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One-dimensional magnetism of Rh chains on the Ag(001) surface

D. I. Bazhanov,[1] W. Hergert,[2] V. S. Stepanyuk,[2] A. A. Katsnelson,[1] P. Rennert,[2] K. Kokko,[3] and C. Demangeat[4]
[1]*Department of Physics, Moscow State University, Ru-117189 Moscow, Russia*
[2]*Fachbereich Physik, Martin-Luther-Universität, Friedemann-Bach-Platz 6, D-06099 Halle, Germany*
[3]*Department of Physics, University of Turku, FIN-20014 Turku, Finland*
[4]*Institut de Physique et de Chimie des Matériaux de Strasbourg, 23 rue du Loess, 67037 Strasbourg, France*

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The electronic and magnetic properties of one-dimensional Rh structures deposited on Ag(001) surfaces are investigated. The ⟨010⟩ and ⟨110⟩ chain directions with Rh atoms at ideal adatom positions are considered. A semiempirical tight-binding method in a chain orbital representation is implemented to exploit the translational symmetry along the chain directions. All structures considered display a sizable magnetic moment for the Rh atoms in the chains. A nonconventional magnetic behavior due to interchain interactions is observed. The results are in a good agreement with Korringa-Kohn-Rostoker calculations for small supported clusters.

I. INTRODUCTION

The electronic and magnetic properties of a low-dimensional metallic surface system depend significantly on the structure of the system. The enhancement of magnetic moment in traditionally ferromagnetic materials and the transfer of nonmagnetic materials into magnetic ones has been obtained by reducing the size and dimensionality of the considered systems[1] suggesting interesting magnetic materials, e.g., for compact magnetic storage devices. In the past mainly two-dimensional magnetic systems on single-crystal surfaces have been studied.[1] However, modern experimental tools (e.g., diffusion controlled aggregation,[2] moving of atoms by the tip of a scanning tunneling microscope,[3] decoration of steps[4]) can be used to produce nanostructures of various size and shape on different metallic substrates.

Very recently Gambardella *et al.*[5] have demonstrated, that high density arrays of parallel nanowires of Ag and Cu can be deposited on a vicinal Pt(997) surface. Measurements of Dallmeyer *et al.*[6] at Co nonowires on the vicinal Pt(997) surface suggest the presence of a one-dimensional exchange-split band and of local magnetic moments.

Transition metal (TM) structures on noble metal surfaces attract special interest since in this case TM systems can be considered as quasifree systems due to the relatively weak interaction between transition metals and noble metals. First-principles calculations for $3d$, $4d$, and $5d$ transition metal clusters on Cu(001) and Ag(001) substrates have shown (cf. Refs. 7 and 8), that transition-metal elements which are nonmagnetic in the bulk, could become magnetic due to the increase of the lattice constants and the reduction of the dimensionality. Some of the theoretical predictions have been confirmed experimentally.[9]

The nonmagnetic $4d$ element Rh has a special interest due to its unexpected properties. Cox *et al.*[10] showed that free standing Rh clusters are magnetic. Moreover, the average magnetic moment of free Rh clusters depends on the symmetry and size of the clusters in a complicated way.[11,12] Therefore investigations on Rh systems could give better insight on the interplay between the structure and the electronic and magnetic properties of low-dimensional metallic sytems.

According to *ab initio*[13–17] and semiempirical calculations[18] pseudomorphically grown Rh monolayers on Ag(001) could be ferromagnetically ordered with a magnetic moment of $1\mu_B$. However, experiments did not show any magnetism for Rh monolayers. No magnetic moment was found either with magneto-optical Kerr effect (MOKE),[19,20] or with photoelectron spectroscopy.[21] This discrepancy is suggested to be connected with the structural defects found in real surfaces.[22,23] Detailed experimental investigations of Rh surface layers have shown that the ideal layer structure assumed in the calculations does not exist in real samples: it is impossible to grow a Rh monolayer on Ag(001) pseudomorphically without an additional Ag layer on top of the structure. The direct interdiffusion process between Rh and Ag atoms and the growth of mixed islands were observed at Rh-Ag interface.[24] Thus experimental investigations suggest that structural effects (island formation, roughness at surface, step defects, interdiffusion) have strong influence on the magnetic properties of low-dimensional metallic systems.

