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Magnetic properties of mixed Co–Cu clusters on Cu(0 0 1)

V.S. Stepanyuk [a,*], A.N. Baranov [b,c], D.I. Bazhanov [b,d], W. Hergert [a], A.A. Katsnelson [b]

[a] *Fachbereich Physik, Martin-Luther-Universität, HalleWittenberg, Friedemann-Bach-Platz 6, D-06099 Halle, Germany*
[b] *Solid State Physics Department, Moscow State University, 119899 Moscow, Russian Federation*
[c] *Institut für Festkörperforschung, Forschungszentrum Jülich, D-52425 Jülich, Germany*
[d] *Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, 06120 Halle, Germany*

Abstract

The aim of this article is to present ab initio calculations of the effect of intermixing at Co/Cu interface on magnetic properties of small Co islands. We find that coating of Co islands with Cu atoms reduce magnetic moments. The spin polarization of Cu atoms near Co islands is revealed. RKKY interaction between Co impurities in Cu layers is calculated. © 2001 Elsevier Science B.V. All rights reserved.

Keywords: Density functional calculations; Green's function methods; Magnetic phenomena (cyclotron resonance, phase transitions, etc.); Cobalt; Copper

Magnetic properties of Co thin films on Cu(0 0 1) are of great interest in the area of magnetoelectronics. In the initial stage of Co heteroepitaxy small Co clusters are formed [1].

Recently the interfacial intermixing at Co/Cu interface was observed despite the fact that Co and Cu are immiscible in the bulk [2]. Atomic exchange processes lead to a bimodal initial growth of Co/Cu(0 0 1): large Cu islands and small Co islands were observed in STM experiments [1]. One of the most striking features of an interface mixing in Co/Cu(0 0 1) has been recently discovered [3]. It was found that Co particles burrow into clean Cu(0 0 1) substrate.

Magnetic properties of Co nanostructures on Cu substrate can be strongly influenced by Cu atoms. For example, copper coverages as small as three hundredths of a monolayer drastically affect the magnetization of Co films [4]. Experiments and theoretical studies demonstrated that magnetization of mixed clusters of Co and Cu depends on the relative concentration of Co and Cu in a nonobvious way [5,6]. Quenching of ferromagnetism in cobalt clusters embedded in copper was reported [5].

The main goal of this paper is to study the effect of Cu atoms on magnetic properties of small Co islands on the Cu(0 0 1). Our results are based on the density functional theory in the local-spin density approximation and the Korringa–Kohn–Rostoker (KKR) Green's function method [7–9]. In this approach, the surface is considered as a two-dimensional perturbation of the bulk. We apply the multiple-scattering theory to obtain the

* Corresponding author. Tel.: +49-345-552-5439; fax: +49-345-552-5446.
E-mail address: stepan@valinux.physik.uni-halle.de (V.S. Stepanyuk).

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Green's function via a Dyson equation. The structural Green's function of the surface is then used as the reference Green's function for the calculations of the pure and mixed clusters on the Cu substrate. The full charge density is taken into account. Details of the method and several its applications can be found elsewhere [7–9].

Our previous calculations by means of a quasi-ab initio molecular dynamics showed that surface alloying is energetically favourable in the case of Co/Cu(0 0 1) and mixed Co–Cu clusters are formed in the early stages of heteroepitaxy [10]. Recent experiments [1] suggest that mixed Co–Cu clusters indeed exist.

First, we consider the effect of a single Cu atom on the magnetic moments of small Co islands. In Fig. 1 we present magnetic moments in the Co_9 and Co_8Cu islands. Because of hybridization with Co atoms, the sizeable magnetic moment on the central Cu atoms is induced. Small moments on the Cu atoms in the topmost surface Cu layer are also revealed. One can see that the central Cu atom exhibit a ferromagnetic polarization with respect to Co, while the substrate Cu atoms are antiferromagnetically polarized. Magnetic moments on Co and Cu atoms in small mixed Co–Cu clusters are presented in Fig. 2. The small magnetic polarization of Cu atoms is well seen.

