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Understanding the magnetoelastic behavior of pure and Co substituted GdNi[1] DURGA PAUDYAL, Y. MUDRYK, The Ames Laboratory, Iowa State University, Ames, IA 50011, V. K. PECHARSKY, K. A. GSCHNEIDNER, JR., The Ames Laboratory and Department of Materials Science and Engineering, Iowa State University, Ames, IA 50011 — Total-energy calculations employing local spin density approximation including Hubbard U (onsite electron correlation) parameter and temperature and magnetic field dependent x-ray diffraction experiments show large anisotropic shifts in lattice parameters and a giant linear magnetostriction without a structural transformation and a negligible volume magnetostriction in GdNi. In agreement with the magnetization and heat-capacity experiments, the total-energy and band splitting results confirm that the anisotropic shape changes in GdNi are associated with the second-order ferromagnetic to paramagnetic transformation. When the band splitting due to the ferromagnetic ordering of the $4f$ moments increases, the concomitant anisotropic changes in the lattice minimize the total free energy of the crystal indicating an unusual interplay between magnetism and crystal structure. The positive formation energy at 0K and the nature of the density of states at the Fermi level confirm an unstable equiatomic Gd compound when Ni is fully substituted by Co. However, the enhanced effective exchange interactions with small Co substitutions increase the Curie temperature without losing the chemical stability.

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