Magnetocrystalline anisotropy calculations of $Fe_{13}Co_{19}C$ SQS

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In bcc Fe and Fe-Co alloys the interstitial C atoms can cause a tetragonal distortion, which may lead to increase of the magnetocrystalline anisotropy energy (MAE) of the samples. In the search for the rare earth free permanent magnets we carried out the electronic band structures calculations of bcc Fe-Co alloys doped with C located into octahedral interstitial positions [1]. Fe/Co concentration of about 40/60 is the most promising to give the highest MAE value. The 40/60 ratio is modeled within 32 atoms bcc supercell by using "mcsqs" Monte Carlo algorithm [2] to generate "special quasirandom structures" (SQS's) [3]. Generated $Fe_{13}Co_{19}$ supercell represents $Fe_{41}Co_{59}$ alloy. A single C atom is put into $Fe_{13}Co_{19}$ SQS interstitial position which indicates 3 at.% (1/33) of C. The electronic band structure is calculated using FP–LAPW method implemented in WIEN2k code [4].

References:

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