MM 14: Topical session (Symposium MM): High entropy and compositionally complex alloys

Sessions: Properties II and Diffusion

Time: Tuesday 10:15–13:15 Location: H43

Topical Talk MM 14.1 Tue 10:15 H43

Nanocrystalline high-entropy alloys studied by atomistic computer simulations — Daniel Utt, Leonie Koch, Alexander Stukowski, and •Karsten Albe — TU Darmstadt, FB 11, FG Materialmodellierung, Otto-Berndt-Str. 3, D-64287 Darmstadt

The superior mechanical properties of high-entropy alloys (HEA) can be mainly attributed to the fact that multiple principle elements tend to strengthen materials markedly by the solid-solution hardening mechanism. Randomly distributed elements in grain interiors can, however, also affect relative grain-boundary energies and minimize thermodynamic driving forces for grain- boundary migration. Moroever, segregation may occur at grain boundaries and work as barriers to prevent grain-boundary motion. These effects become particular imporant in the small grain-size regime. In this contribution results from combined molecular dynamics and Monte-Carlo simulations for a four-component model alloy are presented, which were carried out using an embedded-atom approach and an average potential method. After discussing the impact of local disorder on phonons and stacking fault energies, we present results on the structure and mobility of grain boundaries in bicrystal geometry and compare to result obtained from polycrytalline model structures. The simulations provide no evidence for a change in migration mechanisms, but show the influence of GB segregation and secondary phase formation. Furthermore, samples are studied under mechanical load and deformation mechanisms -in particular twin formation- are investigated.

MM 14.2 Tue 10:45 H43

Quinary TWIP-TRIP high-entropy alloys: design, microstructure and mechanical properties — •Xiaoxiang Wu, Yuji Ikeda, Fritz Körmann, Dierk Raabe, and Zhiming Li — Max-Planck-Institut für Eisenforschung,Düsseldorf,Germany

Quinary FeMnNiCoCr HEAs have shown great potential in obtaining excellent combination of strength and ductility. By adjusting the atomic ratios of the five principal elements to reach appropriately low stacking fault energy (SFE), twinning-induced plasticity (TWIP) and/or transformation-induced plasticity (TRIP) effects can be introduced in the non-equiatomic quinary FeMnNiCoCr HEAs, leading to enhanced strength, ductility and working hardening capacity compared to the equiatomic HEA. In the present work, we combine ab initio calculation and experimental investigation to design various non-equiatomic quinary Fe60-x-yMnxNiyCo20Cr20 (at.%) HEAs. Three typical HEA compositions with comparably low SFE were chosen and alloys were then prepared and characterized. The results show that enhanced work hardening has been achieved by changing Ni concentration from 11 at.% to 6 at.% in the probed HEA system. In spite of the similar SFE level, the three HEAs under investigation demonstrate different primary deformation modes, changing from TRIP-dominant (with considerable TWIP), complete TWIP to TWIP-dominant (with negligible TRIP). The influences of SFE and the individual elements on the deformation modes are discussed to provide new insights into the further design of quinary TWIP-TRIP HEAs.

MM 14.3 Tue 11:00 H43

Strengthening in solid solutions of the system Au-Cu-Ni-Pd-Pt — •Felix Thiel[1,2], Christina Bollnow[1,2], Jens Freudenberger[1,3], David Geissler[1], Alexander Kauffmann[4], Hans Chen[4], Martin Heilmaier[4], and Kornelius Nielsch[1,2] — [1]IFW Dresden, Helmholtzstr. 20, 01069 Dresden — [2]TU Dresden, Institut für Werkstoffwissenschaft, Helmholtzstr. 7, 01069 Dresden — [3]TU Bergakademie Freiberg, Institut für Werkstoffwissenschaft, Gustav-Zeuner-Str. 5, 09599 Freiberg — [4]KIT, Institut für Angewandte Materialien - Werkstoffkunde, Engelbert-Arnold-Str. 4, 76131 Karlsruhe

High Entropy Alloys (HEAs) show outstanding mechanical and physical properties, which would not have been expected upon their simple crystal structure and the fact that they are single phased. The Au-Cu-Ni-Pd-Pt system and their including subsystems show crystallization into the same Cu-type crystal structure within the whole concentration range. Therefore,this system is unique and particularly suitable to study the alloying effect on the properties within a large concentration range without the necessity of considering other phases. The present study shows the effect of alloying a multi-component solid solution on the properties of medium and high entropy alloys in this system. In particular, effects such as solid solution hardening and work hardening are assessed.

