Effect of interstitial doping on atomic structure and magnetic properties of FeCo alloy

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We have investigated the magnetocrystalline anisotropy of carbon and nitrogen interstitially doped FeCo alloy by means of full potential-linearized augmented plane-wave method within the generalized gradient approximation. By impurity doping we found a tetragonal distortion in FeCo lattice. The local magnetic moment of Fe atom around the impurity site was highly suppressed, while no pronounced change was found in the local magnetic moment of Co atom. Using the torque method we found a magnetocrystalline anisotropy constant of 0.65 and 0.58 MJ/m^3 for C and N doped bulk FeCo. This was mainly due to the tetragonal distortion induced by C and N impurity and not because of hybridization effect with Fe or Co atom because no substantial changes in magnetocrystalline anisotropy constant was found even without C and N impurity in the lattice distorted systems. Additionally, the estimated maximum energy product and coercive field were 81.4, 72.5 MGOe and 600, 530 kA/m for C or N doped FeCo, respectively. These investigations show a broader perspective for the role of interstitial doping on atomic structure and magnetic properties of FeCo alloy.

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