 187 MPa at 1473 K) and shows a drop of flow stress after yielding. Some fine dynamic recrystallized grains form at the grain boundaries which is responsible for the strain softening.
32. The paper *Design and Tensile Properties of a BCC Ti-Rich High-Entropy Alloy with Transformation-Induced Plasticity* presents the design and tensile properties of a new

bcc Ti-rich high-entropy alloy (HEA) of composition Ti<sub>35</sub>Zr<sub>27.5</sub>Hf<sub>27.5</sub>Nb<sub>5</sub>Ta<sub>5</sub>, developed using the ‘d-electron alloy design’ approach. The tensile behavior displays a marked transformation-induced plasticity effect resulting in a high normalized work-hardening rate of 0.103 without loss of ductility when compared to the reference composition Ti<sub>20</sub>Zr<sub>20</sub>Hf<sub>20</sub>Nb<sub>20</sub>Ta<sub>20</sub>. In this study, a detailed microstructural analysis was performed to understand the deformation process, revealing architectural-type microstructures and a high volume fraction (65%) of internally twinned stress-induced martensite  $\alpha''$  after mechanical testing. This study opens the way to mechanical properties optimization and enhancement of titanium-based HEAs by combining multiple alloying designs. In conclusion, a new TRIP alloy was found within the HEA family. According to the Bo–Md diagram developed for titanium alloys, the HEA of composition Ti<sub>35</sub>Zr<sub>27.5</sub>Hf<sub>27.5</sub>Nb<sub>5</sub>Ta<sub>5</sub> was considered as a good  $\beta$ -metastable candidate. Successful thermo-mechanical treatments were performed on the as-cast alloy in order to obtain a bcc single solid solution. Tensile tests were performed and microstructural analyses demonstrate that this alloy is deformed by stress-induced phase transformation, conferring it a very high work-hardening rate compared to classical multi-component alloys. The tools developed for the Ti-alloys design proved to be efficient to predict the deformation mechanism in this optimized composition. This allows creating work hardening in a bcc HEA. The study of this composition also illustrates the ‘cocktail effect’, meaning that the properties of the multi-component alloy can be adjusted by varying the concentration of one of the elements, here titanium. A proof of concept is given in this study that TRIP mechanism can be triggered in bcc HEAs. No further optimization was done, and future efforts will be dedicated to improve the microstructure and composition, with the aim to enhance the mechanical properties presented here.

33. The paper *Microstructure and Mechanical Properties of a Refractory HfNbTiVSi<sub>0.5</sub> High-Entropy Alloy Composite* reports on the synthesis of a refractory high-entropy alloy of HfNbTiVSi<sub>0.5</sub> by induction levitation melting. The alloy is a composite composed mainly of a body-centered cubic (BCC) solid solution and a multi-component silicide ((Hf, Nb, Ti)-Si). This alloy displays a balanced combination of strength at high temperature and ductility at room temperature. The studied results show that the compressive yield strength (YS) is as high as 1399 MPa, with a fracture strain of 10.9% at room temperature. At 800 °C and 1000 °C, the YS is still preserved at 875 MPa and 240 MPa, respectively, due to the higher load-carrying capacity of the silicide at elevated temperatures. Comparison to similar refractory HEAs shows that the composite microstructure is beneficial for better room temperature strength and ductility as well as the elevated temperature properties. To summarize, a new refractory HfNbTiVSi<sub>0.5</sub> alloy mainly composed of a BCC solid solution and a simple multi-component silicide has been successfully developed. The alloy density is 8.60 g/cm<sup>3</sup> and the overall hardness is 490 HV. At room temperature, the YS is 1399 MPa, and the fracture strain is 10.9%. At 800 °C and 1000 °C, no fracture occurs at the strain of 50%, and YS values of 875 MPa and 240 MPa, respectively, are obtained. Compared to similar refractory HEAs, the composite structure incorporating the silicide shows superior comprehensive strength and highly improved elevated temperature properties.

34. The paper *Microstructure and Mechanical Properties of a New Refractory HfNbSi<sub>0.5</sub>TiVZr High Entropy Alloy* presents a study on a new refractory alloy HfNbSi<sub>0.5</sub>TiVZr synthesized by induction levitation melting with the aim to achieve an excellent strength and toughness balance of the Hf-Nb-Ti-Zr-based alloy. The as-cast alloy with a density of  $\rho=7.75 \text{ g/cm}^3$  and microhardness of  $H_v=464$  had a microstructure consisting of a BCC solid solution with little vanadium-rich phase and fine intermetallic phase presenting a dendritic structure. Mixing entropy and formation enthalpy can explain this behavior. After heat treatment at 1373 K for 4 hours, no new phase came into being, but elements solute more fully. The compressive yield strength of the alloy gradually decreased from 1540 MPa at room temperature to 371 MPa at 1073 K in the as-cast state and decreased from 1483 MPa at room temperature to 102 MPa at 1073 K after annealing. Comparing with similar high-entropy alloys, the structure combining silicide and continuous solid phase greatly benefits the balance of strength and ductility. In summary, a new refractory alloy HfNbSi<sub>0.5</sub>TiVZr consisting of three phases, including the BCC solid solution with little vanadium-rich phase and fine silicide of Hf and Zr, was synthesized by induction levitation melting. Part of the alloy was heat-treated at 1100°C for 4 hours, and no new phase came into being after heat treatment, but elements solute more fully. The density of the alloy is  $7.75 \text{ g/cm}^3$  and the Vickers hardness is 455.3 as-cast and 495.8 after heat treatment. Higher Vickers hardness is observed after heat treatment. The yield strength is 1540 MPa as-cast and 1483 MPa after annealing, and the ductility is 16.8% and 9.5%, respectively. The yield strength and maximum pressure stress decline as the temperature increases; at 1073 K, the yield strength was 371 MPa as-cast and 102 MPa after annealing, respectively. Meanwhile, the alloy tends to perform plastic deformation rather than brittle fracture. The total mechanical properties as-cast are better than annealed, reflected in the yield strength and ductility, which is connected with vanadium diffusion in the solid solution causing the depression of the matrix melting point, and the elements of the alloy dissolved more sufficiently after heat treatment with the solid solution strengthening effect reduced. Comparing with similar high-entropy alloys, the structure combining silicide and continuous solid phase greatly benefits the balance of strength and ductility.
35. The paper *Thermodynamic Instability of a Nanocrystalline, Single-Phase TiZrNbHfTa Alloy and Its Impact on the Mechanical Properties* investigates the thermodynamic stability and mechanical properties of an equiatomic, single-phase TiZrNbHfTa high-entropy alloy subjected to high-pressure torsion (HPT), resulting in a grain size below 100 nm. Introducing a nanocrystalline microstructure to the material aimed to accelerate a possible phase decomposition through fast diffusion pathways and grain boundary nucleation sites. To test thermodynamic stability, the nanocrystalline high-entropy alloy was subjected to various heat treatments at temperatures between 300°C and 1100°C. Isochronal heat treatments (1 h) revealed a hardness increase from 420 HV1 in the as-processed state to 530 HV1 at 500°C, while softening occurred at temperatures of 700°C and above. To understand this annealing response, selected microstructural states were analyzed using electron microscopy, x-ray diffraction, and mechanical testing, complemented by thermodynamic simulations via the Calphad approach. A phase decomposition from the original equimolar single-phase high-entropy alloy into a NbTa-rich body-centered cubic phase and ZrHf-rich phases (in two different crystal structures depending on the annealing temperature) was identified as the main cause for the property changes. The study demonstrates the impact of newly forming phases on mechanical properties and implications for potential applications of



this alloy. In conclusion, to evaluate the thermodynamic stability of the equiatomic, single-phase TiZrNbHfTa alloy, nanostructured samples processed by HPT were comprehensively studied after annealing. HPT processing resulted in significant grain refinement to approximately 50 nm, doubling the tensile strength to 1900 MPa without losing the single-phase character. Annealing treatments below 1000°C showed a clear phase decomposition tendency, with temperatures between 800°C and 900°C leading to decomposition into two bcc phases (Nb-Ta rich and Zr-Hf rich), and lower temperatures resulting in a second Zr-Hf rich phase with an hcp crystal structure. The phase decomposition strongly affected mechanical performance, as annealing caused severe embrittlement compared to the excellent strength and ductility observed after HPT processing. Thermodynamic simulations aligned well with experimentally observed phases. These findings shed light on the phases of the former single-phase TiZrNbHfTa alloy and their mechanical impact, suggesting that the alloy could serve as a basis for synthesizing complex nanocomposite structures. Volume fractions of individual phases could be tailored through appropriate annealing times and temperatures to optimize strength-ductility trade-offs.

