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Generalized Kanzaki-Krivoglaz model of lattice relaxations in concentrated size-mismatched substitutional alloys applied to Cu-Au and Fe-Pt systems IVAN ZHURAVLEV, JOONHEE AN, KIRILL BELASHCHENKO, Department of Physics and Astronomy and Nebraska Center for Materials and Nanoscience, University of Nebraska-Lincoln, Lincoln, Nebraska 68588, USA — A generalization of the Kanzaki-Krivoglaz model to concentrated alloys was developed and applied to $Cu_{1-x}Au_x$ and $Fe_{1-x}Pt_x$ alloys at x = 0.25, 0.5, and 0.75. This model is based on many-body cluster expansions of the configuration-dependent Kanzaki forces and force constants defined with respect to the ideal fcc lattice. The parameters of these expansions were directly fitted to the forces calculated from first-principles for a number of ordered structures at fixed concentration and volume. The Kanzaki forces are dominated by nearest-neighbor terms, which are strongly asymmetric between the atomic species. This asymmetry leads to a non-pairwise effective interaction with a long-range elastic singularity. The ability to capture this singular non-pairwise interaction accurately is a major advantage of the generalized Kanzaki-Krivoglaz model. The comparison of the predicted stable phases and ordering temperatures with experiment is generally favorable; while the prediction for $Cu_{0.25}Au_{0.75}$ is wrong due to a known failure of semi-local functionals, the remaining discrepancies for $Cu_{0.5}Au_{0.5}$ and $Fe_{0.25}Pt_{0.75}$ are attributed to the contributions from the strong tetragonal striction in the $L1_0$ phase and of magnetic disorder, respectively.

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