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New structures in Pd-rich ordered alloys JACQUELINE CORBITT, ERIN GILMARTIN, GUS HART, Brigham Young University — 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 binary systems have been observed to exhibit this curious structure (Pt_8Zr , Pd_8Mo , Ni_8Nb , etc). 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 and Pd-Cu. In collaboration with Candace Lang's group at University of Capetown South Africa, we are working to experimentally validate the predicted ground states.

Prefer Oral Session
 Prefer Poster Session

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