Abstract

First principles study of the magnetic anisotropy of Mn_2VIn (001) films show perpendicular magnetic anisotropy (PMA), which increases as a function of the thickness of the film. Density functional theory (DFT) as implemented in the Vienna Ab initio simulation package (VASP) is employed here to perform a comprehensive theoretical investigation of the structural, electronic and magnetic properties of the Mn_2VIn(001) films of varying thickness. Our calculations were performed on fully relaxed structures, with five to seventeen mono layers (ML). The degree of spin polarization is higher in the (001) Mn_2VIn thin films as compared to the bulk in contrast to what is usually the case and as in Mn_2VAl, which is isoelectronic to Mn_2VIn as well as inCo_2VIn (001) films studied for comparison. Tetragonal distortions are found in all the systems after relaxation. The distortion in the Mn_2VIn system persists even for the 17ML thin film, resulting in PMA in the Mn_2VIn system. This significant finding has potential to contribute to spin transfer torque (STT) and magnetic random access memory MRAM applications, as materials with PMA derived from volume magnetocrystalline anisotropy are being proposed as ideal magnetic electrodes