MM 14.4 Tue 11:15 H43

abnormal magnetic behavior of FeNiCoMnCu high entropy alloys — •ziyuan rao[1], zhiming li[1], fritz körmann[1,2], biswanath dutta[2], dirk ponge[1], lukas schäfer[3], konstantin skokov[3], oliver gutfleisch[3], and dierk raabe[1] — [1]Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Straße 1, 40237 Düsseldorf, Germany — [2]Materials Science and Engineering, Delft University of Technology, 2628 CD Delft, The Netherlands — [3]Institut für Materialwissenschaft, Technische Universität Darmstadt, Darmstadt, Germany

In this project experimental and theoretical calculations are combined to unveil an abnormal magnetic behavior caused by the addition of nonmagnetic element Cu in face-centered cubic FeNiCoMn-based high entropy alloys (HEAs). We found that saturation magnetization of the as-cast HEAs at room temperature increases by 77% and 177% at Cu contents of 11 at. % and 25 at. %, respectively, compared to the equiatomic FeNiCoMn HEA without Cu addition. For HEAs homogenized at 1273 K for 2 h and water-quenched, the magnetic state transforms from paramagnetism to ferromagnetism at room temperature after 25 at. % Cu addition. For homogenized HEAs, ab initio calculations reveal an increase of Curie temperature caused by Cu addition and agree well with experimental results. By coupling the experimental and theoretic results, we unveiled the mechanisms responsible for the Cu effect on the magnetic properties of FeNiCoMn HEAs, which is fundamentally different from that reported in conventional binary or ternary alloys.

15 min. break

Topical Talk MM 14.5 Tue 11:45 H43

Bulk and grain boundary diffusion in high entropy alloys — •Mayur Vaidya, Sandipan Sen, Daniel Gartner, Gerhard Wilde, and Sergiy Divinski — Institute of Materials Physics, University of Münster, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany

An intriguing aspect of High entropy alloys (HEAs) is their diffusion behaviour and there is yet a lack of consensus on the factors governing atomic transport rates in HEAs. The present talk attempts to provide a critical analysis of the diffusion measurements reported so far for HEAs and gives glimpses of current diffusion studies being performed at the research lab of University of Münster. The anticipated *sluggish* diffusion is clearly absent in FCC CoCrFeNi and CoCrFeMnNi HEAs, both in the lattice and along grain boundaries. Ni is slowest diffusing species in both the HEAs, while Mn diffusion is fastest in the quinary HEA. The diffusion rates are lower (by maximum an order of magnitude) in these HEAs when compared to lower component alloys only when a homologous temperature scale is used for the comparison. Diffusivity measurements in single crystals of these HEAs have hinted towards a possible contribution of dislocations to the penetration profile. The preliminary results of solute diffusion in HCP HEAs are also presented.

MM 14.6 Tue 12:15 H43

Radiotracer diffusion in single crystalline CoCrFeNi and CoCrFeMnNihigh entropy alloys — •Daniel Gaertner[1], Josua Kottke[1], Yury Chumlyakov[2], Gerhard Wilde[1], and Sergiy V. Divinski[1] — [1]Institute of Materials Physics, University of Münster, Münster, Germany — [2]Department of Physics of Metals, Tomsk State University, Tomsk, Russia.

High entropy alloys are multicomponent alloys, which consist of five or more elements in equiatomic or nearly equiatomic concentrations. These materials are hypothesized to show significantly decreased self-diffusivities. For the first time, diffusion of all constituent elements in equiatomic CoCrFeNi and CoCrFeMnNi single crystals and additionally solute diffusion of Mn in the quaternary alloy is investigated using the radiotracer technique, thereby the tracer diffusion coefficients of

^{57}Co, ^{51}Cr, ^{59}Fe, ^{54}Mn and ^{63}Ni are determined in a temperature range between 923 K and 1373 K. The components are characterized by significantly different diffusion rates, with Mn being the fastest element and Ni and Co being the slowest ones in the quinary composition. In the quaternary composition Mn and Cr are the slowest elements at low temperatures and the situation is reversed with increasing temperature. Furthermore, solute diffusion of Cu in the CoCrFeNi single crystal is investigated in the temperature range of $973 - 1173$ K using the ^{64}Cu isotope. In the quaternary alloy, Cu is found to be a fast diffuser at the moderate temperatures below 1273 K and its diffusion rate follows an Arrhenius law with an activation enthalpy of about 149 kJ/mol.

