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Thermodynamically stable superstructures in binary alloys
LANCE NELSON, Brigham Young Universty — Adding a second metal to another can induce the formation of ordered superstructures. These ordered phases have properties that are desireable in many industrial, manufacturing and technological applications. Our goal is to find which of the thousands of possible superstructures are thermodynamically stable through the use of computational tools. Owing to the many superstructures that are possible, as well as the complex nature of some of these, DFT calculations become impractical for searching for these superstructures. We employ a cluster expansion method, which uses energy information from a relatively small number of structures and fits that information to a set of interaction types. Because the resulting expansion provides a fast way to compute energies, we can use it to calculate the energies of the thousands of other superstructures. Specifically, I discuss the use of the cluster expansion on two binary alloys: AgPd and MgZn. Palladium alloys are of interest in the fabrication of jewelry, and a stable ordered phase at some concentrations would be a breakthrough for the jewelry manufacturers. Magnesium alloys are of interest because of their strength and light weight. They are being used increasingly in the manufacturing of things such as airplanes and automobiles. A cheap alloying agent that promotes the formation of an ordered structure would be a breakthrough.

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