36. The paper *Microstructure and Properties of a Refractory High-Entropy Alloy After Cold Working* investigates the microstructural and mechanical properties of a refractory high-entropy alloy, HfNbTaTiZr, after cold rolling and subsequent annealing. A refractory high-entropy alloy HfNbTaTiZr was successfully rolled at room temperature up to 86.4% reduction in thickness (true thickness strain is  $-2.3$ ). This represents the first successful attempt to cold roll a HEA with a BCC crystal structure. The microstructure and properties of the rolled sheets were determined in the as-rolled condition and after annealing at 800 °C, 1000 °C, and 1200 °C. Cold rolling resulted in extensive grain elongation, formation of deformation bands within the grains, and development of crystallographic textures that depended on the rolling reduction. The 86.4% cold-rolled sheet had true tensile stress of 1295 MPa and tensile ductility of 4.7%. After annealing at 1000 °C and 1200 °C, complete recrystallization of the cold-rolled sheet occurred. After annealing at 1000 °C, the true tensile stress and ductility of the sheet were 1262 MPa and 9.7%, respectively. In conclusion, a refractory high-entropy alloy, HfNbTaTiZr, was successfully cold rolled to 86.4% total thickness reduction. This represents the first successful attempt to cold roll such a material with a BCC crystal structure. Cold rolling resulted in extensive grain elongation, the formation of a “cellular” structure with deformation bands within the grains, and the development of crystallographic textures that depended on the rolling reduction. After 65% reduction, the textures were characterized by  $jj$  ND,  $jj$  ND,  $jj$  RD, and  $jj$  RD. An increase in strain to 86.4% reduction intensified the  $jj$  RD component, retained the  $jj$  ND component, and weakened the  $jj$  ND component considerably. The 86.4% cold-rolled sheet had the true tensile stress of 1295 MPa and tensile ductility of 4.7%. Annealing the cold-rolled sheet at 800 °C for 2 h resulted in partial recrystallization and precipitation of second-phase particles in non-recrystallized regions. The particles were slightly enriched in Nb and Ta and had a BCC crystal structure. Concurrently, the matrix was slightly enriched in Hf and Zr and also had a BCC crystal structure. After annealing at 800 °C, the true tensile stress of the sheet increased to 1334 MPa, but the true tensile ductility decreased to 1.9%. Despite the low macroscopic ductility, the

fracture behavior appeared entirely ductile. After annealing at 1000 °C and 1200 °C, complete recrystallization of the cold-rolled sheet occurred with the formation of large equiaxed grains. The average grain size increased with an increase in the annealing temperature. In the 86.4% cold-rolled sheet, it was ~22 μm and 76 μm, respectively, for the two annealing temperatures. The annealed samples were essentially a single-phase BCC structure. However, they also contained a very small amount (~1e2 vol.%) of fine second-phase precipitates. After annealing at 1000 °C, the true tensile strength and ductility were 1262 MPa and 9.7%, respectively.

37. The paper *Simultaneously Increasing the Strength and Ductility of a Refractory High-Entropy Alloy via Grain Refining* investigates the grain growth kinetics and tensile properties of the HfNbTaTiZr refractory high-entropy alloy. The HfNbTaTiZr refractory high-entropy alloy was investigated on the grain growth kinetics and tensile properties. Grain growth at 1200–1350 °C is rather slow. The activation energy is 389 kJ/mol and the growth exponent is 3.5. The HfNbTaTiZr alloy has high strength, small work hardening, and high ductility. Grain refining is found to enhance the tensile strength and ductility simultaneously. In conclusion, the grain growth kinetics and tensile properties in the HfNbTaTiZr BCC refractory high-entropy alloy were investigated. The activation energy of grain growth at 1200~1350 °C is 389 kJ/mol, and the growth exponent is 3.5. The grain growth rate is controlled by the slowest two components, i.e., Nb and Ta. The slow grain boundary migration is a result of the solute-drag mechanism. Grain refinement increases both strength and ductility. The tensile yield strength, elongation, and true fracture strain of HfNbTaTiZr HEA with the smallest grain size of 38 μm are 958 MPa, 20%, and 1.23, respectively. The grain size strengthening is significant and obeys the Hall–Petch relationship.
38. The paper *Study of a BCC Multi-Principal Element Alloy: Tensile and Simple Shear Properties and Underlying Deformation Mechanisms* investigates the impact of a concentrated solid solution on the deformation mechanisms of a BCC multi-principal elements alloy. The room temperature mechanical properties in tension and simple shear are studied on samples with controlled microstructure. The partition of the various stress components is performed, as well as the determination of the activation volumes and the analysis of the dislocation density and velocity. The study of the mechanical behavior is coupled to a complete TEM investigation. The alloy displays a high yield strength that is explained by a strong impact of the short-range obstacles to the dislocation glide, with an enhancement of the effective stress due to the concentrated solid solution. The increase of the backstress is related to the formation of a heterogeneous dislocation structure, with dense dislocation bands acting as long-range obstacles. Deformation is controlled by screw dislocation glide. The  $a/2\langle 111 \rangle$  screw dislocations are rectilinear, indicating a high lattice friction effect. Evolution of both dislocation velocity and density during multirelaxation transients suggests a low mobility. If activation volumes are consistent with a Peierls mechanism, other considerations rather head towards the hypothesis of a transitory regime where the solid solution could impact further the dislocation glide. In conclusion, this paper provides an in-depth study of the deformation mechanisms of a quinary BCC MPEA at room temperature. To achieve reproducible results, all the analyses are performed on samples

with recrystallized microstructure. The analysis is done both on a mechanical side (stress partitioning, calculation of the activation volumes) and on a microstructural side, with the TEM analysis of the deformation features. The principal results are summarized below. A high yield strength is obtained by uniaxial tensile testing. Stress partitioning evidences that it is linked to the strong effect of short distance obstacles on gliding dislocations, with a major impact of the solid solution. The work-hardening occurring in the alloy is mostly due to the formation of a microstructure with dense bands, acting as long range obstacles. The deformation is controlled by dislocation glide. The dislocations are mostly screw and rectilinear. Their mobility is low, as confirmed by the evolution of the dislocation density and velocity along multi-relaxation series. Calculation of the activation volumes and TEM observations (strong lattice friction) tend to indicate that Peierls mechanisms are active. However, the classical kink-pair mechanism could not explain alone the experimental values. The hypothesis of a transitory regime with some influence of the pinning is highly suggested. A concept that has already been suggested is that the concentration fluctuation, due to the statistic repartition of the different elements onto the lattice position, would favor the notion of an “effective medium” over that of a classical solid solution. In good agreement with the results of Rao et al., this study rather concludes that the solid solution plays a significant role, probably related to the local fluctuations impacting the dislocation core configuration.

39. The paper *Microstructure and Room Temperature Properties of a High-Entropy TaNbHfZrTi Alloy* presents a new refractory alloy, Ta<sub>20</sub>Nb<sub>20</sub>Hf<sub>20</sub>Zr<sub>20</sub>Ti<sub>20</sub>, produced by vacuum arc-melting followed by hot isostatic pressing (HIPing) at T = 1473 K and P = 207 MPa for 3 h. The alloy has predominantly a single-phase body-centered cubic (BCC) structure with the lattice parameter a = 340.4 pm. The alloy density and Vickers microhardness are  $\rho = 9.94 \text{ g/cm}^3$  and Hv = 3826 MPa. The alloy has high compression yield strength ( $\sigma_{0.2} = 929 \text{ MPa}$ ) and ductility ( $\epsilon > 50\%$ ). The alloy shows considerable strain hardening and homogeneous deformation. A simple model of solid-solution strengthening is proposed to explain the behavior. In conclusion, a refractory alloy, Ta<sub>20</sub>Nb<sub>20</sub>Hf<sub>20</sub>Zr<sub>20</sub>Ti<sub>20</sub>, produced by vacuum arc-melting, has a single-phase body-centered cubic (BCC) structure with the lattice parameter a = 340.44 pm. No phase changes occur after HIPing the alloy at 1473 K, 207 MPa for 3 h. The alloy density and Vickers microhardness after HIPing were  $\rho = 9.94 \text{ g/cm}^3$  and Hv = 3826 MPa. The alloy has high compression yield strength ( $\sigma_{0.2} = 929 \text{ MPa}$ ) and ductility ( $\epsilon > 50\%$ ). The alloy shows considerable strengthening and homogeneous deformation. The high stress is explained by solid-solution strengthening.
  
40. The paper *On the Room Temperature Deformation Mechanisms of a TiZrHfNbTa Refractory High-Entropy Alloy* analyzes the deformation micro-mechanisms of an as-cast equimolar refractory high-entropy alloy composed of Ti, Zr, Hf, Nb, and Ta through monotonic and relaxation compression tests coupled with transmission electron microscopy observations. The evolution of the work hardening with plastic strain displays three stages. After a sharp decrease until a plastic strain of approximately 3%,

work hardening stabilizes at  $1300 \pm 50$  MPa and finally decreases again. The measured apparent activation volumes  $V_{app}$  slightly evolve with plastic strain and decrease from approximately  $50b^3$  to  $30b^3$ . These values are coherent with a Peierls mechanism due to strong intrinsic lattice friction. In addition, the measured activation volumes correlate well with TEM observations, which provide evidence that dislocation glide is controlled – in the first stages – by the movement of screw dislocations. The deformation is rapidly localized in bands in which dislocation dipoles, loops, and tangles are induced at higher plastic strains. In conclusion, dislocation structures have been studied in a solid solution of a refractory Ti<sub>20</sub>Zr<sub>20</sub>Hf<sub>20</sub>Nb<sub>20</sub>Ta<sub>20</sub> HEA after mechanical tests and TEM observations. These observations allow the clarification of the deformation mechanisms at room temperature of the multi-component alloy. From the TEM observations at different plastic strains, our investigation gives evidence that the first stages of the plastic deformation are governed by the motion of screw dislocations with  $b=a/2$  Burgers vector aligned in directions, giving also evidence of a strong intrinsic friction stress. Microstructures often are heterogeneous with soft and hard zones and the presence of such like shear bands containing screw dislocations, loops, and dipoles. At higher strains, the bands from early deformation stages tend to homogenize with a multiplication of the dislocations in the soft zones, and numerous debris are observed. The analysis of the mechanical behavior of the HEA in compression gives evidence of three stages. The first stage corresponds to a rapid decrease of work-hardening, the second to a stabilization of the latter close to 1300 MPa, and a final decrease after approximately 10% of plastic strain. From relaxation testing, the measured apparent activation volumes evolve rather a little with plastic strain and are comprised between approximately  $50b^3$  and  $30b^3$ , values compatible with a Peierls mechanism and comparable to other bcc metals and alloys.

