Magnetic anisotropy and structural phase transition in ultrathin Fe (111) films: first-principles study

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Experimental research proves, that the phase transition from Fe-fcc (c/a 1.4) to bcc (c/a 1.0) system was accomplished by depositing iron by molecular beam epitaxy onto a Cu_3Au (001) substrate. This phase transition is observed with layer thicknesses somewhere between 4 - 12 monolayers of iron [1]. In our research we consider Fe layers with a triangular lattice surface, which are known to form an fcc structure and are stable for thicknesses of a few monolayers. In the limit of large thicknesses, the bcc structure is stable. We show at what thickness the structural transition from fcc to bcc should be expected. In the presented calculations, the Perdew-Burk-Erzerhof (PBE) potential was used. Our calculations show the anisotropy characteristics of magnetocrystalline energy and magnetic spin moments for the considered thickness ranges of an iron layer suspended in vacuum, which does not take into account substrate-related effects. Through calculations, we show that the studied layers have stable magnetic configurations. The studied set is consistent with experimental results [3].

References:

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