Strain effects on magnetocrystalline anisotropy of bulk CoFe and its (011) films: A density functional study

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In this study, we carry out first principle calculations of strain effects on MCA energies of CoFein bulk, using the VASP code. The strains are assumed to be forced on the (001) and (011) planes by adjusting 2-D lattice constants of the (001) and (011) planes. Exchange-correlation interaction is described in general gradient approximation. In the bulk system, MCA energydecreases from 1.1 to -0.5 erg/cm^{2}for the (011) strain and from 0.3 to -0.3 erg/cm^2 for the (001) strain as the 2-D lattice increases from2.62 Å to 3.00 Å, as shown in Fig. 1: The strain effect of the (011) plane is relatively significant.

For CoFe(011) thin films of the thickness of from 2-MLs to 7-MLs, their MCA energies are also investigatedas functions of the 2-D strain of the (011) plane and compared to the MCA behaviorin bulk. In the film systems, interestingly perpendicular MCA getslarger as the 2-D lattice constant decreases. For anenhanced 2-D lattice, the easy axis turns to be [0-11] and for a reduced 2-D lattice constant gets a perpendicular MCA. In particular, the film with a reduced 2-D lattice constant of 2.62 Å hasa relatively large saturated perpendicular MCA energy of ~4.0 erg/cm^2 when the film becomes thicker than 5-ML.

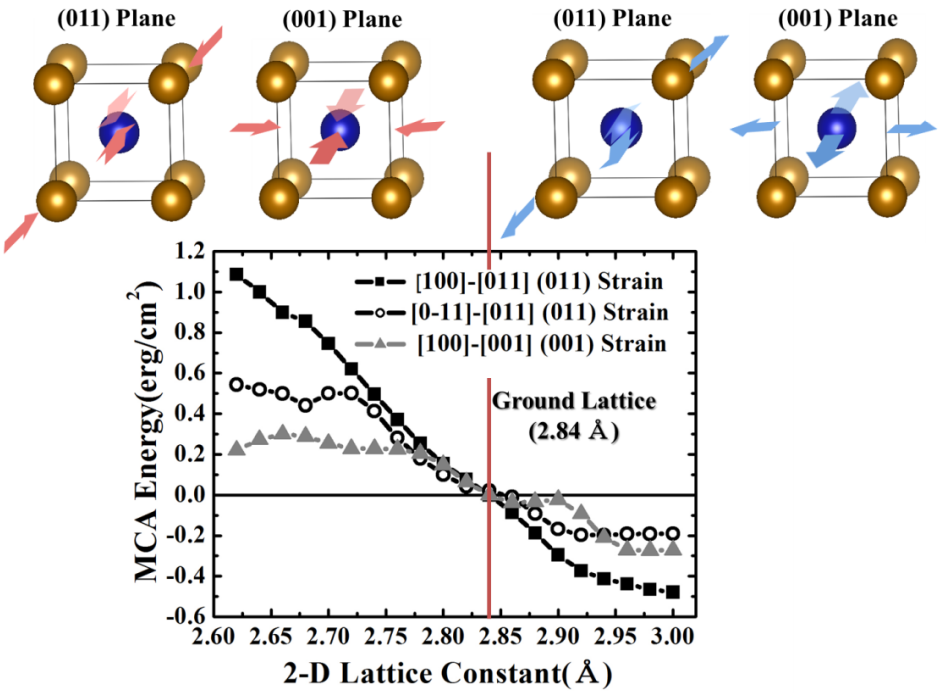

Fig 1. MCA energies as functions of 2-D lattice strains. Black lines are for the strain of the (011) plane and gray line the strain of the (001) plane. Squaresrepresent MCA energy between [100] and [011] magnetic orientations and circles MCA energy between [0-11] and [011] orientations. The vertical red line indicates the lattice constant (2.84 Å)of the bulk CoFe in equilibrium.