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Theoretical study on the magnetic structure of ultrathin Fe on Cu(100) LASZLO UDVARDI, LASZLO SZYUNYOGH, Department of Theoretical Physics, Budapest University of Technology and Economics, PETER WEIN-BERGER, Center for Computational Material Science, TU Wien — Thin films of Fe on Cu (100) surface exhibit rich variety of magnetic and structural phases. As it is accepted by most of the experimental work at large thickness a bcc phase is formed and below 4 atomic layers a ferromagnetic fct structure is realized. In the present paper the magnetic structure of the intermediate region between 4 and 10 monolayers has been studied by means of an extended Heisenberg model. All the parameters appearing in the model, namely the exchange, anisotropic symmetric-exchange and the on-site uniaxial anisotropy has been determined from first principle by a method described in Ref.[1]. The ground state and the finite temperature behavior of the thin film has been investigated by Monte Carlo simulations. The results of magneto optical Kerr effect and depth-resolved x-ray dichroism measurements suggested that the ground state of the system is a spin density wave. The averages of the layer resolved magnetization resulted by our simulations qualitatively agree the experimental results. We were also able to reproduce the different shape of the magnetization curve for films consist of odd and even number of atomic layers. [1] L. Udvardi, L. Szunyogh, K. Palotas, and P. Weinberger, Phys. Rev. B 68, 104436 (2003)

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