Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Prediction of high entropy alloys with sublattice order BOJUN FENG, MICHAEL WIDOM, Carnegie Mellon Univ, WALTER STEURER, ETH Zurich — Multicomponent high entropy alloys form simple Bravais lattice structures such as body-centered cubic (Pearson type cI2), in which all species occupy every lattice site equally. Here we seek to generalize this notion to lattices with inequivalent sites, such as with cube vertex and body center favoring different subsets of species (Pearson type cP2), or more complex order with three inequivalent sites (Pearson type cF16). A thorough investigation of stability of Al-TM1-TM2 (TM=Transition Metal) BCC-based ternary alloys is done by means of first principles DFT calculation. Energies of disordered structures are estimated using special quasi-random structures (SQS), where those special quasi-random structures are artificial structures that have the same short range order as cP2 and cI2 up to as many as several nearest neighbors. Application of a simple entropy model predicts sequences of temperatures over which differing degrees of order are stabilized up to the alloy melting point. Comparing with experiment, we find substantial but not complete agreement with experiment in cases where the phase diagrams are known. The source of disagreement is analyzed. Additionally, we find many examples where we predict partially ordered structures that have not yet been reported experimentally.

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Date submitted: 03 Nov 2016 Electronic form version 1.4