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Hybrid MC/MD Method For High Entropy Alloy[1] BOJUN FENG, MICHAEL WIDOM, Carnegie Mellon University — High entropy alloys (HEA) are materials that contain multiple components of elements consisting of a single solid solution phase which could make the entropy of mixing very high. From recent investigations, HEAs possess promising properties such as strength at high temperature, tensile strength, thermal stability and corrosion resistance. In this talk, a hybrid Molecular Dynamics (MD)/Monte Carlo (MC) simulation method is introduced to the computational analysis of HEA, treating atomic displacement by MD as well as swapping atomic species by MC. This method efficiently models the phase separation and short range order by swapping between different types of atoms, while structural deviation from the perfect lattice sites of atoms is equilibrated quickly by MD. We apply this method to HfNbTaZr HEA modeled using an embedded-atom potential. The result gives a strong phase separation of Hf-Zr and Nb-Ta pairs shown by the pair correlation function. Diffuse scattering patterns are predicted and compared to experiments.

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