MM 14.7 Tue 12:30 H43

Heat capacity, defect annihilation and tracer diffusion in the Ni–CoCrFeMn system: transition from a dilute solid solution to a high entropy alloy — •Josua Kottke[1], Jonas Lübke[1], Adnan Fareed[1], Daniel Gaertner[1], Mathilde Laurent-Brocq[2], Loïc Perrière[2], Łukasz Rogal[3], Sergiy V. Divinski[1], and Gerhard Wilde[1] — [1]Institute of Materials Physics, University of Münster, Münster, Germany — [2]Université Paris Est, ICMPE (UMR 7182), CNRS, UPEC, F-94320, Thiais, France — [3]Institute of Metallurgy and Materials Science of the Polish Academy of Sciences, 30-059 Krakow, Poland

High-entropy alloys, i.e. multicomponent alloys with a large number of constituting elements in equiatomic or nearly equiatomic composition, attract an increased attention as potential structural materials due to their favorable physical and mechanical properties, especially at elevated temperatures. Here, we report on the changes in thermodynamic and kinetic properties regarding the transition from a dilute solid solution to a high entropy alloy.

The true heat capacity and tracer diffusion of all elements are measured in $Co_{20}Cr_{20}Fe_{20}Mn_{20}Ni_{20}$, $Co_{10}Cr_{10}Fe_{10}Mn_{10}Ni_{60}$ and $Co_2Cr_2Fe_2Mn_2Ni_{92}$ and compared to those in pure Ni. Furthermore, the annihilation of deformation-induced vacancies and the recrystallisation kinetics are investigated using differential scanning calorimetry. While tracer diffusion does not reveal any abrupt transition, the defect evolution and the microstructural response are shown to be distinct in the $Co_{10}Cr_{10}Fe_{10}Mn_{10}Ni_{60}$ alloy.

MM 14.8 Tue 12:45 H43

Solute diffusion in HCP high entropy alloys — •Sandipan Sen[1], Mayur Vaidya[1], Lukasz Rogal[2], Blazej Grabowski[3], Sankaran Shanmugam[1,4], Gerhard Wilde[1], and Sergiy Divinski[1] — [1]Institute of Materials Physics, University of Münster, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany — [2]Institute of Metallurgy and Materials Science of the Polish Academy of Sciences, 30-059 Krakow, Poland — [3]Max-Planck-Institut für Eisenforschung GmbH D-40237 Düsseldorf, Germany — [4]Department of Metallurgical and Materials Engineering, Indian Institute of Technology Madras, Chennai-600036, India

Diffusion studies in high entropy alloys are still scarce and practically limited to FCC systems. For the first time, diffusion in HCP high entropy alloys is investigated using a radiotracer technique. Diffusion of Co (the so-called ultra-fast diffuser in α-Ti) is systematically measured in HfZr, HfZrTi, and Al-Hf-Sc-Ti-Zr alloys in the temperature range between 400°C - 800°C and, thus, the impact of the number of constituting elements on solute diffusion is examined. Two quinary systems (Al15Hf20Sc10Ti20Zr20 and Al5Hf20Sc20Ti20Zr20) are studied to elucidate the influence of the Al addition and of a possible short-range ordering on ultra-fast diffusion. The phase composition of the alloys was characterized by X-ray diffraction and transmission electron microscopy. The temperature dependence of the diffusion coefficients of Co is shown to follow Arrhenius behavior for all the alloys. The obtained results are compared on the homologous temperature scale with the solute diffusivities in other HCP matrices.

MM 14.9 Tue 13:00 H43

Microstructure and diffusion behavior of pseudobinary multicomponent intermetallic compounds — •Mohan Muralikrishna Garlapati[1,2], Mayur Vaidya[2], Gerhard Wilde[2], Kaustubh N. Kulkarni[3], Sergiy Divinski[2], and Murty B.S.[1] — [1]Department of Metallurgical and Materials Engineering, Indian Institute of Technology Madras, Chennai 600036, India — [2]Institute of Materials Physics, University of Muenster, Muenster 48149, Germany — [3]Indian Institute of Technology Kanpur, Kalyanpur, U.P. 208 016, India

The current study investigates the possible formation of ordered B2 intermetallic compounds with the addition of multiple elements. In order to have the advantage of a light weight and high strength, a novel pseudo binary approach has been employed for alloy synthesis from binary to quinary. In each alloy, Al content is maintained as 50 at.% and other elements (Co, Fe, Mn and Ni) constitute the remaining 50 at.%. The alloys have been processed using vacuum arc melting followed by suction casting. Synthesized alloys have been homogenized at 1100° C for 5 days. X-ray diffraction analysis confirms the presence of B2 phase in all the alloys. Scanning electron microscopy validates a uniform phase composition and coarse grain microstructure. Self-diffusivities of the constituent elements in each of the alloys have been determined at 1100° C using radiotracer technique. Diffusion coefficients have been measured using tracer penetration profiles and are compared with literature and the impact of multi-element matrix on diffusion is discussed.