41. The paper *Mechanical Behavior and Microstructure of Ti<sub>20</sub>Hf<sub>20</sub>Zr<sub>20</sub>Ta<sub>20</sub>Nb<sub>20</sub> High-Entropy Alloy Loaded Under Quasi-Static and Dynamic Compression Conditions* investigates the microstructure and mechanical behavior of equimolar Ti<sub>20</sub>Hf<sub>20</sub>Zr<sub>20</sub>Ta<sub>20</sub>Nb<sub>20</sub> high-entropy alloy across a wide range of initial strain rates between  $\sim 10^{-3} \text{ s}^{-1}$  and  $\sim 3.4 \times 10^3 \text{ s}^{-1}$ . A significant increment in the yield strength with increasing strain rate was observed, with the yield strength at  $\sim 3.4 \times 10^3 \text{ s}^{-1}$  being about 40% higher than that measured at  $\sim 10^{-3} \text{ s}^{-1}$ . Analysis by electron backscatter diffraction (EBSD) shows that in the low strain rate regime (up to  $\sim 10 \text{ s}^{-1}$ ), deformation occurs mainly in evenly distributed bands, while in the dynamic regime, deformation is strongly localized in macroscopic shear bands accompanied by softening even after the onset of yielding. The Kernel Average Misorientation technique reveals a high level of lattice rotation within these bands that also carries intense shear. Additionally, X-ray diffraction line profile analysis indicates that the sharp increase in the flow stress is mostly related to an increase in the dislocation density. In conclusion, the effect of strain rate on the plastic behavior of equimolar Ti<sub>20</sub>Hf<sub>20</sub>Zr<sub>20</sub>Ta<sub>20</sub>Nb<sub>20</sub> high-entropy alloy was studied in the range of  $\sim 10^{-3} \text{ s}^{-1}$ – $3.4 \times 10^3 \text{ s}^{-1}$ . The difference in mechanical performance at various strain rates was explained with post-mortem microstructure investigations using EBSD and XRD. The yield strength increased with increasing strain rate, with the strength at  $3.4 \times 10^3 \text{ s}^{-1}$  being about 40% higher than that measured at the strain rate of  $\sim 10^{-3} \text{ s}^{-1}$ , and the increment in strength becoming faster for strain rates between  $\sim 10^3$  and  $\sim 3.4 \times 10^3 \text{ s}^{-1}$ . At low and medium strain rates, the compression behavior up to a strain of about 0.3 is characterized by continuous hardening, while at high strain rates, softening was observed shortly after the onset of plastic deformation.

This difference is manifested in the difference between the yield strength and the flow stress measured at a strain of 0.05: at strain rates lower than  $10 \text{ s}^{-1}$ , the yield strength is lower than the flow stress, while for larger strain rates, the trend is opposite. EBSD investigations revealed strong strain localization in the samples deformed at high strain rates, which may cause early softening during compression. It was found that the dispersion of shear bands was reduced with increasing strain rate, as the density and thickness of bands decreased and increased, respectively. The flow stress measured for the material impacted at a velocity of 10.34 m/s up to a true strain of  $\sim 0.49$  agrees well with the value calculated from the Taylor equation using the average dislocation density obtained by X-ray line profile analysis. This observation suggests that besides the high friction stress, the large dislocation density ( $47 \pm 7 \times 10^{14} \text{ m}^{-2}$ ) is the main reason for the high flow stress of the samples impacted at high strain rates.

42. The paper *Elastic and Plastic Properties of As-Cast Equimolar TiHfZrTaNb High-Entropy Alloy* investigates the elastic properties of as-cast TiHfZrTaNb high-entropy alloy through ultrasound measurements, yielding  $C_{44}=28 \text{ GPa}$  and  $C_{11}=172 \text{ GPa}$ , effective isotropic elastic constants. This allowed the computation of the Young's modulus (E), the bulk modulus (B), and Poisson's ratio ( $\nu$ ) as about 78.5 GPa, 134.6 GPa, and 0.402, respectively. A Pugh ratio (G/B) as low as 0.208 and a high positive Cauchy pressure ( $C_{12}-C_{44}=80 \text{ GPa}$ ) were calculated, suggesting ductile behavior. Tensile tests were carried out on specimens taken along the ingot diameter to address micro-segregation effects on the macroscopic behavior. Micro-segregations were further addressed at a smaller scale via nano-hardness measurements. Given the observed low deviations from both tensile and nano-indentation experiments, the influence of micro-segregation was concluded to be negligible. The necking and fracture surface investigations revealed multiple slip bands, grain boundary distortions, and a mixture of shallow and profound dimples of varying sizes, all of which characterize high tensile ductility behavior in line with elasticity measurements predictions. Post-mortem EBSD investigations revealed lattice distortions mainly at the grain boundaries' vicinity as a consequence of dislocation accumulation. In conclusion, the elastic and plastic properties of as-cast TiHfZrTaNb high-entropy alloy were investigated by ultrasound measurements and tensile tests up to failure. Both the Rayleigh surface acoustic wave and the longitudinal sound velocity allowed computation of the Young's modulus (E), the bulk modulus (B), and Poisson's ratio ( $\nu$ ) of about 78.5 GPa, 134.6 GPa, and 0.402, respectively, in close agreement with the Reuss average estimates from DFT calculations, potentially suggesting an isostress situation in all grains. The obtained Young's modulus is about 30% higher than reported after compression tests (apparent modulus  $\sim 55 \text{ GPa}$ ) by Lin et al. The Pugh ratio (G/B) as low as 0.208 and a high positive Cauchy pressure ( $C_{12}-C_{44}=80 \text{ GPa}$ ) were computed, suggesting a ductile behavior for the investigated material, which was confirmed by tensile tests and SEM examination of the necking and fracture surfaces. Room temperature tensile tests showed only remote micro-segregation effects on the mechanical behavior of the as-cast materials: depending on the specimen location, yield strengths at 0.002 offset in the range  $\sim 800\text{--}840 \text{ MPa}$  were obtained. The latter are within experimental error. Local hardness measurements by nano-indentation exhibited

similar results for either dendrites or interdendritic zones, confirming no influence of micro-segregation on mechanical behavior. Post-mortem EBSD investigations revealed high levels of lattice distortions at the grain boundaries' vicinity, which were at the origin of the strengthening of the investigated HEA and are in line with the available literature reports.

43. The paper Microstructure and Elevated Temperature Properties of a Refractory TaNbHfZrTi Alloy examines the compression properties of a refractory multi-component alloy, Ta<sub>20</sub>Nb<sub>20</sub>Hf<sub>20</sub>Zr<sub>20</sub>Ti<sub>20</sub>, in the temperature range of 296–1473 K and strain rate range of  $10^{-1}$ – $10^{-5}$  s<sup>-1</sup>. The properties were correlated with the microstructure developed during compression testing. The alloy was produced by vacuum arc melting, hot isostatically pressed (HIPd), and homogenized at 1473 K for 24 h prior to testing. It had a single-phase body-centered cubic structure with the lattice parameter  $a = 340.4$  pm. The grain size ranged from 100–200  $\mu\text{m}$ . During compression at a strain rate of  $10^{-3}$  s<sup>-1</sup>, the alloy had yield strengths of 929 MPa at 296 K, 790 MPa at 673 K, 675 MPa at 873 K, 535 MPa at 1073 K, 295 MPa at 1273 K, and 92 MPa at 1473 K. Continuous strain hardening and good ductility ( $\epsilon \geq 50\%$ ) were observed in the temperature range from 296 to 873 K. Deformation at  $T = 1073$  K and strain rate  $\geq 10^{-3}$  s<sup>-1</sup> was accompanied by intergranular cracking and cavitation, explained by insufficient dislocation and diffusion mobility to accommodate grain boundary sliding activated at this temperature. The intergranular cracking and cavitation disappeared with an increase in deformation temperature to 1273 and 1473 K or a decrease in strain rate to  $\sim 10^{-5}$  s<sup>-1</sup>. At these high temperatures and/or low strain rates, the alloy deformed homogeneously and showed steady-state flow at a nearly constant flow stress. Partial dynamic recrystallization, leading to the formation of fine equiaxed grains near grain boundaries, was observed in specimens deformed at 1073 and 1273 K, while complete dynamic recrystallization was observed at 1473 K. In conclusion, compression properties of a new refractory multi-component alloy, TaNbHfZrTi, were determined in the temperature range of 296–1473 K and strain rate range of  $10^{-1}$ – $10^{-5}$  s<sup>-1</sup>, with the properties correlated to the microstructure developed during compression testing. Three temperature regions with different deformation behaviors were identified. In the temperature range of 296–873 K, the alloy showed temperature-independent strain hardening, deformation twinning, and shear band formation. High yield strength ( $\sigma_{0.2} = 929$  MPa), strong work hardening ( $d\sigma/d\epsilon = 3360$  MPa), homogeneous macroscopic flow, and excellent compression ductility ( $\epsilon > 50\%$ ) were observed at room temperature. Strain localization and formation of deformation shear bands occurred at 673 and 873 K, with macro-cracks detected only in specimens deformed at 873 K. During compression at 1073 K, heavy cavitation and the formation of very fine equiaxed grains along the boundaries of deformed grains were observed at strain rates  $\geq 10^{-3}$  s<sup>-1</sup>, and no deformation twinning was detected. The cavitation sufficiently reduced, and large notched cracks were replaced with finer round-shaped pores at strain rates  $< 10^{-3}$  s<sup>-1</sup>, explained by grain boundary sliding creating stress concentrations at grain boundary ledges and triple junctions. During deformation at 1273–1473 K, the alloy showed a rapid drop in flow stress after yielding followed by steady-state flow, with no cavitation or cracks observed in specimens compressed to at least 50% strain. Partial (at 1273 K) or complete (at 1473 K) dynamic recrystallization occurred, likely responsible for strain softening and steady-state flow at these temperatures.

