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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 advanced magnetics material applications, such as high density magnetic cording media. The stacking fault effects on free surfaces wasexamined by first-principles calculations based on density functional theory (DFT), within the pseudopotential plane wavemethod as implemented in VASP (Vienna Ab initio SimulationPackage). The projector augmented wave method with exchange correlation function is used for spin polarized generalized gradient approximation (GGA). The layer atomic relaxation for free surfaces show a compression on the relative displacementamount to about 1.35 %, 9.02 % for Fe and FeFe surfaces respectively, the magnetic moment decrease about 3.90 % for FeFe surfaces.

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