Ab initio design of high entropy alloys

We recently studied various aspects of multi-principal element alloys or often called high entropy alloys (HEAs). HEAs have attracted remarkable attention since their discovery in 2004 due to their various excellent materials properties and the sheer endless possibilities to explore new alloys. The alloys are mostly investigated by experiments, but ab initio calculations have emerged as a powerful approach that complements experiment and can serve as a predictive tool to explore materials properties of new promising alloys.

Two examples are given below. In [1] we utilized a combination of ab initio calculations by means of density functional theory (DFT) and lattice Monte Carlo simulations. Effective chemical interactions are computed based on DFT. We identified a sequence of transitions from the ground state to the solid solution and identified the chemical ordering temperatures.

Fig. 1: Sketch of ordering in bcc NbMoTaW refractory HEA.

At high temperatures, materials properties are strongly affected by lattice vibrations (phonons). Phonons critically influence thermal stability, thermodynamic and elastic properties, as well as thermal conductivity. In contrast to perfect crystals and ordered alloys, the inherently present mass and force constant fluctuations in HEAs can induce significant phonon scattering and broadening. We employed DFT calculations to systematically study the impact of force constant and mass fluctuations on the phonon spectral functions of 12 bcc random alloys, from binaries up to 5-component HEAs, addressing the key question of how chemical complexity impacts phonons.

Fig. 2: Sketch of phonon broadening for eight different refractory alloys, from binaries up to 5-component HEAs.

KEY PUBLICATIONS in 2017

OTHER ACHIEVEMENTS in 2017
- VIDI grant (NWO/STW)
- Invited talk at TMS (March ‘17, San Diego, USA)