44. The paper *Structural-disorder and its effect on mechanical properties in single-phase TaNbHfZr high-entropy alloy* investigates equiatomic TaNbHfZr refractory high-entropy alloys (HEAs) synthesized by arc-melting. The HEAs were annealed at 1800 °C for different times, at maximum up to 8 days. Their on-average body-centered cubic (bcc) solid-solution structure was confirmed by X-ray (XRD) and neutron (ND) diffraction, respectively. The HEAs are characterized by high average values of the static atomic displacements from the ideal lattice positions and the local internal strain. The short-range clustering (SRC) of a subset of atoms, enriched in Hf and Zr, takes place perpendicular to the  $\langle 100 \rangle$  directions. Furthermore, it becomes increasingly interconnected as a function of the annealing time. This is revealed by the evaluation of diffuse XRD intensities, high-resolution transmission electron microscopy (HRTEM) images, and atom probe tomography (APT). The local structural disorder and distortions at the SRC were modeled by molecular dynamics (MD) relaxations. The hardness and compressive yield strength of the as-cast HEA is found to be many times of what can be expected from the rule of mixture. The yield strength further increases by 76% after 1 day of annealing, which can be explained by a strengthening mechanism resulting from the SRC. With further annealing to 4 days, a minor phase with hexagonal close packed (hcp) structure and rich in Hf and Zr nucleates at the larger connecting nodes of the SRCs. The TaNbHfZr HEA shows a bcc average structure in the as-cast and the long-term annealed condition. The average structure reflects the high degree of local lattice distortion by the large static ADP based on the single-crystal XRD and the powder ND experiments. With longer annealing time at 1800 °C, an increasing degree of SRC perpendicular to the principal axes is observed. APT analysis reveals that the local composition of the SRC is high in Zr and depleted in Ta and Nb. But, after 4 days of annealing Hf and Zr cluster together in the SRCs. The SRCs cause local tetragonal lattice relaxation as evidenced from the direct HRTEM imaging and the diffuse scattering intensities in SAED and single-crystal XRD. The asymmetric streak-like nature of the diffuse scattering intensities could be partially reproduced by the MD relaxations of a model structure containing SRCs. With longer annealing times, the SRCs become more interconnected forming clustering nodes and grid-like repeating domains. The as-cast yield strength (1315 MPa) of the HEA is 4.9 times that expected from the expected value due to solid-solution strengthening-like mechanism. But, the peak of yield strength (2310 MPa) and hardness accompanied by a minimum of plasticity is observed after 1 day of annealing. The increase in yield strength could be adequately explained with the local energy minimization by SRCs as calculated by the MD relaxation of a model structure. After 4 days of annealing, nucleation of a hcp  $\beta$  phase is evidenced at the larger nodes of the SRCs as observed from the XRD and the HRTEM studies. This  $\beta$  phase precipitation lowers the internal stress of the matrix, causing the yield strength to drop and plasticity to improve again beyond 1 day of annealing. Under compression, barreling is only observed for the as-cast HEA, whereas the brittle annealed HEAs fracture predominantly by shearing. Our study reveals the details of the local disorder present, their mechanism of evolution with long annealing time, and its effect on the mechanical properties at ambient temperature.
45. The paper *A refractory Hf<sub>25</sub>Nb<sub>25</sub>Ti<sub>25</sub>Zr<sub>25</sub> high-entropy alloy with excellent structural stability and tensile properties* introduces a novel refractory Hf<sub>25</sub>Nb<sub>25</sub>Ti<sub>25</sub>Zr<sub>25</sub> high

entropy alloy (HEA) with a single body-centered cubic (BCC) structure, prepared by the copper mold cast method. This HEA retains the single BCC phase even after furnace cooling from homogenization at 1573 K for 6 h. The fracture strength and plastic strain of this HEA reach about 969 MPa and 14.9%, respectively. There is a significant work hardening effect in this HEA, which is considered as resulting from the movement and multiplication of dislocations. In summary, a novel refractory HfNbTiZr high-entropy alloy with a single BCC phase has been successfully developed. This new HEA alloy exhibits excellent phase stability at high temperature and no phase separation during furnace cooling from 1573 K homogenization. In the as-cast state, tensile YS is 879 MPa, UTS is 969 MPa, and the plastic elongation is 14.9%. The YS and UTS obtained in tensile tests are much higher than most of the reported FCC type of HEAs. The remarkable tensile elongation is seldom found in BCC HEAs. The TEM study confirms that dense dislocations have been formed during the deformation, resulting in large plasticity and significant work hardening for this HEA.

46. The paper *Phase composition and solid solution strengthening effect in TiZrNbMoV high-entropy alloys* investigates TiZrNbMoxVy high-entropy alloys (HEAs) with  $x = 0-2$ ,  $y = 1$  and  $y = 0.3$ , respectively, designed and prepared by copper mold casting technology. The phase composition and stability of these HEAs were investigated. It is shown that the HEAs with low content of V are composed of only one type of bcc solid solution phase (SSP) and demonstrate excellent phase stability at 1273 K. The high content of V and Mo results in the formation of two types of bcc SSPs and the decrease of phase stability in the HEAs. Based on the previously proposed criteria, the formation ability of solid solution phase for this kind of HEAs was comprehensively evaluated. The compressive mechanical properties of the as-cast and annealed HEAs were measured. It has been found that Mo plays a strong solid solution strengthening effect on this kind of HEAs. Especially, TiZrNbMo0.3V0.3 has the yield strength and plastic strain of 1312 MPa and >50%, respectively, and still maintains the excellent plastic deformation ability even after annealed at 1273 K for 72 h. The strengthening effect in this kind of HEAs is considered to be due to the shear modulus mismatch. The solubility limit of HEAs is correspondent to shear modulus mismatch of 29. In this study, the microstructural evolution and compressive properties of a series of TiZrNbMoV HEAs were investigated. The alloying effects of Mo and V on the phase formation and strengthening effect of these HEAs were discussed. Based on the obtained results, conclusive remarks are drawn as following: The phase formation is strongly affected by both the addition of Mo and V. For G-MV10 HEAs, there is a bcc type of structure as the Mo is lower than 25%, and two kinds of bcc phases as the Mo content is higher than 25%. Only one single bcc phase is formed in G-MV3 HEAs. After annealed at 1273 K for 72 h, M3V3 still maintains single bcc phase, while the microstructure of M7V3 has been changed to two bcc phases and C15 type of Laves phases. By using the existing criteria including  $\delta$ ,  $\Delta H_{mix}$ ,  $\Delta S_{mix}$ ,  $\Omega$  and  $\Delta\chi$ , the phase composition were predicted for the present HEAs. It is found that all these parameters for the present HEAs fall in the region of solid solution phase proposed based on these criteria. It is also found that the G-MV3 HEAs are more liable to form solid solution microstructure than G-MV10 HEAs. Mo plays a strong solid solution strengthening effect on this kind of HEAs. M3V3 demonstrates excellent comprehensive compressive mechanical properties with yield strength of 1312 MPa and plastic strain higher than 50%. The M3V3 and M7V3 HEAs maintain equivalent plastic deformation abilities to those of



as-cast alloys after annealed at 1273 K for 72 h. The TiZrNbMoV HEAs investigated in this work possesses relative high SYS among all the bcc HEAs. This strengthening effect is found to be correlated to the shear modulus mismatch. The solubility limit of current HEAs was found to be consist with  $\Delta G = 29$ , when prepared by copper mould casting.

