Precipitate phase and local strain in high-entropy alloys: A first-principles assessment

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Multi-component systems with predominantly simple phase are an area of current focus in alloy development. Termed High Entropy Alloys (HEAs), different empirical rules have been introduced to understand phase formation in these systems, and determine what the dominant phases may be. The mixture of bcc/fcc in Fe-based HEAs materials is expected to possess balanced mechanical properties, e.g., both high strength and good ductility. However, experimental investigation has revealed that the micro-structures of certain "HEAs" can be very complicated since they often undergo the spinodal decomposition, and ordered and disordered phase precipitate at lower temperatures. Our recent studies of phase stability of ternary fcc and bcc Fe-Cr-Ni alloys using a combination of density functional theory (DFT) with both conventional and magnetic cluster expansion methods show that the dependence of local chemical short-range orders as function of temperature and composition can be the origin of precipitate phases present in HEAs [1]. In the first part of this talk, an integrated modelling and experimental approach is proposed for magnetic HEAs systems by taking electronic structure effects into account in prediction of the phase most likely too be found in multi-component alloys. Good agreement is found when the calculations are confronted with data from experiments, including new magnetic HEAs system CoFeNiV where the precipitate σ phase is predicted to be more stable than the fcc one when the valence electron concentration n $\leq$ 7.6 [2].

In the second part of this contribution, a methodology to investigate one of the main contributions to the yield strength from solid solution hardening (SSH) in HEAs is proposed by comparing DFT calculations and atomistic simulations that accurately describe the distortion in the lattice produced by the interaction of the different chemical species. The benchmark HEAs are the equimolar bcc MoNbWTaV and its 5 sub-quaternary systems [3]. The local atomic strains are described by the forces acting between different pairs of atoms. The interatomic spacing distribution is obtained by imposing force equilibrium for all atomic bonds. The effect of short-range order, which deviates the lattice configurations from randomness, can be studies by means of a elastic system, where the first and second nearest neighbours of each atom are the most influential. The atomic coordinates computed by this method can be used as a better starting point for DFT calculations and to quantify the SSH in HEAs.

Finally, we briefly discuss a generalisation of the first-principles assessment for the radiation-induced segregation phenomenon in a non-equilibrium system of multi-component alloys [4].

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