Magnetic destabilization of Ni_7Al

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Previously unknown cubic ordered Ni_7Al and Cu_7Pt compounds have recently been theoretically predicted to be stable phases in the Ni-Al and Cu-Pt systems. While Cu_7Pt was subsequently synthesized and identified,

to an Ising-like model, which was then used to predict the energies of other phases not calculated ~such as $D7$). ~ii! The previous approach for Ni-Al ~but not Cu-Pt! ~Ref. 3! utilized LDA energies based on the method of linear muffin-tin orbitals within the atomic sphere approximation ~LMTO-ASA! rather than a full-potential approach. ~iii! Nonmagnetic calculations were employed. Due to the absence of experimen-

values of exchange splitting and bandwidth.[18–21] The calculated magnetic moment in pure Ni (0.59 m_B/atom) is in good agreement with the observed value (0.61 m_B/atom); however, as in previous calculations,[22–25] the calculated magnetic moment of Ni in the Ni_3Al compound (0.20 m_B/atom) is higher than the experimental value 0.08 m_B/atom).[26]

~3! *Implication of Magnetism on Superlattice Stability*: The destabilization of the Ni_7Al structure with spin polarization also has interesting consequences on the calculated Ni/Ni_3Al interfacial energies. The energy of a coherent A_pB_p superlattice between materials *A* and *B* can be separated into two components:[27] ~a! *Coherency Strain*: the strain energy required to maintain coherency between the ~lattice mismatched! materials *A* and *B*, and ~b! *Interfacial Energy*: the energy associated with the interactions between materials at the *A*/*B* interface~s!. To define these terms, it is useful to first

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[1] T. B. Massalski, *Binary Alloy Phase Diagrams* ~ASM International, Metals Park, OH, 1986!.

[2] R. Hultgren, R. D. Desai, D. T. Hawkins, M. Gleiser, and K. K. Kelley, *Selected Values of the Thermodynamic Properties of Binary Alloys* ~