The most interesting results have been obtained for Co island coated by Cu atoms. We have found a strong effect of Cu atoms on the moments of Co atoms. These results are shown in Fig. 3. The Cu

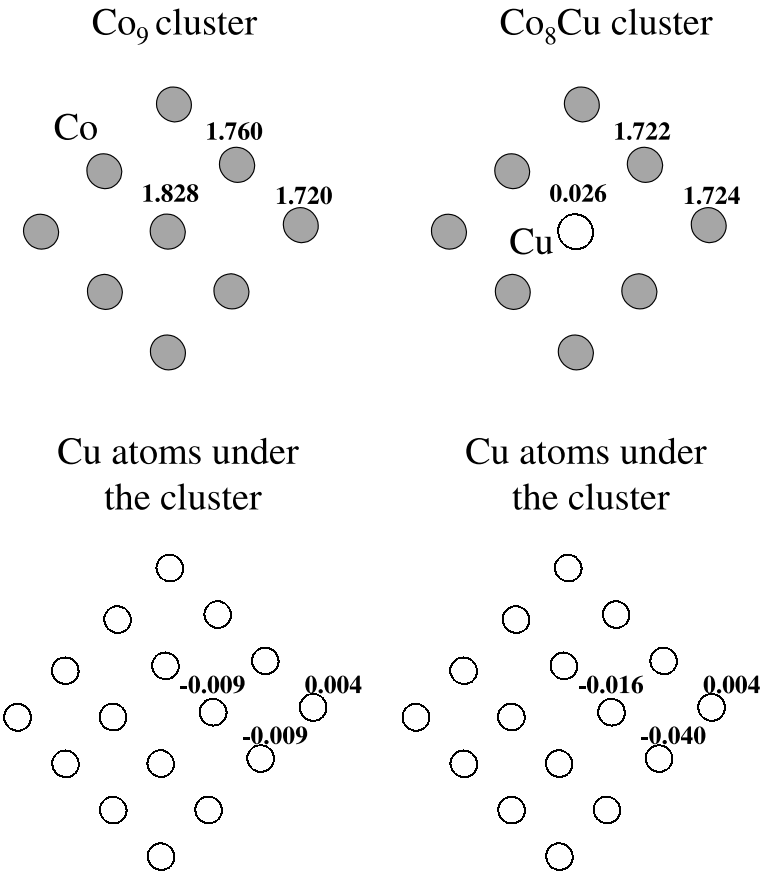

Fig. 1. Spin polarization of Co_9 and Co_8Cu clusters on Cu(0 0 1). The induced magnetic moment on Cu atoms under the islands are shown. Magnetic moments in Bohr magnetons are given for all inequivalent sites.

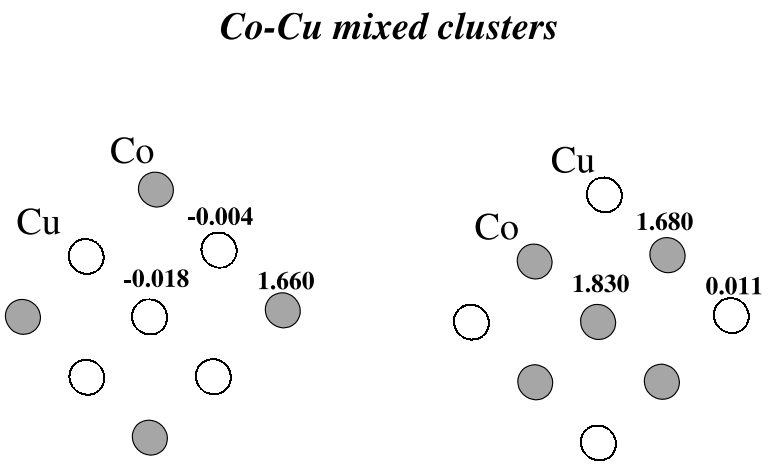

Fig. 2. Spin polarization of Co–Cu mixed cluster on Cu(0 0 1). Magnetic moments in Bohr magnetons are given for all inequivalent sites.

