

Abstract Submitted
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Electronic structure calculations of the temperature dependence of magnetocrystalline anisotropy in $(\text{Fe}_{1-x}\text{Co}_x)_2\text{B}$ alloys¹ IVAN ZHURAVLEV, Department of Physics and Astronomy, University of Nebraska-Lincoln, Lincoln, Nebraska 68588, USA, LIQIN KE, VLADIMIR ANTROPOV, Ames Laboratory, Ames, Iowa 50011, USA, KIRILL BELASHCHENKO, Department of Physics and Astronomy, University of Nebraska-Lincoln, Lincoln, Nebraska 68588, USA — A number of important magnetic systems exhibit anomalous temperature dependence of the magnetocrystalline anisotropy (MCA), such as a spin-reorientation transition or an MCA increasing with temperature. The mechanisms of such anomalies vary. In Nd-Fe-B magnets the spin-reorientation transition is likely due to the disordering of Nd spins, while in MnBi the MCA quickly increases with temperature due to thermal expansion. $(\text{Fe}_{1-x}\text{Co}_x)_2\text{B}$ alloys present another example of highly anomalous temperature-dependent MCA. Our calculations show that these anomalies are not due to thermal expansion. We therefore study the effects of spin disorder on MCA and on the electronic structure of this system using our implementation of the vector disordered-local moment (DLM) method with spin-orbit coupling within the Green's function-based linear muffin-tin orbital (LMTO) method. We also consider the influence on MCA of the magnitude of the spin moments of Fe and Co. The results show that the observed anomalies are associated with the effects of thermal spin fluctuations on the electronic structure.

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