Structural and magnetic properties of Fe bi-layer on W(110)

I. Zasada and M. Rybicki

Solid State Physics Department, University of Lodz, Poland

The magnetic and structural properties of pseudomorphic iron on tungsten substrate has been studied within the density functional generalized gradient approximation [1]. By studying the spectrum of surface phonons within the direct method, a strong dependence of lattice dynamics on magnetic interaction has been revealed. The ferromagnetic interactions have been found to be crucial element in stabilizing the Fe monolayer on W(110) [1].
In the present work we focus on the crystallographic and magnetic structure of Fe bi-layer on the W(110) surface using LEED technique, DFT and thermodynamic calculations. The structural results of LEED were confirmed by the calculation within the density functional generalized gradient approximation approach implemented in the VASP program. For completeness, we have performed first-principles calculations of the phonon excitation spectrum [2] for the iron bi-layer on the tungsten (110) surface. The stability of the system is analyzed in connection with its magnetic properties. The magnetic moments distribution is than discussed in terms of the thermodynamics of inhomogeneous low-dimensional systems based on a Néel sublattices concept while using a spin 1 Heisenberg Hamiltonian. The model allows us to investigate in a straightforward manner the layer-dependent phenomena. At the end we compare our results with those for Fe monolayer as well as thicker Fe films grown on W(110) surface.

Acknowledgments: This work was supported by Polish government (MNiSW) within the contract No. N N202 259539.

[1] J. Łażewski, P. Piekarz, A. M. Oleś, K. Korecki, and K. Pariński, Phys. Rev. B76, 205427 (2007).
[2] K. Pariński, PHONON software, Cracow, (2007).