

Abstract Submitted
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New structures in Pd-rich ordered alloys¹ JACQUELINE CORBITT, ERIN GILMARTIN, GUS HART, BYU-Provo — An intriguing intermetallic structure with 8:1 stoichiometry was discovered in the 1950s in the Pt-Ti system. Since then a handful of other Pt/Pd/Ni-X binary systems have been observed to exhibit this curious structure (Pt₈Zr, Pd₈Mo, Ni₈Nb, etc). Precipitates of this ordered structure can significantly increase the hardness of an alloy. For jewelry applications involving Pt and Pd, international hallmarking standards require that the alloys be at least 95% pure by weight. However, Pt- and Pd-rich alloys are often soft when purity is high if the minority atoms are disordered. Because the 8:1 structure maintains a high weight percentage of Pt/Pd, it can satisfy purity standards while increasing performance. Recent calculations and experiments suggest that the 8:1 structure may form in about 20 previously unsuspected Pt/Pd binary systems. Using first-principles calculations and cluster expansion modeling, we have performed a ground state search to find the stable structures in Pd-Nb, Pd-Cu, and Pd-Mg, and predict the temperatures at which the new structures may form.

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