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Journal of Magnetism and Magnetic Materials 272–276 (2004) 1658–1659
Journal of magnetism and magnetic materials
www.elsevier.com/locate/jmmm

Magnetic properties of finite iron wires on Cu(1 1 1)

B. Lazarovits[a,*], L. Szunyogh[a,b], P. Weinberger[a]

[a] *Center for Computational Materials Science, Vienna University of Technology, Gumpendorferstrasse 1/a, Vienna A-1060, Austria*
[b] *Department of Theoretical Physics and Center for Applied Mathematics and Computational Physics, Budapest University of Technology and Economics, Budafoki út 8., Budapest H-1521, Hungary*

Abstract

We present a systematic study of the magnetic moments and of the magneto-crystalline anisotropy of finite monoatomic Fe_n ($1 \leqslant n \leqslant 9$) chains along the ($1\,\bar{1}\,0$) direction deposited on top of an FCC Cu(1 1 1) surface. Exploring the magnetic anisotropy properties of these systems we obtained a strong out-of-plane easy axis and an in-plane anisotropy agreeing remarkably well with the experimental findings.

PACS: 75.30.Hx; 73.22.−f; 75.30.Gw

Keywords: Magnetic nanowires; Green's function technique; Orbital magnetization; Magnetic anisotropy

The fast development of manufacturing and observation techniques made available a large number of different geometrical arrangements of magnetic impurities on metallic surfaces like dots, wires, stripes or corrals. Due to their sensitivity on the local environment, the magnetic properties of transition metal structures can thus be greatly modulated, exploring a wide spectrum of magnetic phenomena, e.g., increased spin and orbital magnetization, strong magnetic anisotropies as well as a temperature and time dependence of the magnetization.

In this contribution in terms of the embedding technique within the relativistic KKR method [1] we present results for the magnetic moments and the magneto-crystalline anisotropy (MAE) of finite monoatomic Fe_n ($1 \leqslant n \leqslant 9$) chains deposited along the ($1\,\bar{1}\,0$) direction on top of an FCC Cu(1 1 1) surface. For the Cu atoms adjacent to the Fe impurities we found a relatively weak magnetic polarization even in the surface layer, where the spin-polarization of the host atoms is expected to be the strongest. The calculated spin moments of these host atoms (S_z^{Cu}) were about 0.02 μ_B and the corresponding orbital moments (L_z^{Cu}) were less than 10^{-3} μ_B.

Placing the Fe impurity on the top of the surface and within the uppermost (surface) Cu layer one can selectively trace the effect of hybridization between the impurity and the host atoms. The orbital moment of the Fe adatom is about 5.5 times larger on top of the surface (0.65 μ_B) than in the Cu surface layer (0.12 μ_B). This change is much larger than the corresponding change in the spin moment ($\sim 12\%$) which is 3.27 μ_B on the surface and 2.91 μ_B within the surface layer. For an adatom placed on top of the surface an easy magnetization axis pointing perpendicular to the surface is favored, with a corresponding MAE, $\Delta E_{x-z} = 4.30$ meV, while within the surface layer we found that the in-plane direction is preferred, $\Delta E_{x-z} = -0.08$ meV. The calculated MAE and orbital moment anisotropy are in this case consistent with the qualitative rule obtained from perturbation theory: the easy axis corresponds to a maximum of the orbital moment. Within the surface layer the hybridization of the d_{xy}- and $d_{x^2-y^2}$-like states of the impurities mostly with sp-like states of the adjacent Cu atoms leading thus to a broadening and to a corresponding lowering of these components of the density of states at the Fermi level serves as the reason for the change of the easy-axis.

Investigating longer chains a transition from a point-like (0D) to a quasi-one-dimensional (1D) system can be traced in terms of the spin- and orbital moments of the

*Corresponding author. Tel.: +43-158-801-15840; fax: +43-158-801-15898.
E-mail address: bl@cms.tuwien.ac.at (B. Lazarovits).

