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Effects of the stacking fault on free surfaceFePt L10

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Abstract : Chemical ordered FePt L10, which is characterizedby a tetragonal distortion of a few percent along the c-axis,accompanied by an alternating stacking of elemental layers alongthe [001] direction, is attractive candidate for many advancedmagnetics material applications, such as high density magneticrecording media. The stacking fault effects on free surfaces wasexamined by first-principles calculations based on densityfunctional theory (DFT), within the pseudopotential plane wavemethod as implemented in VASP (Vienna Ab initio SimulationPackage). The projector augmented wave method with exchangecorrelation function is used for spin polarized generalizedgradient approximation (GGA). The layer atomic relaxation forfree surfaces show a compression on the relative displacementamount to about 1.35 %, 9.02 % for Fe and FeFe surfacesrespectively, the magnetic moment decrease about 3.90 % forFeFe surfaces.

Keywords : L1 0 FePt, FePt; stacking fault, free surfaces