47. The paper *Mechanical properties of refractory high-entropy alloys: Experiments and modeling* explores the potential of refractory high-entropy alloys for high-temperature applications beyond the capability of Ni-based superalloys, focusing on their solid solution formation characteristics and mechanical properties. Designed using the CALPHAD method, the formation of as-cast arc-melted body-centered cubic MoNbTaTiV was experimentally verified using X-ray diffraction and scanning electron microscopy. The measured density and lattice parameter for MoNbTaTiV are and 3.224 Å, which obey the rule of mixtures (ROM). The alloy exhibits high hardness at 443 Hv, high yield strength at 1.4 GPa, and good compressive fracture strength at 2.45 GPa with a fracture strain of at room temperature. The yield strength and hardness values of this alloy, and other single-phase refractory high-entropy alloys, are estimated using a simple model of solid solution strengthening. Reasonable agreement between modeling prediction and experiments is obtained. In addition, first-principles density functional theory calculations predict an enthalpy of formation of  $-0.865$  kJ/mol for the MoNbTaTiV alloy, with calculated atomic volume and elastic properties (e.g., bulk and elastic moduli) obeying the ROM. In summary, this study confirmed a single BCC phase in as-cast MoNbTaTiV HEA fabricated via arc-melting, as predicted by CALPHAD modeling using the TCNI8 database. The microstructure was examined using XRD and SEM. Mechanical properties were characterized through compression testing and Vickers hardness tests. The elastic properties of the MoNbTaTiV alloy and its constituent elements were studied using the DFT method. The following conclusions can be reached: The measured density and lattice parameter for MoNbTaTiV are and 3.224 Å, which obey the ROM. The DFT calculated lattice parameter for MoNbTaTiV is 3.2130 Å, and the enthalpy of formation is  $-0.865$  kJ/mol. The calculated elastic properties derived from the stress-strain relation are: , , ,  $B = 181.20$  GPa,  $G = 50.71$  GPa,  $E = 139.15$  GPa, and  $\nu = 0.372$ . The bulk modulus calculated from EOS is 174.47 GPa. The calculated atomic volume and elastic properties (e.g., bulk and shear moduli) for the alloy obey the ROM within the computation uncertainties. Microsegregation was observed in the casting through segregation in the dendritic microstructure: For as-cast MoNbTaTiV, Mo and Ta are enriched in the dendrite arms, while Ti and V are enriched in the interdendritic regions. The observed microsegregation behavior is consistent with non-equilibrium solidification modeling using CALPHAD. The calculated empirical parameters for MoNbTaTiV favor the formation of a single-phase solid solution with the BCC structure: kJ/mol,  $\delta = 3.36\%$ ,  $\Omega = 14.1$ ,  $VEC = 5$ , , and  $\phi = 31.32$ . The alloy exhibits substantial solid solution strengthening, large work hardening capability, and a compression fracture strain of 30% at room temperature. The measured yield strength, fracture strength, and hardness are 1.4 GPa, 2.45 GPa, and 443 Hv, respectively. The simple SSS model predicts well the yield strength of MoNbTaTiV and other reported single-phase refractory HEAs; the hardness values are approximately three times the yield strength. For HfMoxNbTaTiZr ( $x \leq 1$ ) alloys, the

SSS model predicts that Zr and Mo dominate the contributions to the SSS in HfMo<sub>x</sub>NbTaTiZr.

48. The paper *Effect of Ti additions on mechanical properties of NbMoTaW and VNbMoTaW refractory high entropy alloys* explores the development of a new refractory high entropy alloy (HEA) of TiNbMoTaW with Ti addition in a NbMoTaW alloy. It has been found that this HEA possesses a single body-centered cubic (BCC) phase structure and could sustain the phase structure even after annealing at 1200 °C for 24 h. In comparison with the mechanical properties of the NbMoTaW and VNbMoTaW HEAs, the room-temperature yield strengths and compressive plastic strains of the TiNbMoTaW and TiVNbMoTaW HEAs are significantly enhanced. In particular, the TiNbMoTaW and TiVNbMoTaW HEAs also show very promising high-temperature strength, with yield strengths as high as ~586 and ~659 MPa at 1200 °C, respectively. The present results indicate that Ti addition is beneficial to the strength and the compressive ductility of the refractory HEAs at room temperature. It is suggested that the present refractory HEAs possess the potentials in applications of high-temperature structural materials. With Ti additions, a new refractory TiNbMoTaW high entropy alloy with a single BCC phase structure has been developed. The Ti-containing HEAs possess high thermal stability and sustain a BCC phase even when annealed at 1200 °C for 24 h. Owing to the Ti alloying in the NbMoTaW and VNbMoTaW HEAs, the TiNbMoTaW and TiVNbTaMoW HEAs show enhanced strength and ductility. The room-temperature yield strengths of the TiNbMoTaW and TiVNbMoTaW HEAs are 1343 MPa and 1515 MPa, respectively. Meanwhile, their compressive plastic strains at room temperature are above 10%. The effect of Ti additions on the mechanical properties of these HEAs can be interpreted in terms of a solid solution hardening model. It has been found that both the TiNbMoTaW and TiVNbTaMoW HEAs exhibit yield strengths higher than 550 MPa at 1200 °C. The high-temperature mechanical performance of these two HEAs makes them potential materials for high-temperature applications.
49. The paper *Microstructures and mechanical properties of TixNbMoTaW refractory high-entropy alloys* explores the development of TixNbMoTaW refractory high-entropy alloys (RHEAs) by alloying Ti in the NbMoTaW RHEA, a material with excellent mechanical properties, high strength, and thermal stability at elevated temperatures but limited room temperature ductility. The study shows that the room temperature ductility of the RHEAs increases from 1.9% of the NbMoTaW RHEA to 11.5% of the TiNbMoTaW RHEA, and the yield strength increases from 996 MPa of the NbMoTaW RHEA to 1455 MPa of the TiNbMoTaW RHEA. In addition, the TixNbMoTaW RHEAs maintain a stable single BCC structure up to their melt points. The present result indicates that Ti addition could effectively enhance both the ductility and strength of the NbMoTaW RHEA. The combined performance of superior mechanical properties and high thermal stability of the TixNbMoTaW RHEAs

promises them an important role in engineering applications. With Ti additions,  $\text{Ti}_x\text{NbMoTaW}$  RHEAs ( $x = 0, 0.25, 0.5, 0.75$  and  $1$ ) have been developed. The  $\text{Ti}_x\text{NbMoTaW}$  RHEAs possess a single BCC crystal structure, which keeps stable up to their melt points. Alloying with Ti element effectively improves both the strength and ductility of the  $\text{Ti}_x\text{NbMoTaW}$  RHEAs at room temperature. Specifically, the yield strength of the  $\text{TiNbMoTaW}$  alloy is 1455 MPa, which is 46% higher than that of  $\text{NbMoTaW}$  RHEA, while its ductility at room temperature is as high as 11.5%, which is about 5 times higher than that of  $\text{NbMoTaW}$  RHEA. The strength enhancement of the  $\text{Ti}_x\text{NbMoTaW}$  RHEAs can be interpreted by the solid solution hardening effect. The improved ductility of the  $\text{Ti}_x\text{NbMoTaW}$  RHEAs can be understood by the grain boundary cohesion improvement, ductile elemental segregation, and shear instability. The excellent mechanical performance and high thermal stability of these RHEAs make them hold potentials for applications as structural materials.

50. The paper *TiZrNbTaMo high-entropy alloy designed for orthopedic implants: As-cast microstructure and mechanical properties* combines the high-entropy alloy (HEA) concept with property requirements for orthopedic implants, resulting in the design of a  $\text{Ti}_{20}\text{Zr}_{20}\text{Nb}_{20}\text{Ta}_{20}\text{Mo}_{20}$  equiatomic HEA. The arc-melted microstructures, compressive properties, and potentiodynamic polarization behavior in phosphate buffer solution (PBS) were studied in detail. It was revealed that the as-cast  $\text{TiZrNbTaMo}$  HEA consisted of dual phases with bcc structure, major bcc1 and minor bcc2 phases, with the lattice parameters of 0.3310 nm and 0.3379 nm, respectively. As confirmed by nanoindentation tests, the bcc1 phase is somewhat harder and stiffer than the bcc2 phase. The  $\text{TiZrNbTaMo}$  HEA exhibited Young's modulus of 153 GPa, Vickers microhardness of 4.9 GPa, compressive yield strength of  $\sigma_y = 1390$  MPa, and apparent plastic strain of  $\epsilon_p \approx 6\%$  prior to failure. Moreover, the  $\text{TiZrNbTaMo}$  HEA manifested excellent corrosion resistance in PBS, comparable to the Ti6Al4V alloy, and pitting resistance remarkably superior to the 316L SS and CoCrMo alloys. These preliminary advantages of the  $\text{TiZrNbTaMo}$  HEA over the current orthopedic implant metals in mechanical properties and corrosion resistance offer an opportunity to explore new orthopedic-implant alloys based on the  $\text{TiZrNbTaMo}$  concentrated composition. Combining the HEAs concept with property requirement for orthopedic implants, we used the equiatomic  $\text{Ti}_{20}\text{Zr}_{20}\text{Nb}_{20}\text{Ta}_{20}\text{Mo}_{20}$  quinary alloy as the starting point to screen the potential orthopedic-implant HEA. Based on preliminary investigation on this alloy, several conclusions are drawn as follows: 1. The as-cast  $\text{Ti}_{20}\text{Zr}_{20}\text{Nb}_{20}\text{Ta}_{20}\text{Mo}_{20}$  HEA structurally consisted of major bcc1 and minor bcc2 in fraction, without formation of intermetallic phases. Difference in melting temperature between constituent elements results in chemical microsegregation in some extent in the microstructures, ultimately forming the Ta- and Mo-rich bcc1 phase as dendrites of  $\text{Ti}_{15}\text{Zr}_{10}\text{Nb}_{20}\text{Ta}_{31}\text{Mo}_{24}$  and the Ta- and Mo-depleted bcc2 phase resided at interdendritic regions as the  $\text{Ti}_{24}\text{Zr}_{43}\text{Nb}_{12}\text{Ta}_8\text{Mo}_{13}$ . The lattice parameters of bcc1 and bcc2 solid-solution phases were determined to be 0.3310 nm and 0.3379 nm, respectively. 2. As confirmed by nanoindentation tests, dominant bcc1 phase containing more refractory elements is somewhat harder and stiffer than minor bcc2 phase with less refractory elements, at the levels of  $H_v = 6.4$  GPa and  $E = 161$  GPa for bcc1 phase, and  $H_v = 5.7$  GPa and  $E = 133$  GPa for bcc2 phase. In the average case, Vickers microhardness and Young's modulus of the as-cast  $\text{TiZrNbTaMo}$  HEA were 4.9 GPa and 153 GPa, respectively. Against the rule of mixtures, the alloying-induced hardening effect is remarkable. The strengthening mechanism of this solid-solution-like HEA was

