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Prediction of A2 to B2 Phase Transition in the High Entropy Alloy Mo-Nb-Ta-W[1] WILLIAM HUHN, MICHAEL WIDOM, Carnegie Mellon University — In this talk we show that an effective Hamiltonian fit with first principles calculations predicts an order/disorder transition occurs in the high entropy alloy Mo-Nb-Ta-W. Using the Alloy Theoretic Automated Toolset, we find T=0K enthalpies of formation for all binaries containing Mo, Nb, Ta, and W, and in particular we find the stable structures for binaries at equiatomic concentrations are close in energy to the associated B2 structure, suggesting that at intermediate temperatures a B2 phase is stabilized in Mo-Nb-Ta-W. Our "hybrid Monte Carlo/molecular dynamics" results for the Mo-Nb-Ta-W system are analyzed to identify certain preferred chemical bonding types. A mean field free energy model incorporating nearest neighbor bonds will be presented, allowing us to predict the mechanism of the order/disorder transition. We find the temperature evolution of the system is driven by strong Mo-Ta bonding. Comparison of the free energy model and our MC/MD results suggest the existence of additional low-temperature phase transitions in the system likely ending with phase segregation into binary phases.

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