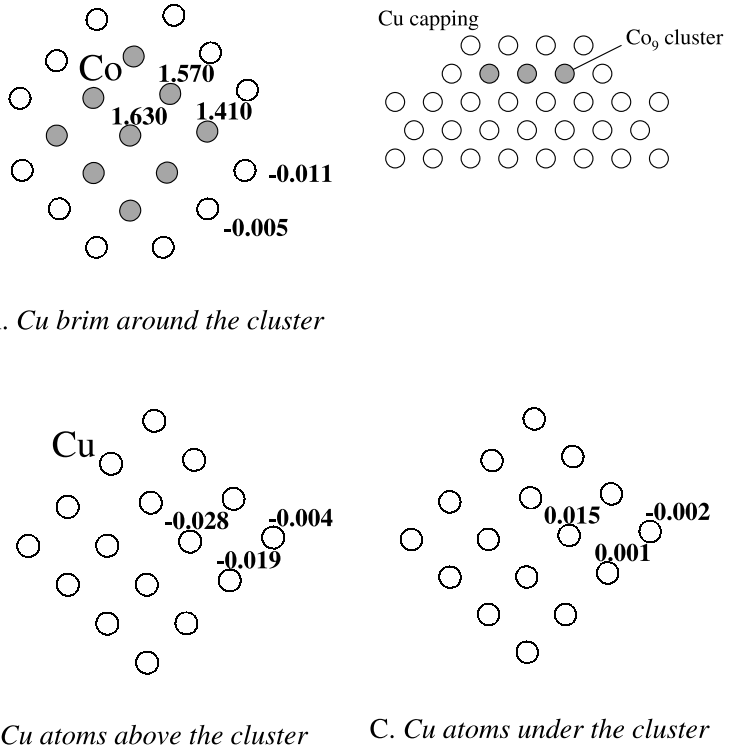

Fig. 3. Spin polarization of Co_9 cluster coated by Cu atoms on Cu(0 0 1). Magnetic moments in Bohr magnetons are given for all inequivalent sites.

atoms in the capping layer and in the substrate have different sign of spin polarization. The average magnetic moment of the Co_9 cluster with Cu capping is reduced by 14% compared to the pure

Co_9 cluster. A strong reduction of the average moment of Co clusters can have a strong impact on magnetic properties at Co/Cu interface in the early stages of growth. Coating of Co clusters with Cu atoms has been recently found in the experiments [3].

Finally, we consider the exchange interaction between Co impurities in Cu surface layers. The interaction between two Co impurities is calculated employing the frozen potential (FP) approximation [11]. Within this approximation the total energy difference between the ferro and antiferromagnetic configuration is simply given by the difference of the single particle energies $E_{ex} = E_{sp}^{F} - E_{sp}^{AF}$. The single particle energies are calculated using the Lloyd's formula [11].

Firstly, we demonstrate that within the FP approximation the single-particle energies alone allow a reliable calculation of the exchange coupling between impurities. Table 1 shows the calculated exchange interaction energies in the FP approximation and in a fully self-consistent calculations (SCC) for the topmost surface layer. One can see that the FP values agree very well with the self-consistent results. Thus the exchange interaction between surface impurities can be reliably calculated from the single-particle energies only.

Table 1
Exchange interaction between Co impurities in the Cu(0 0 1) surface in the first surface layer

Neighbours	Full SCC	FP
First	−0.22 eV	−0.24 eV
Third	−6.6 meV	−6.3 meV
Sixth	8.5 meV	6.8 meV

The values FP refer to the frozen potential approximation and are compared with the total-energy results from full SCC.

In Fig. 4 we present our results for the exchange interaction energies of two Co impurities on Cu surface and in the topmost surface layer. The existence of slowly decaying oscillations is evident from this figure in qualitative agreement with the RKKY picture. Our results also demonstrate that the RKKY-like interactions are strongly different for the adatom positions and for the surface layer. Detailed studies of the RKKY interactions will be presented elsewhere.

In summary, we have demonstrated that the coating of the Co clusters with Cu atoms leads to a reduction of the average magnetic moment.

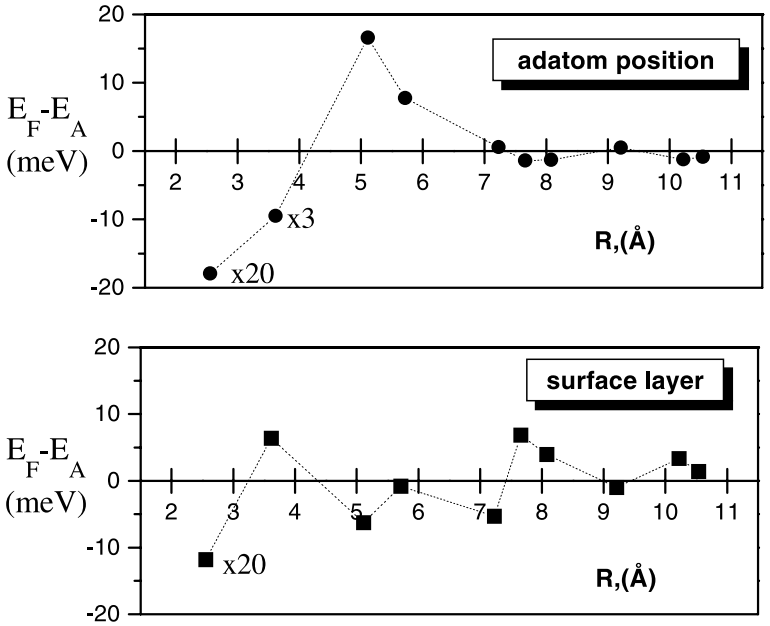

Fig. 4. Exchange interaction energies for two Co impurities in Cu(0 0 1) surface.

The first ab initio calculations of RKKY interactions between surface impurities are presented.

Acknowledgements

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