Strain effects and defect study on Sr_2FeMoO_6 bulk and films from first-principles

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Spin polarized half-metallic ferromagnetic complex oxides like double perovskite Sr_2FeMoO_6 (SFMO) have attracted intensive interest in materials science. They are considered as a good material for creating spin-polarized current for next-generation spintronics devices especially as magnetic tunnel junctions (MTJs). The Curie temperature, T_C, in its bulk state is exceptionally high, around 410 K to 450 K [1]. For potential application, we need thin films rather than polycrystalline or bulk samples. Therefore, the production of high quality thin films with high T_C and magnetic properties close to the bulk material is desired but hindered by various imperfections such as anti-site disorder (ASD), oxygen vacancies (V_O) or epitaxial strain during the growth process.

To investigate some of these imperfections, we have carried out first-principles calculations based on the density functional theory using the pseudo-potential code, Vienna *ab initio* simulation package (VASP), with the implemented projector augmented wave (PAW) method and the on-site Coulomb interaction correction taken into account with PBE+U [2].

The order of defects or the stability of imperfections are classified with respect to their formation energies. We investigated the role of biaxial strains which might result from the lattice mismatch of the various substrates on which the SFMO films are grown. Concerning possible applications, the half-metallic character of SFMO with its high spin polarization is crucial. In the bulk, this is still preserved for a small strain or the presence of V_O in agreement with previous *ab initio* calculations [3]. The magnetic moment reduction of $2\,\mu_B$ per vacancy is also observed for V_O. In contrast, ASD alone or together with an V_O as a defect complex reduces the spin polarization. In agreement with experiment, the slab calculations show the presence of compressive strains which decrease with increasing film thickness.

References

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