

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

New potential structure for jewelry application. Does it exist in Pt-Mo, Pt-Hf, or other systems? ERIN GILMARTIN, JACQUELINE CORBITT, GUS HART, Brigham Young University — The only known intermetallic structure with an 8:1 stoichiometry is that of Pt_8Ti . It is intriguing that an ordered phase would occur at such low concentrations of the minority atom, but this structure occurs in about a dozen binary intermetallic systems. The formation of an ordered phase in an alloy can significantly enhance the performance of the material, particularly the hardness. We have taken a broad look at possible systems where this phase forms. Using first-principles, we calculated the stability of this structure relative to experimentally known phases for more than 70 Pt/Pd binary systems. We find the Pt_8Ti structure is a possible ground state in more than 20 cases. Our experimental collaborators have verified our prediction in Pt-Mo and observed order-hardening in Pt-Hf. We discuss the discovery of new ground states via the cluster expansion that are likely to be verified experimentally and their impact on Pt- and Pd-based jewelry and catalysts.

Erin Gilmartin
Brigham Young University

Date submitted: 25 Sep 2009

Electronic form version 1.4