rationalized by virtue of Labusch approach, proving the major contributor responsible for strengthening is the modulus misfit effect. 3. The TiZrNbTaMo HEA exhibits room-temperature compressive yield strength of  $\sigma_y = 1390 \pm 75$  MPa and apparent plastic strain of  $\epsilon_p \approx 6\%$  prior to failure. Its fracture mode and fractography reveal its brittleness and limited plasticity under deformation. Even so, it initiates the future effort direction to improve the ductility and toughness of the TiZrNbTaMo-based HEAs chemically away from the equiatomic composition. 4. Under PBS medium to simulate physiological environment, the TiZrNbTaMo HEA exhibits excellent corrosion resistance comparable to the Ti6Al4V alloy, and pitting resistance remarkably superior to the 316 L SS and CoCrMo alloy. Characterization of chemical and physical features of passive oxide film on the alloy surface is on-going work.

51. The paper *Novel TiNbTaZrMo high-entropy alloys for metallic biomaterials* presents a novel equiatomic TiNbTaZrMo high-entropy alloy (HEA) developed as a new metallic biomaterial. The constituent elements of the HEA were biocomparable, and the HEA was designed based on parameters such as the mixing enthalpy ( $\Delta H_{mix}$ ), the omega parameter ( $\Omega$ ), the delta parameter ( $\delta$ ), and the valence electron concentration (VEC) theory. The bcc solid solution phases with the different lattice constants were obtained in as-cast and annealed states. The HEA showed considerable strength with deformability and superior biocompatibility comparable to pure Ti. This study demonstrated the possibility of using HEAs as a new class of metallic biomaterials. In conclusion, a novel equiatomic TiNbTaZrMo HEA composed of biocomparable elements was successfully developed as a metallic biomaterial. Two bcc solid solution phases were obtained in the TiNbTaZrMo HEA. An equi-axis fine dendrite structure was observed in the ingots. The HEA showed excellent biocompatibility compared to that of pure Ti, together with superior mechanical properties, indicating the possibility of using HEAs as a new class of metallic biomaterials.
  
52. The paper *MoNbTaV medium-entropy alloy* describes the synthesis of the refractory medium-entropy alloy MoNbTaV, guided by CALPHAD (Calculation of Phase Diagrams) modeling, using vacuum arc melting under a high-purity argon atmosphere. A body-centered cubic solid solution phase was experimentally confirmed in the as-cast ingot using X-ray diffraction and scanning electron microscopy. The measured lattice parameter of the alloy (3.208 Å) obeys the rule of mixtures (ROM), but the Vickers microhardness (4.95 GPa) and the yield strength (1.5 GPa) are about 4.5 and 4.6 times those estimated from the ROM, respectively. Using a simple model on solid solution strengthening predicts a yield strength of approximately 1.5 GPa. Thermodynamic analysis shows that the total entropy of the alloy is more than three times the configurational entropy at room temperature, and the entropy of mixing exhibits a small negative departure from ideal mixing. In conclusion, the refractory MoNbTaV HEA is designed by CALPHAD modeling and synthesized by vacuum arc melting. The as-cast alloy with a single BCC structure based on XRD and SEM analyses exhibits a high yield stress of  $\sim 1.5$  GPa and a large compression fracture strain of  $\sim 21\%$  at room temperature, both of which are significantly greater than what was found for the MoNbTaW alloy. CALPHAD modeling is useful in predicting phase formation and

analyzing the elemental segregation that occurs during solidification. The total entropy of the alloy is nearly four times that of the configurational entropy even at room temperature, and the entropy of mixing shows slightly negative departure from ideal. The Vickers microhardness value (and the yield stress) of the alloy are about 4.5 (and 4.6) times that estimated from the simple ROM. This behavior has been explained by a simple solid solution strengthening modeling based on traditional elasticity theory. The predicted yield stress agrees very well with experimental value.

53. The paper *Ultra-high strength WNbMoTaV high-entropy alloys with fine grain structure fabricated by powder metallurgical process* discusses the fabrication of an equi-atomic WNbMoTaV high entropy alloy (HEA) with a single body-centered cubic structure (BCC) by the powder metallurgical process of mechanical alloying (MA) and spark plasma sintering (SPS). Mechanical alloying behavior, microstructure, and mechanical properties of the WNbMoTaV HEA were studied systematically. During MA, a single BCC phase was formed and the average particle size and crystallite size were refined to 1.83  $\mu\text{m}$  and 66.1 nm, respectively, after 6 hours of MA. Afterward, the as-milled powders were sintered in the temperature range of 1500–1700  $^{\circ}\text{C}$ . The microstructure of the sintered sample exhibits a few micrometer-scale grain sizes and a homogeneous BCC matrix with a small amount of oxide inclusion originating from oxidation during the powder metallurgical process. The bulk sample of the WNbMoTaV HEA sintered at 1500  $^{\circ}\text{C}$  shows an ultra-high compressive yield strength of 2612 MPa with a failure strain of 8.8% at room temperature, respectively. These mechanical properties of the WNbMoTaV HEA fabricated by the powder metallurgical process were attributed to the combined effects of grain boundary strengthening, substitutional solid solution strengthening, interstitial solid solution strengthening, and Orowan strengthening by the oxide inclusions. Through a Hall-Petch analysis, the Hall-Petch coefficient of the WNbMoTaV HEA was derived. The WNbMoTaV HEA fabricated via the powder metallurgical process showed the best compressive yield strength when compared with other reported refractory HEAs processed with arc-melting and casting. In conclusion, the WNbMoTaV HEA with a BCC matrix was fabricated by MA and SPS powder metallurgical processes. Phase and microstructural characterization of the WNbMoTaV HEA powder indicated that 6 hours of MA was the minimum milling time to mitigate contamination during the MA process while being adequate for the subsequent sintering process. The 6-hour milled powders and bulk WNbMoTaV HEA exhibited a single BCC solid solution phase, in accordance with theoretical criteria for the formation of a single solid solution. After SPS at 1500–1700  $^{\circ}\text{C}$ , the bulk material had a relative density exceeding 99.5%. The microstructure of the bulk alloy consisted of a BCC matrix with a small volume fraction of oxide inclusions that were probably  $\text{Ta}_2\text{VO}_6$ . Therefore, this work established a route to a WNbMoTaV HEA with a homogeneous microstructure and high relative density. The bulk material sintered at 1500  $^{\circ}\text{C}$  had a compressive yield strength and plastic strain of 2612 MPa and 8.8%, respectively, when measured at room temperature. The outstanding mechanical properties of the WNbMoTaV HEA were attributed primarily to intrinsic solid solution strengthening, with the combined effect of grain boundary strengthening, interstitial solid solution strengthening, and Orowan strengthening. The interstitial strengthening, which was introduced by the powder metallurgical process, particularly contributed to the strength and suggested that it is an important strengthening mechanism of HEAs in general. The Hall-Petch coefficient of the

WNbMoTaV HEA was deduced to have a range of 1462 ~ 1774 MPa  $\mu\text{m}^{0.5}$  depending on the contribution of the interstitial solid-solution strengthening. The compressive yield strength of WNbMoTaV HEA fabricated using MA and SPS was much higher than that of other reported HEAs processed by arc-melting and casting.