According to *ab initio* calculations by Freeman[17] and Blügel[25] the additional Ag layer on top of the Rh layer reduces the magnetic moment of Rh to $0.55\mu_B$. Semiempirical investigations[18,26] showed that an ordered layer $Rh_{50}Ag_{50}$ on the Ag(001) surface destroys the magnetism of the Rh monolayer on the Ag(001) surface. Later on Turek *et al.*[27] studied the change of the magnetic properties in dependence on intermixture by means of the *ab initio* tight-binding (TB)- linear muffin-tin orbital (LMTO)- coherent potential approximation (CPA) method. The magnetic moments in the two mixed layers of $Rh_{1-x}Ag_x/Rh_xAg_{1-x}/Ag(001)$ have been found to be a minimum in the concentration range $0.5 \leqslant x \leqslant 0.6$. The moments are $0.3\mu_B$ in the topmost layer and $0.2\mu_B$ in the subsurface layer. In contrast with this theoretical analysis of magnetic properties in the monolayer regime the moments of small supported Rh adislands are enhanced due to the interdiffusion with Ag atoms.[28] Using weak localization and anomalous Hall effect Beckmann and Bergmann[30] have found an enhancement of the magnetic moment of small Rh clusters compared to single Rh adatoms

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on the Ag (001) surface. An unusual behavior for Rh dimers on the Ag(001) surface is found by means of *ab initio* calculations.[29] The magnetic moment per Rh atom decreases strongly with increasing Rh-Rh interatomic distance. This is in contrast with results obtained for all other transition-metal adatoms.

From all this it is now clear that the role of structural effects on the magnetism of Rh supported nanostructures is not fully understood. Especially one-dimensional (1D) structures, which occur on anisotropic surfaces or in the vicinity of steps have not been investigated in detail yet. Here we report on the magnetic properties of ideal 1D Rh chains at the Ag(001) surface. Two chain directions $\langle 010\rangle$ and $\langle 110\rangle$ are considered. A semiempirical tight-binding Hamiltonian in the framework of the recursion method is applied to clusters of chains.

II. THEORETICAL METHOD

A. Calculation of magnetic properties

The semiempirical TB method is a suitable tool for the calculation of the electronic and magnetic properties of rough metal surfaces, clusters on surfaces, nonperfect metallic layered systems, etc.[1] This method is specifically devoted to the study of very large low-dimensional systems with a considerable number of inequivalent atoms which is far beyond the possibilities of *ab initio* methods because every loss of translational symmetry leads to a dramatic increase of numerical effort.

Very recently Robles *et al.* used the TB method to study monoatomic Co wires on the Pd(110) surface.[31] In contrast to our approach, a pure real-space formulation of the tight-binding method was applied, i.e., the one-dimensional translational symmetry along the chains was not used in their calculation.

We have derived an Hamiltonian, which contains a one-particle interaction and an electron-electron interaction suitable to investigate the magnetic properties of infinite linear metallic chains on metal surfaces. The interaction Hamiltonian is treated in the unrestricted Hartree-Fock approximation to the Hubbard-Hamiltonian (cf. Refs. 32 and 33). The hopping integrals are spin independent and the spin-dependent diagonal terms are given by

$$\epsilon_{Ai\nu\sigma}=\epsilon^{0}_{Ai\nu}+\sum_{\nu'}\left(U^{A}_{\nu\nu'}\triangle N_{Ai\nu'}-\sigma\frac{J^{A}_{\nu\nu'}}{2}\mu_{Ai\nu'}\right), \qquad (1)$$

where i is the chain index, ν describes the angular momentum ($\nu=s,p,d$) of the basis functions, σ gives the spin polarization ($\sigma=\pm 1$), and A denotes the type of atoms. $J^{A}_{\nu\nu'}$ is the exchange integral and $\mu_{Ai\nu}$ is the magnetic moment per atom of type A in the ith chain. $\triangle N_{Ai\nu}$ is the deviation of the number of electrons of angular momentum ν at an atom of type A in the ith chain from a reference level. The reference values to calculate $\triangle N_{Ai\nu'}$ are conventionally the electron numbers in the bulk material. $U^{A}_{\nu\nu'}$, the effective intra-atomic Coulomb interection, is usually taken from the literature or chosen in such a way that local neutrality is preserved.

