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Strain-induced interactions in size-mismatched alloys: A Kanzaki force approach[1] ALEJANDRO DIAZ-ORTIZ, OLEG SHCHYGLO, VLADIMIR BUGAEV, HELMUT DOSCH, ALEXANDER UDYANSKY, HARALD REICHERT, Max Planck Institute for Metals Research, RALF DRAUTZ, Department of Materials, University of Oxford — A perturbative approach to determining the strain-induced effective interactions in binary alloys with large atomic-size mismatch is presented. Using the chemical energy as the reference state, the strain-induced energy of the alloy is cast into a many-body (Kanzaki) force expansion that depends on both the configurational and displacive degrees of freedom. It is shown that the k-space energy expansion is valid for all wave-lengths. The theory is then applied to the Cu_3Au alloy where, due to the large difference between atomic sizes, considerable relaxations are observed from first-principles calculations. We found that the inhomogeneous contribution ($\boldsymbol{k}\neq 0$) dominates the strain energy in Cu_3Au, whereas the homogeneous part ($\boldsymbol{k}=0$), notwithstanding its configurational dependence, contributes only a few percent.

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