54. The paper *Mechanical properties of Nb<sub>25</sub>Mo<sub>25</sub>Ta<sub>25</sub>W<sub>25</sub> and V<sub>20</sub>Nb<sub>20</sub>Mo<sub>20</sub>Ta<sub>20</sub>W<sub>20</sub> refractory high entropy alloys* investigates two refractory high entropy alloys with compositions near Nb<sub>25</sub>Mo<sub>25</sub>Ta<sub>25</sub>W<sub>25</sub> and V<sub>20</sub>Nb<sub>20</sub>Mo<sub>20</sub>Ta<sub>20</sub>W<sub>20</sub>, produced by vacuum arc-melting. Despite containing many constituents, both alloys had a single-phase body-centered cubic (BCC) structure that remained not only stable after exposure to 1400 °C but also disordered, as confirmed by the absence of superlattice reflections in neutron diffraction data. Compressive flow properties and microstructure development of these alloys were determined from room temperature up to 1600 °C. Limited compressive plasticity and quasi-cleavage fracture at room temperature suggest that the ductile-to-brittle transition for these alloys occurs above room temperature. At 600 °C and above, both alloys showed extensive compressive plastic strain. The yield stress of both alloys dropped by 30–40% between room temperature and 600 °C, but was relatively insensitive to temperature above 600 °C, comparing favorably with conventional superalloys. In conclusion, the phase stability, microstructure development, and mechanical behavior of two refractory high entropy alloys, Nb<sub>25</sub>Mo<sub>25</sub>Ta<sub>25</sub>W<sub>25</sub> and V<sub>20</sub>Nb<sub>20</sub>Mo<sub>20</sub>Ta<sub>20</sub>W<sub>20</sub>, were investigated from room temperature up to 1600 °C. Neutron diffraction analysis in material tested at room temperature and annealed at 1400 °C indicated that both alloys had a single-phase, BCC crystal structure. The lattice parameter for the 4-element alloy was  $a = 3.220 \text{ \AA}$ , both in as-solidified and annealed conditions. The 5-element alloy had a lattice parameter  $a = 3.185 \text{ \AA}$  in the as-solidified condition and  $a = 3.187 \text{ \AA}$  in the annealed condition. No superlattice reflections were observed at either temperature confirming that both alloys were disordered and lacked an order–disorder transition or other instability over the studied temperature range. During deformation at room temperature, the alloys showed high yield stress of 1058 MPa and 1246 MPa, but a limited ductility of about 2.0% and 1.5% of plastic strain, for the Nb<sub>25</sub>Mo<sub>25</sub>Ta<sub>25</sub>W<sub>25</sub> and V<sub>20</sub>Nb<sub>20</sub>Mo<sub>20</sub>Ta<sub>20</sub>W<sub>20</sub> alloys, respectively. Quasi-cleavage fracture by splitting along the surfaces that were almost parallel to the compression direction suggests that fracture occurred under tensile stresses and that the brittle-to-ductile transition temperature for these BCC refractory alloys is above room temperature. Over the temperature range of 600 °C–1000 °C, both alloys demonstrated good plastic flow with compressive strain exceeding 10–15% prior to localized shear accompanied by a drop in strength, suggesting that the DBTT for each alloy is located between room temperature and 600 °C. In the Nb<sub>25</sub>Mo<sub>25</sub>Ta<sub>25</sub>W<sub>25</sub> alloy, the yield stress was 561 MPa at 600 °C and it continuously decreased with temperature down to 405 MPa at 1600 °C. The V<sub>20</sub>Nb<sub>20</sub>Mo<sub>20</sub>Ta<sub>20</sub>W<sub>20</sub> alloy was ~200 MPa stronger in the temperature range of 600 °C–1200 °C. However, the yield stress of the V<sub>20</sub>Nb<sub>20</sub>Mo<sub>20</sub>Ta<sub>20</sub>W<sub>20</sub> alloy decreased more rapidly than that of the Nb<sub>25</sub>Mo<sub>25</sub>Ta<sub>25</sub>W<sub>25</sub> alloy in the temperature range of 1200 °C–1600 °C, so that its yield stress at 1600 °C (477 MPa) was close to

that of the Nb<sub>25</sub>Mo<sub>25</sub>Ta<sub>25</sub>W<sub>25</sub> alloy (405 MPa). While near-steady state flow occurred at 1200–1600 °C in the Nb<sub>25</sub>Mo<sub>25</sub>Ta<sub>25</sub>W<sub>25</sub> alloy, the V<sub>20</sub>Nb<sub>20</sub>Mo<sub>20</sub>Ta<sub>20</sub>W<sub>20</sub> alloy showed considerable softening shortly after yielding in this temperature range. This apparent softening of the 5-element alloy was concomitant with material spallation from the side surfaces of deforming samples, obfuscating stress measurement during compression, and dynamic recrystallization. Microstructural examination of both materials indicated that grain boundary sliding occurred at these temperatures. It was responsible for void formation and fracture along grain boundaries. These observations, combined with the fact that the dendritic structure was retained even at 1400 °C, anecdotally support the concept that the high configurational entropy of these alloys is capable of strongly suppressing constituent diffusivity for accommodation of the grain-boundary sliding.

55. The paper *Alloy Design and Properties Optimization of High-Entropy Alloys* reviews the recent work on the high-entropy alloys (HEAs) in our group and others. HEAs usually contain five or more elements, and thus, the phase diagram of HEAs is often not available to be used to design the alloys. We have proposed that the parameters of  $\delta$  and  $\Omega$  can be used to predict the phase formation of HEAs, namely  $\Omega \geq 1.1$  and  $\delta \leq 6.6\%$ , which are required to form solid-solution phases. To test this criterion, alloys of TiZrNbMoV  $x$  and CoCrFeNiAlNb  $x$  were prepared. Their microstructures mainly consist of simple body-centered cubic solid solutions at low Nb contents. TiZrNbMoV  $x$  alloys possess excellent mechanical properties. Bridgman solidification was also used to control the microstructure of the CoCrFeNiAl alloy, and its plasticity was improved to be about 30%. To our surprise, the CoCrFeNiAl HEAs exhibit no apparent ductile-to-brittle transition even when the temperatures are lowered from 298 K to 77 K. In conclusion, by statistically analyzing the parameters  $\delta$  and  $\Omega$  for reported multicomponent HEAs, a criterion  $\Omega \geq 1.1$  and  $\delta \leq 6.6\%$ , for forming high-entropy stabilized solid-solution phases, has been proposed, which can be used to assist in developing advanced metallic alloys. TiZrNbMoV  $x$  and CoCrFeNiAlNb  $x$  HEAs mainly contain a simple bcc solid-solution phase. Persistent bcc phase separation was observed in TiZrNbMoV  $x$ . The Nb addition induces the change of microstructures from hypoeutectic to hypereutectic structures in CoCrFeNiAlNb  $x$  alloys. An ordered hexagonal Laves phase forms with higher Nb contents. TiZrNbMoV  $x$  alloys exhibit high yielding strengths, fracture strengths, and good plasticity. Compared to the as-cast sample, the plasticity for the CoCrFeNiAl alloy synthesized by Bridgman solidification was improved by a maximum of 30%, and the morphology changes from dendrites to equiaxed grains in this alloy after Bridgman solidification. The mechanical properties of single-phase bcc AlCoCrFeNi HEA were measured at different temperatures. It is concluded that the yielding strengths and fracture strengths increase and the fracture strains change very gently as the temperatures decrease from 298 K to 77 K.
56. The paper *NbTaV-(Ti,W) refractory high-entropy alloys: Experiments and modeling* reports the design and development of ductile and strong refractory single-phase high-entropy alloys (HEAs) for high temperature applications, based on NbTaV with addition of Ti and W. Assisted by CALPHAD modeling, a single body-centered cubic

solid solution phase was experimentally confirmed in the as-cast ingots using X-ray diffraction and scanning electron microscopy. The observed elemental segregation in each alloy qualitatively agrees with CALPHAD prediction. The Vickers microhardnesses (and yield strengths) of the alloys are about 3 (and 3.5–4.4) times that those estimated from the rule of mixture. While NbTaTiVW shows an impressive yield strength of 1420 MPa with fracture strain of 20%, NbTaTiV exhibits exceptional compressive ductility at room temperature. In summary, three refractory HEAs, NbTaTiV, NbTaVW, and NbTaTiVW, were designed by CALPHAD modeling and synthesized by vacuum arc melting. A single BCC solid solution phase was observed in the as-cast alloys using a combination of XRD and SEM analyses. The following conclusions were reached: 1. While NbTaTiV is very ductile and does not fracture up to 50% strain, NbTaTiVW has a yield strength of 1420 MPa with a fracture plastic strain of 20%. 2. The Vickers microhardness values (and the yield strengths) of the HEAs are about 3 (and 3.5–4.4) times that those estimated from the rule of mixture, suggesting contribution from matrix solid solution strengthening. 3. The microsegregation behavior of the elements is closely related to their melting points, and the experimental results are consistent with CALPHAD prediction. 4. The entropies of mixing for both liquid and BCC phases for HEA NbTaTiV are predicted to be ideal. Conversely, HEAs NbTaVW and NbTaTiVW show negative departure from ideal.

