Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Ab initio **Prediction of Yield-Stress Anomalies in $L1_2$ Ni_3Ge-Fe_3Ge Psuedo-Binaries** JIANBO LIU, DUANE JOHNSON, Materials Science and Engineering, U. of Illinois – Urbana-Champaign, Urbana, IL 61801 — $L1_2$-based $(Ni_{1-c}Fe_c)_3Ge$ is an ideal system to study yield-strength anomaly and its origin as it is a continuous solid-solution versus c, and Ni_3Ge exhibits an anomaly while Fe_3Ge does not. We calculated planar-fault energies, i.e. antiphase boundaries (APB) and generalized stacking faults as a function of c. We predict to loss of yield-strength anomaly via an energy-based, *necessary* condition using APB energy anisotropy and elastic anisotropy in combination with a *sufficiency* condition that APB(111) is stable against formation of a superlattice intrinsic stacking fault. We predict the transition from anomalous to normal temperature dependence of yield strength for $c \gtrsim 0.35$ (or 26 *at.*% Fe), as is observed. The APB energies agree quantitatively with experimentally assessed values when antisite disorder (either thermal or off-stoichiometric), which is intrinsic to the characterization data, is taken into account. *Support through the DOE at the Frederick Seitz Materials Research Laboratory (DEFG02-91ER45439), and the NSF at the Materials Computation Center (DMR-0312448)

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Date submitted: 27 Mar 2013 Electronic form version 1.4