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Local-to-average crystal structures and mechanical properties in High-Entropy and Compositionally Complex fcc, bcc and hcp-based alloys studied by synchrotron methods

New technologies require high operating temperatures for many applications. The research into refractory HEAs (RHEAs) is motivated by their potential to rival Ni-based superalloys, limited by melting and solvus temperatures **[Senkov2018]**. From the beginning, the *bcc*-based RHEAs attracted interest because of their ability to retain strength up to 1600°C, contrarily to the *fcc*-based ones. However, most of them show ductility only in compression, and only few of them have a practical tensile ductility at room temperature, due to a drastic rise of the ductile-to-brittle transition temperature, a mechanism not yet fully understood **[Senkov2018]**. The *bcc*-based RHEAs that show at least some tensile ductility are mostly based on the Ti–Zr–Nb–Hf–Ta system: the as-cast *bcc* equiatomic TiZrNbHfTa alloy shows high strength (σ_y of 800-1000 MPa), good ductility at room temperature (tensile plastic strain >10%), and can be heat treated in single phase *bcc* structure **[Senkov2018]**. On the other hand, *hcp*-HEAs are still rare, as they can intrinsically suffer from brittleness due to the limited number of slip systems. Recently, an Al-Sc-Ti-Zr-Hf system was investigated by mainly computational methods by **Rogal2017**, resulting in a new *hcp*-structured HEA showing a partially ordered crystal structure ($D0_{19}$-type superstructure), never shown before in *hcp*-based HEA, and a fully disordered *hcp*-A3 structure, depending on the annealing temperature. Its ordered-disordered phase transition is of great interest for investigating the local chemical ordering and its relation to the mechanical properties in both phases, such as hardness values and compressive stress-strain plots, shown in **Rogal2017**.

In this project, an overall comparison between a typical *fcc*-based compositionally complex alloy composed by transition metal elements, $Al_8Co_{17}Cr_{17}Cu_8Fe_{17}Ni_{33}$ (*cf.* results reported e.g. in **Fantin2020**, **Kasatikov2021**), the most investigated in literature *bcc* RHEA (TiZrHfNbTa), and a novel *hcp* based HEA ($Al_{15}Sc_{10}Ti_{25}Zr_{25}Hf_{25}$) will be carried out based on a structural point of view. The different solid grounds for the alloy choice were established on the experimental experience raised during the first part of the SPP funding period (*cf.* BA1170/39-1). The main question this project aims to answer is the following: *will the high entropy concept, based on ordering and distortions in the solid solution, be different depending on the crystal structure?*

Several experimental synchrotron techniques will be employed: X-ray absorption spectroscopy, High-resolution X-ray diffraction and Pair Distribution Function, investigating in detail the crystal structure at all spatial scales. Focus will be, more specifically, on local distortions and their spatial extension, preferred bonding partners, atomic size change upon alloying, order-disorder phase transition (*hcp* alloy) and correlation to mechanical properties such as diffusion, hardness and those derived from tensile testing.

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[Fantin2020] Fantin et al., Acta Materialia **193**, (2020) Pages 329-337

[Kasatikov2021] Kasatikov et al., **857** (2021) 157597

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[Senkov2018] Senkov et al., *J. Materials Research* **33**, (2018), 3092-3128