Abstract Submitted
for the 4CF09 Meeting of
The American Physical Society

Platinum-Palladium Crystal Structures WESTON PRATT, BYU — Being able to predict Platinum-Palladium ordering is important in discovering new alloys that have commercial and industrial applications. Using direct quantum mechanical calculations coupled with a lattice-based Hamiltonian called a cluster expansion, we can predict which crystal structures are thermodynamically stable for. In addition, a Monte Carlo simulation can be used in this model to determine the order-disorder transition temperatures. Knowing which structures are thermodynamically stable and their respective transition temperatures may help develop useful platinum palladium alloys.

Weston Pratt
BYU

Date submitted: 29 Sep 2009 Electronic form version 1.4