Surface reconstruction and magnetic phase of the FePt thin films on Pt (110) substrate

Hanchul Kim and Miyoung Kim*
Dept of Nano Physics, Sookmyung Women's University, Korea
*kimmy@sookmyung.ac.kr

The FePt3 alloy is one of the most investigated materials for high density storage applications due to its rich variety of magnetic structures which transform sensitively depending on change in its local structure. Here, we present the *ab-initio* total energy and electronic structure calculations within the framework of density functional theory for the FePt3 film of 0.5 nm in thickness on a Pt (110) surface. The precise all-electron FLAPW calculation reveals that the FePt thin film with a missing-row surface reconstruction along the [110] direction is energetically more preferred to an unreconstructed clean surface. From the analysis of the electronic structures, this is attributed to the energy gain by the *p*-electron charge spill-out to the large (110) facet area, which was mostly from Pt atoms at the second and third atomic layers. The missing-row reconstruction is found to enhance the stability of the ferromagnetic phase over the antiferromagnetic phase which is the ground phase for bulk, and to induce possible concurrence of a meta-stable atomic structure with an in-plane anti-phase boundary along the orientation of missing-row in addition to the conventional $L1_2$ surface, implying the possible observation of various magnetic phases.