0304-8853/$ - see front matter © 2003 Published by Elsevier B.V.
doi:10.1016/j.jmmm.2003.12.349

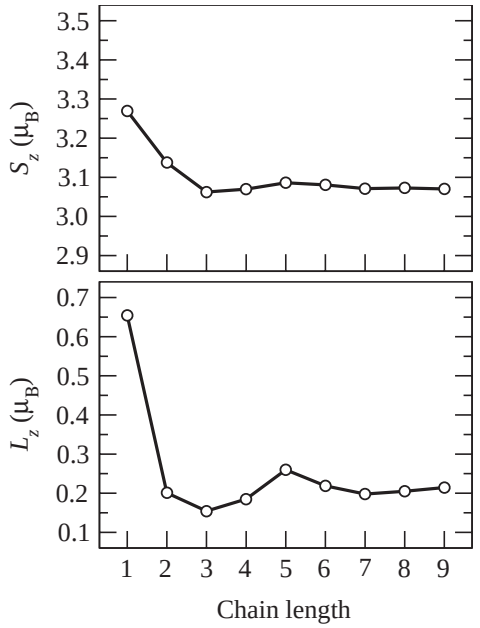

Fig. 1. Calculated spin (S_z) and orbital moments (L_z) of the central (most symmetric) Fe atom in Fe_n ($n = 2, \ldots, 9$) chains along the ($1\,\bar{1}\,0$) direction Cu(1 1 1) surfaces with a magnetization pointing normal to the surface.

central atoms shown in Fig. 1 as a function of the length of the chains, n. The results for the chains show that up to $n = 3$ the magnetic moments decrease systematically and then seem to converge to a well-defined value. The value of S_z^{Fe} and L_z^{Fe} extrapolated numerically from the data in Fig. 1 to $n = \infty$, 3.07 and 0.22 μ_B, respectively, can be interpreted as an estimate for the moments in an infinite chain. A systematic trend of the reduction of S_z and L_z when increasing the dimensionality of the magnetic nanostructures, 0D $\rightarrow$ 1D $\rightarrow$ 2D has been explored also experimentally [2]. Our estimated values of L_z for infinite monoatomic chains on top (0.22 μ_B) and in the surface layer (0.10 μ_B) of Cu(1 1 1) fit well into the tendency of the experimental values when reducing the thickness of the Fe film as reported in Ref. [3]. The experimental value approximated to the wire case ($\sim$0.13 μ_B) is somewhat smaller than the calculated values of L_z, most possibly since step-edge positions of the chains are supposed in the experiments.

For chains deposited onto the surface, the direction normal to planes remains the easy axis. For shorter chains ($n \leqslant 5$) typically rapid variations of the contributions of the individual Fe atoms along the chains apply. For longer chains ($n \geqslant 6$) we found that the largest contributions to ΔE_{y-z} come from the outermost atoms, while the inner and the outermost sites add nearly the same contribution to ΔE_{x-z}. Similar to the orbital moment, our estimated values of ΔE_{x-z} for infinite wires, $\sim$1.5 meV, is in good agreement with that deduced from the experiments, $\sim$1.6 meV [3]. The *in-plane* magnetic anisotropy energies, ΔE_{y-x}, of chains on top of the surfaces are also calculated with respect to the length of Fe chains. ΔE_{y-x} shows rapid oscillations (with a period of 2 atoms) indicating that the in-plane MAE is influenced by confinement effects. The extrapolated value of the in-plane MAE for an infinite chain on a Cu(1 1 1) surface, $\sim$0.5 meV, which is very close to the experimental value of about 0.4 meV reported by Boeglin et al. [3].

This paper was sponsored by the RTN network "Computational Magnetoelectronics" (Contract No. HPRN–CT–2000-00143), the Center for Computational Materials Science (Contract No. GZ 45.531), the Austrian Science Foundation (Contract No. W004), and the Hungarian National Scientific Research Foundation (OTKA T037856 and OTKA T038162).

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