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Cluster Expansion for Pt/Pd-Al binary alloys DEREK CARR, Brigham Young University — Pure platinum and pure palladium are too soft for typical jewelry applications. Adding small amounts of other metals can significantly increase their performance. However, international hallmarking standards require the alloys to be 95% pure by weight. How does one achieve significant improvements in performance adding only small amounts (5 wt-%) of other metals? Significant improvements are possible with small additions when the added element forms an ordered array in the Pt/Pd matrix. Our task is to identify, among an infinite set of possibilities, arrangements that are stable and which will form easily. One solution is to use a cluster expansion. A cluster expansion is a fast method which can calculate the energy of all candidate crystal superstructures. Using the cluster expansion, we identify the "ground states," the atomic arrangements that are the most stable. After the ground states are identified, Monte Carlo simulations are used to predict the order-disorder transition temperatures. The transition temperatures indicate the feasibility of making the ordered alloys in the laboratory.

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