Abstract Submitted for the MAR08 Meeting of The American Physical Society

Strain-induced interactions in size-mismatched alloys: A Kanzaki force approach<sup>1</sup> ALEJANDRO DIAZ-ORTIZ, OLEG SHCHYGLO, VLADIMIR BUGAEV, HELMUT DOSCH, ALEXANDER UDYANSKY, HARALD RE-ICHERT, 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<sub>3</sub>Au alloy where, due to the large difference between atomic sizes, considerable relaxations are observed from first-principles calculations. We found that the inhomogeneous contribution ( $k \neq 0$ ) dominates the strain energy in Cu<sub>3</sub>Au, whereas the homogeneous part (k=0), notwithstanding its configurational dependence, contributes only a few percent.

<sup>1</sup>Work supported by the Alexander von Humboldt Foundation.

Alejandro Diaz-Ortiz Max Planck Institute for Metals Research

Date submitted: 29 Nov 2007

Electronic form version 1.4