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Theoretical Study of Structural, Magnetic, and Magneto-Optical Properties of Ultrathin Films of Fe/Cu (001)

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Abstract : By means of the first principle calculation, we have investigated the structural, magnetic and magneto-optical properties of the ultra-thin films of Fen/Cu(001) with (n=1, 2, 3). We adopted a relativistic approach using DFT theorem with local spin density approximation (LSDA). The electronic structure is performed within the framework of the Spin-Polarized Relativistic (SPR) Linear Muffin-Tin Orbitals (LMTO) with the Atomic Sphere Approximation (ASA) method. During the variational principle, the crystal wave function is expressed as a linear combination of the Bloch sums of the so-called relativistic muffin-tin orbitals centered on the atomic sites. The crystalline structure is calculated after an atomic relaxation process using the optimization of the total energy with respect to the atomic interplane distance. A body-centered tetragonal (BCT) pseudomorphic crystalline structure with a tetragonality ratio c/a larger than unity is found. The magnetic behaviour is characterized by an enhanced magnetic moment and a ferromagnetic interplane coupling. The polar magneto-optical Kerr effect spectra are given over a photon energy range extended to 15eV and the microscopic origin of the most interesting features are interpreted by interband transitions. Unlike thin layers, the anisotropy in the ultra-thin films is characterized by a perpendicular magnetization which is perpendicular to the film plane.

Keywords : ultrathin films, magnetism, magneto-optics, pseudomorphic structure
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