Only exchange integrals for d electrons of Rh and Ag are assumed to be nonzero and their values are taken from Ref. 18 ($J^{Ag}_{dd}=0.041Ry$, $J^{Rh}_{dd}=0.044Ry$). The local magnetic moments $\mu_{Ai\nu}$ at an atom of type A in the ith chain are given by

$$\mu_{Ai\nu}=N_{Ai\nu\uparrow}-N_{Ai\nu\downarrow}, \qquad (2)$$

$$N_{Ai\nu\sigma}=\int_{-\infty}^{\varepsilon_F}\rho_{Ai\nu\sigma}(\epsilon)d\epsilon.$$

The local density of states $\rho_{Ai\nu\sigma}(\epsilon)$ (LDOS) per spin is connected directly with the corresponding diagonal element of the Green's function and is calculated by the recursion method.

The magnetic moments $\mu_{Ai\nu}$ are evaluated self-consistently in the local charge neutrality approximation.[34] Self-consistency is achieved if changes in the electron numbers and in the magnetic moments were less than 10^{-5}. It is assumed that the local charge distribution corresponds to the bulk value $N^{\nu}_{i\sigma 0}$.[34,35]

B. Systems with 1D translational symmetry

The recursion method permits to calculate the LDOS for systems with arbitrarily placed atoms within the TB method. Hopefully the calculation of electronic properties can be simplified considerably by implementing the Bloch theorem. An important property of **k**-space representation is the separability property of the Hamiltonian, which allows us to treat each **k** vector separately. The **k**-space formulation of the recursion method was applied to bulk systems with three-dimensional translation symmetry by Anlage and Smith[36] and Woodruff.[37] Later the method was extended for two-dimensional systems.[18,38,39] Layered systems are characterized by a translational symmetry within the layer and an arbitrary staking sequence of layers in the third direction.

In this paper we investigate infinite chains of atoms on the ideal Ag(001) surface. Therefore only one-dimensional translational symmetry is conserved. The system under investigation can be considered as a cluster of chains of atoms. The use of 1D translational symmetry leads to the introduction of the so-called ''chain orbitals,'' which are one-dimensional Bloch functions. The chain orbitals are constructed by summing over all atoms of a certain type A in a given chain i:

$$|AQ\rangle=|A\nu i\sigma\mathbf{k}\rangle=\frac{1}{\sqrt{N_{iA}}}\sum_{\mathbf{R}} e^{i\mathbf{k}(\mathbf{R}+\tau_{iA})}\phi^{A}_{\nu\sigma}(\mathbf{r}-\mathbf{R}-\tau_{iA}). \qquad (3)$$

The chain orbital $|AQ\rangle$ is characterized by the set of quantum numbers $Q=\{\nu,i,\sigma,\mathbf{k}\}$. $\mathbf{k}$ is a vector of the one-dimensional Brillouin zone and $\mathbf{R}$ a one-dimensional lattice vector. N_{iA} is the number of atoms of type A in the chain i. τ_{iA} is a nonprimitive translation of an atom of type A in the chain i. The localized orbitals $\phi^{A}_{\nu\sigma}$ form the basis set of the calculation. The analytical form of the Hamiltonian, taking into account up to second nearest-neighbor interactions, is constructed by means of a computer algebra package.[40] The two-center approximation is used and hopping integrals for Rh and Ag are taken from Ref. 41. Hopping integrals for the

