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New structures in Pd-rich ordered alloys[1] JACQUELINE CORBITT, ERIN GILMARTIN, GUS HART, Brigham Young University, Provo UT 84602 — An intriguing intermetallic structure with 8:1 stoichiometry was discovered in 1959 in the Pt-Ti system. Since then a handful of other Pt/Pd/Ni binary systems have been observed to exhibit this 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 too soft for jewelry applications when purity is high and the minority atoms are disordered. Because the 8:1 structure maintains a high weight percentage of Pt/Pd, it can satisfy hallmarking 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.

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