Potential rare earth free permanent magnetic: The α″-$Fe_{16}N_2$

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Using the first principles method, we have investigated the electronic structure and magnetocrystalline anisotropy of α″-$Fe_{16}N_2$ systems. In order to tune the magnetocrystalline anisotropy of the pure α″-$Fe_{16}N_2$ we follow two routes, firstly the impurity doping both substitutional and interstitial, and secondly the multilayer approach. The impurity doping induces local lattice distortions near the impurity site, however the volume of the cell and total magnetic moment of the doped systems were not much affected. The substitutional heavy 4d, 5d elements were found to be more helpful for the enhancement of magnetocrystalline anisotropy than interstitial doping of 2s and 2p elements. Due to the increased magnetocrystalline anisotropy we found almost 50~58 % enhancement of coercivity for 5d element (W and Pt) doping in α″-$Fe_{16}N_2$. In multilayer approach we have studied two systems, (i.e) α″-$Fe_{16}N_2$/Ag/ α″-$Fe_{16}N_2$ and α″-$Fe_{16}N_2$/Au/ α″-$Fe_{16}N_2$. Here we used a very thin layer (3 monolayer) of Ag and Au. In this approach the magnetocrystalline anisotropy was enhanced almost 60 % of the pure α″-$Fe_{16}N_2$ for Ag doping. Besides the saturation magnetization drops almost 40 % of the pure $Fe_{16}N_2$. Due to enhancement of the magnetocrystalline anisotropy and reduction in saturation magnetization the coercivity was enhanced to almost 80 % of the pure α″-$Fe_{16}N_2$. Besides the maximum energy products were also seen to enhance in impurity doped systems. In the light of the obtained results α″-$Fe_{16}N_2$ could be a potential candidate for the future cost effective rare earth free permanent magnet.