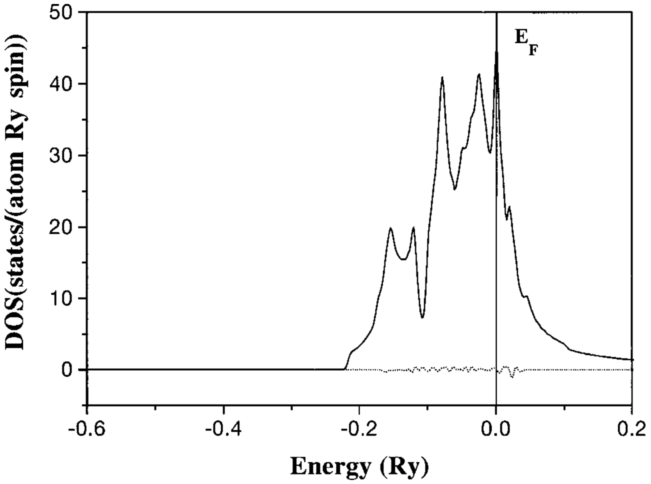

FIG. 1. Paramagnetic DOS of an isolated Rh monolayer with Ag lattice constant calculated in chain orbital representation and difference in the DOS between calculations in layer orbital representation and chain orbital representation [1400 **k** points in 2D Brillouin zone (BZ) are used for the layer orbital calculation, 90 **k** points in 1D BZ, and 100 chains are used in chain orbital calculation].

Rh-Ag interaction are constructed by the rule $\beta_{RhAg}=\sqrt{\beta_{RhRh}\cdot\beta_{AgAg}}$. It should be noted that the parametrization is the same as used in Ref. 18 to describe the magnetic properties of Rh monolayers on Ag(001).

We tested the chain description for the isolated Rh monolayer. With respect to the two-dimensional translational symmetry the Rh monolayer can be described most efficiently in the layer orbital representation. Nevertheless, the layer can be also considered as a ladder of chains. Therefore it can be described also in the chain orbital representation. Both representations have to be numerically identical. Figure 1 compares the paramagnetic density of states, calculated self-consistently in the framework of both layer and chain representation. The DOS in chain representation and the difference of the two calculations is shown. The over all differences of the two calculations are small. The differences are a bit higher near the van Hove singularities of the *d* DOS. This is not surprising because the absolute high of the DOS in the peaks depends also strongly from the details of the DOS calculation.

III. RESULTS AND DISCUSSION

A. Single chains

In the following we discuss how changes in the local environment influence the magnetic properties of Rh wires on the Ag(100) surface. We consider two chain directions, the ⟨110⟩ one, and the ⟨010⟩ one. ⟨110⟩ is the usual direction of steps on the (100) surface, because it is closed packed. Experimental results about the real structure of Rh chains on Ag(001) are not available. therefore it is assumed, that the Rh atoms are located at ideal positions on the Ag(001) surface. This means Rh atoms occupy hollow sites at the Ag(001) surface and have a distance equal to the Ag layer distance to the Ag(001) surface. Experimentally the relaxations of the Ag surfaces are found small ($\Delta_{12}/d_{bulk}<1\%$) and therefore are not taken into account in the present calculation.[42]

Wires on the surface and embedded in the surface are discussed. It is known, that the numbers of neighbors and the changes in the lattice constant play an important role in the magnetic properties of nanostructures. In Table I the local environment is summarized for the structures discussed here, i.e., how many nearest and next-nearest Rh or Ag atoms a Rh atom has. The band width being proportional to the square root of the coordination number is further reduced in the wires with respect to the surface. The Rh lattice constant being about 7% smaller than the Ag lattice constant, this leads generally to a shrinking band width for the supported Rh nanostructures.

Figure 2 presents the self-consistently calculated paramagnetic densities of states for single Rh chains for the two directions considered here. The chains are in ideal adatom position or embedded in the surface. The following effects can be easily seen:

(i) In all cases the Stoner criterion $\rho(E_F)\cdot J_{Rh}>1$ is fulfilled, due to the high density of states at the Fermi energy. The high density of states results from the reduced coordination number and the stretching of the Rh interatomic distance due to the high value of the Ag lattice parameter.

(ii) The magnetic properties of the Rh wires are mainly determined by the number of Rh neighbors. The embedding of the Rh chains into the Ag surface leads to a stronger hybridization with the *sp* bands of silver and reduced magnetic moment (cf. Table II).

