Abstract Submitted
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Intrinsic Magnetic Properties of $L1_0$ Derivates[1] RALPH SKOMSKI, Dept. of Physics & Astronomy and NCMN, University of Nebraska, PRIYANKA MANCHANDA, PANKAJ K. SAHOTA, ARTI KASHYAP, IIT Jaipur, India, BALAMURUGAN BALASUBRAMANIAN, Dept. of Physics & Astronomy and NCMN, University of Nebraska, J.E. SHIELD, Dept. Mechanical Enginering, University of Nebraska, D.J. SELLMYER, Dept. of Physics & Astronomy and NCMN, University of Nebraska — It is investigated how atomic substitutions modify the magnetization, exchange and anisotropy of $L1_0$-ordered ferromagnets. Emphasis is on properties of interest in permanent magnetism, including the reduction of raw-materials costs by substituting iron-series transition metals for expensive heavy ($4d/5d$) transition-metal elements. In particular, VASP calculations are used to determine the magnetizations of the Fe-Co-Pt, Mn-Al-C and Fe-Ni-S systems. We perform supercell calculations to determine the moments of Fe and Co in various $L1_0$ derivates with chemical disorder. The local magnetic moments exhibit a subtle dependence on the environment, not only in each Fe-Co layer but also through alternating $4d/5d$ layers. However, the magnitude of these spatial fluctuations is not very large, and after configurational averaging, the moments exhibit very simple dependencies on the concentrations of the involved atoms. The FeNi system is also interesting because $L1_0$-ordered FeNi was originally discovered in meteorites (tetrataenite), formed with cooling times in excess of one million years.

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