Available online at www.sciencedirect.com
SCIENCE DIRECT®
Journal of Magnetism and Magnetic Materials 272–276 (2004) 1594–1595
Journal of magnetism and magnetic materials
www.elsevier.com/locate/jmmm

Electric transport in nanostructures: real space ab initio investigations

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

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

Abstract

A real-space embedding technique based on the fully relativistic spin-polarized Korringa–Kohn–Rostoker method is combined with the real-space Kubo–Greenwood formula in order to describe electrical transport properties of magnetic nanostructures. Finite Fe and Co chains embedded into the surface layer of FCC Ag(1 0 0) are investigated.

PACS: 73.63.Nm

Keywords: Magnetic nanowires; Green's function technique; Kubo formalism

Ab initio investigations of electric transport have been successfully applied to systems with two- or three-dimensional translational symmetry in the last decades, e.g., for studying GMR, TMR and AMR effects [1]. Investigation of electric transport in magnetic nanostructures is of special interest for nanoscale technologies and diverse applications, although at present experimental studies seem to be very limited.

Multiple scattering theory allows the treatment of a finite cluster of impurities embedded into a translationally invariant host medium,

$$\boldsymbol{\tau}_{\mathrm{clus}} = \boldsymbol{\tau}_{\mathrm{host}}[\mathbf{I} - (\mathbf{t}_{\mathrm{host}}^{-1} - \mathbf{t}_{\mathrm{clus}}^{-1})\boldsymbol{\tau}_{host}]^{-1}, \tag{1}$$

where $\boldsymbol{\tau}_{\mathrm{host}}$ and $\boldsymbol{\tau}_{\mathrm{clus}}$ are site-angular momentum representations of the scattering path operator for the host and for the embedded cluster, respectively, while $\mathbf{t}_{\mathrm{host}}$ and $\mathbf{t}_{\mathrm{clus}}$ are the corresponding single-site scattering matrices. For more details of the embedding technique, see Ref. [2]. It should be noted that no lattice relaxation effects are taken into account.

According to Kubo's formula the conductivity tensor between sites labeled by i and j is of the following form:

$$\sigma_{\mu\nu}^{ij} = -\frac{1}{4\pi V}\sum_{k,l=1}^{2}(-1)^{k+l} \times Tr\left[J_{\mu}^{i}(\varepsilon_k,\varepsilon_l)\tau_{\mathrm{clus}}^{ij}(\varepsilon_l)J_{\nu}^{j}(\varepsilon_l,\varepsilon_k)\tau_{\mathrm{clus}}^{ji}(\varepsilon_k)\right], \tag{2}$$

where $\mu,\nu\in\{x,y,z\}$, V is the atomic volume, $\varepsilon_1 = \varepsilon_{\mathrm{F}} + \mathrm{i}\delta$, $\varepsilon_2 = \varepsilon_{\mathrm{F}} - \mathrm{i}\delta$ with ε_{F} being the Fermi level and $\delta\to 0$, while J_{μ}^{i} stands for the relativistic current matrix in angular momentum space. For more details of the theory as well as numerical tests, see Ref. [3].

In our calculations, we used $l_{\max} = 2$ for the angular momentum expansion and the potentials were treated within the atomic sphere approximation. Furthermore, 210 $k_{\|}$ points were used in the irreducible wedge of the two-dimensional Brillouin zone in order to calculate $\boldsymbol{\tau}_{\mathrm{host}}$ in real space.

We investigated single impurities and finite chains (length of 2–10 atoms) of Fe and Co embedded along the (1 1 0) direction (x) in the surface layer of Ag(1 0 0). We use the notation, e.g., Co4 for a Co chain of 4 atoms. We tested the non-local conductivity by increasing the number of self-consistently calculated atoms for Fe1, Fe2 and Co1, Co2. Since the relative difference between

*Corresponding author. Tel.: +43-1-58801-15841; fax: +43-1-58801-15898.
E-mail address: kp@cms.tuwien.ac.at (K. Palotás).