57. The paper *Ab initio study of Al<sub>x</sub>MoNbTiV high-entropy alloys* investigates the Al<sub>x</sub>MoNbTiV ( $x = 0-1.5$ ) high-entropy alloys (HEAs) that adopt a single solid-solution phase, having the body centered cubic (bcc) crystal structure. Here we employ the ab initio exact muffin-tin orbitals method in combination with the coherent potential approximation to investigate the equilibrium volume, elastic constants, and polycrystalline elastic moduli of Al<sub>x</sub>MoNbTiV HEAs. A comparison between the ab initio and experimental equilibrium volumes demonstrates the validity and accuracy of the present approach. Our results indicate that Al addition decreases the thermodynamic stability of the bcc structure with respect to face-centered cubic and hexagonal close packed lattices. For the elastically isotropic Al<sub>0.4</sub>MoNbTiV HEAs, the valence electron concentration (VEC) is about 4.82, which is slightly different from VEC  $\sim 4.72$  obtained for the isotropic Group metals and refractory—HEAs. The ab initio EMTO-CPA method has been employed to study the equilibrium bulk properties of Al<sub>x</sub>MoNbTiV HEAs with Al fraction ranging between null and  $x = 1.5$ . The theoretical predictions for the equilibrium volume agree well with the available experimental data. The present calculations confirm the stability of the bcc structure relative to the two close packed lattices (fcc and hcp). The addition of Al slightly decreases the thermodynamic stability of the bcc phase, which is in contrast to the common knowledge in the case of steel alloys, for which Al is known as a strong bcc stabilizer. In absence of relevant experimental data, we have presented and discussed the trends of the calculated elastic parameters rather than focusing on their magnitudes. In particular, we have shown that the ab initio Cauchy pressure ( $c_{12} - c_{44}$ ), B/G ratio and Poisson ratio  $\nu$  of Al<sub>x</sub>MoNbTiV HEAs slightly decrease with increasing Al content. According to the Zener ratio and the polycrystalline elastic anisotropy ratio, we predict that Al<sub>x</sub>MoNbTiV HEAs become isotropic when  $x \sim 0.4$  which corresponds to VEC  $\sim 4.82$ .



58. The paper *Elastic properties of high entropy alloys by MaxEnt approach* presents the elastic properties of seven single-phase high-entropy alloys (HEAs) with excellent properties, investigated through first-principles calculations. A new method, Maximum Entropy (MaxEnt), was adopted as an algorithm to study the lattice distortion effect of HEAs. The CP2K first-principles simulation package was employed for calculation. The comparison of calculated elastic properties of TaNbHfZrTi with experimental data shows good agreement. Elastic properties of AlMoNbTiV are close to the calculated data from the Coherent Potential Approximation (CPA), and the reasons for this were discussed. The influence of lattice distortions on elastic properties was also studied. Furthermore, elastic properties of a series of refractory HEAs were predicted. These results demonstrate that the MaxEnt model can properly describe HEAs. We employed the MaxEnt method to investigate the elastic properties of HEAs. All the above HEAs are single-phase HEA. Comparing the data from EMTO-CPA with MaxEnt, MaxEnt is a feasible algorithm to study HEAs and even has advantages to study the influences of local environment. The good agreement between theoretical (with lattice distortion) and measured elastic properties of TaNbHfZrTi further proves its reliability. The theoretical results of TaNbHfZrTi (without lattice distortion) demonstrate that lattice distortion is one of the main features of HEAs, which should be considered. Moreover, MaxEnt structure has the potential to describe the HEAs which have four to ten elements, even unequal concentrations.

59. The paper *Ab initio design of elastically isotropic TiZrNbMoVx high-entropy alloys* investigates the TiZrVNb and TiZrNbMoVx ( $x = 0-1.5$ ) high-entropy alloys (HEAs), which are single-phase solid solutions having the body-centered cubic crystallographic structure. The ab initio exact muffin-tin orbitals method, in combination with the coherent potential approximation, is used to study the equilibrium bulk properties of the above refractory HEAs. A detailed investigation of the effect of alloying elements on the electronic structure and elastic parameters is provided. The results indicate that vanadium enhances the anisotropy of TiZrNbMoVx. As an application of the present theoretical database, the study verifies the often-quoted correlation between the valence electron concentration (VEC) and the micro-mechanical properties in the case of multi-component alloys. Furthermore, it is predicted that the present HEAs become elastically isotropic for VEC approximately 4.72. Ab initio alloy theory has been employed to investigate the electronic structure and the basic bulk properties of TiZrVNb and TiZrNbMoVx HEAs consisting of refractory transition metals. The calculated equilibrium volumes are consistent with the available experiment and the estimated Wigner–Seitz radii. All HEAs considered here are predicted to adopt the bcc structure. The calculated electronic structure of the Mo-containing HEAs indicates anomalous temperature dependence for the elastic parameters of Mo-containing alloys, which should be confirmed by further theoretical and experimental studies. The valence electron concentration increases with increasing V content and shows good correlation with the trends of the polycrystalline elastic moduli and also with the enhanced ductility of TiZrNbMoVx alloys. Except for the Mo-free alloy, all the other HEAs are obtained

to be nearly isotropic. Vanadium addition is predicted to introduce a small anisotropy in TiZrNbMo. The present theoretical trends suggest that the elastic anisotropy of these materials can be fine-tuned by adjusting the composition. It is proposed that by properly balancing the V/Mo content, the TiZrNbMoV<sub>x</sub> alloys can be made fully isotropic. Indeed, it is shown that specific V/Mo content lead to isotropic alloys. Furthermore, it is found that a particular VEC is the criterion for elastic isotropy in refractory HEAs. Since the present results correspond to static conditions, the above conclusion is valid only at low temperatures. Due to the particular electronic structure of the refractory HEA alloys, the elastic anisotropy is expected to depend strongly on temperature. The present theoretical study is a pioneering work describing the bulk properties of refractory HEAs using first-principles theory. In the absence of experimental data, the calculated elastic parameters represent the first predictions that should be verified by experiments.

60. The paper *Alloying effect on the elastic properties of refractory high-entropy alloys* uses ab initio total energy calculations to determine the elastic properties of TiZrVNb, TiZrNbMo, and TiZrVNbMo high-entropy alloys in the body-centered cubic (bcc) crystallographic phase. Calculations are performed using the Vienna Ab initio Simulation Package and the Exact Muffin-Tin Orbitals methods, with compositional disorder treated within the frameworks of the special quasi-random structures technique and the coherent potential approximation, respectively. Special emphasis is given to the effect of local lattice distortion and trends against composition. Significant distortion can be observed in the relaxed cells, which result in an overlap of the first and second nearest neighbor (NN) shells represented in the histograms. When going from the four-component alloys TiZrVNb and TiZrNbMo to the five-component TiZrVNbMo, the changes in the elastic parameters follow the expected trends, except that of C<sub>44</sub>, which decreases upon adding equiatomic Mo to TiZrVNb despite the large shear elastic constant of elemental Mo. Although the rule of mixtures turns out to be a useful tool to estimate the elastic properties of the present HEAs, to capture the more delicate alloying effects, one needs to resort to ab initio results. The elastic properties of bcc TiZrVNb, TiZrNbMo, and TiZrVNbMo random alloys were studied using two first-principles methods in combination with two techniques for random alloys. First, the DFT tools (VASP and EMTO) were assessed by comparing the two sets of ab initio bulk parameters with the available experimental data for pure elements. The two methods provide consistent equations of states for bcc Ti, Zr, V, Nb, and Mo, but systematic deviations are observed for the single-crystal elastic constants, especially for C<sub>12</sub> and C<sub>44</sub>. None of these methods in combination with the present DFT approximation (PBE) is able to provide highly accurate results for all elastic parameters. This means that alloying effects should always be discussed with respect to the data for end members obtained using the same underlying DFT tool. In general, the ab initio results obtained with CPA and SQS for the present HEAs are consistent with each other. Local lattice distortions were investigated by the use of SQS cells and the VASP method. LLD has a significant impact on the mixing energy. Neglecting this effect can lead to strongly overestimated enthalpy of formation, and thus such rough data is completely useless to draw any conclusions concerning the solid solution formation. On the other hand, LLD has a very small effect on the equation of state and elastic constants. For these

properties, CPA is clearly superior to SQS as it gives more flexibility for the number of components and deviations from equiatomic compositions. The two DFT tools in combination with the two alloy theories efficiently complement each other in the ab initio description of complex alloys. The magnitude of the LLDs was measured for the three HEA systems here using histograms to show the data. Here, we were ultimately interested in quantifying the degree of the distortion. An overlap of the first and second nearest neighbor shell was observed in TiZrVNb, TiZrNbMo, and TiZrVNbMo, meaning that significant distortions exist in the relaxed cells. We also studied the alloying effects and found large deviations from the trends expected from simple estimates. In particular, when equiatomic Mo is added to TiZrVNb, the C44 elastic parameter decreases or slightly increases (depending on the employed DFT solver and alloy theory) despite the fact that Mo has the largest C44 among all metals and alloys considered here. Having computed all necessary data for the pure end members and alloys, we had the possibility to assess the rule of mixtures for HEAs. The estimated elastic parameters are found to be rather close to the values obtained from the CPA and SQS calculations, especially on the scale of the present values (0–250 GPa). But this simple estimate turned out to be too rough to resolve delicate alloying effects like the one seen for C44 of TiZrNbMo and TiZrVNbMo. Nevertheless, when based on data obtained for the same crystal lattice, the rule of mixtures can provide very useful first-level estimates for the values of the lattice parameters and elastic constants, including general trends.