Magnetic properties of carbon-doped $Fe_{1-x}Co_x$ supercells studied by conformation space mapping

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$Fe_{1-x}Co_x$ disordered alloy is known to have notable magnetic properties in uniaxially strained body-centred tetragonal structure [1,2]. Such deformation can be, to some extent, obtained by introducing interstitial impurities of small atoms like boron, carbon or nitrogen [3].

A wide range of artificially induced distortions and alloy compositions can be simulated using density functional theory (DFT). Chemical disorder in the alloy can be approximated by various methods, including virtual crystal approximation (VCA) or coherent potential approximation (CPA), as well as by conformational space reduction by specific sampling schemes such as special quasirandom structures (SQS). However, it has been shown that for supercells of a few dozen atoms, a more direct approach by the study of all possible symmetrically inequivalent arrangements of atoms in a stoichiometric concentration is feasible [4].

We present a DFT analysis of $Fe_{1-x}Co_x$ stoichiometric supercells doped with an interstitial carbon atom by sampling a large part of possible geometrically inequivalent atomic positions occupancies by Fe and Co atoms in a full range of Co concentrations. Magnetic, such as magnetocrystalline anisotropy and magnetic moments, as well as structural properties, were calculated using FPLO (full potential local-orbit) scheme and compared with methods of chemical disorder approximation – VCA, CPA and SQS.

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We acknowledge the financial support of the National Science Centre Poland under the decision DEC-2018/30/E/ST3/00267. The work has been co-funded by Polish Ministry of Science and Higher Education.