0304-8853/$ - see front matter © 2003 Published by Elsevier B.V.
doi:10.1016/j.jmmm.2003.12.313

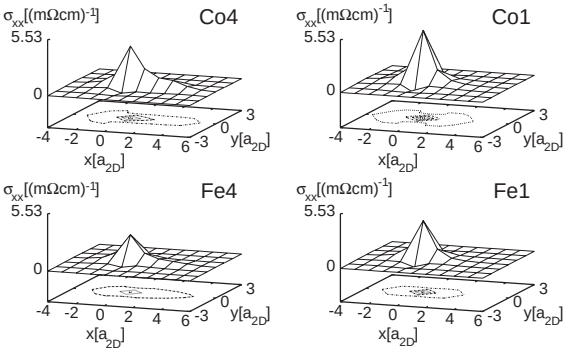

Fig. 1. Non-local conductivities $\sigma^{0j}_{xx}(x_j, y_j)$. The atom labeled by 0 is at the position (0, 0), while the position of atom j is varied in the (1 0 0)-oriented surface plane, ($\delta = 1$ mRy).

the conductivities by taking self-consistently calculated cluster "chain + 1 shell" and "chain + 2 shell" is below 0.2%, we decided to use the "chain + 1 shell" configurations to perform self-consistent calculations for longer chains, thus, saving computer time.

The xx-component of the non-local conductivity tensor between an origin (the impurity or the atom on the brink of the chain) and all other atoms in the plane is shown for the impurity case and for a chain of four atoms for both Co and Fe in Fig. 1. It can be seen that in the impurity case the shape of the conductivity is symmetric to the $x = 0$ plane, while in the chain case the tensor-elements along the $+x$ direction (where the chain lies) are much larger than in other directions, causing an asymmetry. This behavior is true for all chains. Moreover, it can be seen that the site-diagonal conductivity component at the origin (the peak) for Co is larger than for Fe, causing in turn of higher resistivity of Fe chains. Let us define a kind of "residual resistivity" for finite clusters, as follows:

$$\rho^{\alpha}_{\mu\mu}(r) = \left[\frac{1}{n}\sum_{i\in chain}\sum_{j=1}^{N(r)}\sigma^{ij}_{\mu\mu}\right]^{-1}, \qquad (3)$$

where n denotes the number of atoms in the chain of type α (Fe or Co) and $N(r)$ is the number of atoms involved in the cluster (chain + environmental atoms up to the furthermost distance of r). As can be seen from Fig. 2, $\rho^{\alpha}_{xx}(r)$ decrease monotonically, and the difference, $\rho^{Fe}_{xx}(r) - \rho^{Co}_{xx}(r)$ is finite and varies slowly with respect to the cluster size.

We studied the influence on the residual resistivity with respect to the orientation of magnetization. Selected results are listed in Table 1. As can be seen,

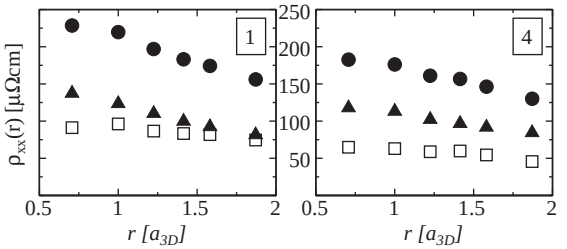

Fig. 2. Residual resistivities of Fe (circles) and Co (triangles) chains. Open squares refer to $\rho^{Fe}_{xx}(r) - \rho^{Co}_{xx}(r)$. The length of the chains is shown explicitly. The orientation of magnetization is normal to the (1 0 0) plane (M_z).

Table 1
Residual resistivities versus orientation of magnetization, $\rho_{xx}(r = a_{3D})$[μΩ cm]

Type	M_x	M_y	M_z
Co1	120.1	126.9	123.5
Fe1	198.3	225.3	219.6
Co4	109.0	113.7	113.2
Fe4	166.7	176.4	176.2

M_x provides the smallest resistivity, while M_y the highest one. In the impurity case, $\rho^{Fe}_{xx}(M_y)$ is by 13.6% larger than $\rho^{Fe}_{xx}(M_x)$, while $\rho^{Co}_{xx}(M_y)$ is only by 5.7% larger than $\rho^{Co}_{xx}(M_x)$ which means a higher sensitivity with respect to the orientation of the magnetization for Fe. The orientation of the magnetization perpendicular to the chain (M_y and M_z) results in minor differences in the resistivity for longer chains.

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 45.451), the Austrian Science Foundation (Contract No. W004) and the Hungarian National Scientific Research Foundation (OTKA T037856, OTKA T038162).

References

[1] P. Weinberger, Phys. Rep. 377 (2003) 281.
[2] B. Lazarovits, L. Szunyogh, P. Weinberger, Phys. Rev. B 65 (2002) 104441.
[3] K. Palotás, P. Weinberger, B. Lazarovits, L. Szunyogh, Phys. Rev. B 67 (2003) 174404.