TABLE I. The number of nearest (NN) and next-nearest-neighbors (NNN) of the Rh atoms of the investigated Rh structures. In the three and four chain Rh wires there are inequivalent Rh chains which are shown separately.

			⟨010⟩				⟨110⟩			
			Rh		Ag		Rh		Ag	
System			NN	NNN	NN	NNN	NN	NNN	NN	NNN
Adchain			0	2	4	1	2	0	4	1
Embedded chain			0	2	8	5	2	0	8	5
Two chains			2	2	4	1	3	2	4	1
Three chains	●^{1}●^{2}●^{3}	(1,3)	2	3	4	1	3	2	4	1
		(2)	4	2	4	1	4	4	4	1
Four chains	●^{1}●^{2}●^{3}●^{4}	(1,4)	2	3	4	1	3	2	4	1
		(2,3)	4	3	4	1	4	4	4	1
Monolayer			4	4	4	1	4	4	4	1

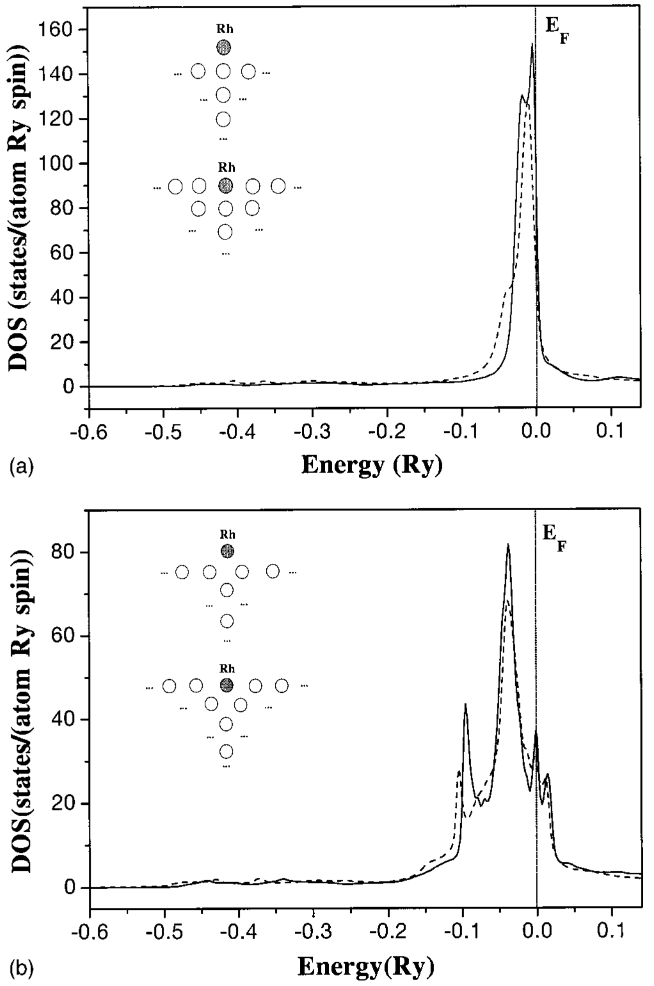

FIG. 2. The paramagnetic density of states of the adsorbed (solid line) and embedded (dashed line) Rh chains in the ⟨010⟩ (a) and ⟨110⟩ (b) directions. The cross sections of the structures are shown too (70 **k** points in 1D BZ, 230 chains in cluster).

(iii) The bandwidth is smaller for the ⟨010⟩ chains than for the ⟨110⟩ chains. This leads to higher $\rho(E_F)$ values and as a consequence to higher magnetic moments. The reason is that in the ⟨010⟩ chain the Rh atoms have only next-nearest Rh neighbors.

The magnetic moment of the infinite ⟨110⟩ Rh chain can be compared with *ab initio* calculations[7] performed for the ferromagnetic state of the linear chain of four Rh atoms (C4) in the ⟨110⟩ direction on the Ag(100) surface and in the topmost surface layer. The magnetic moment for the inner Rh atoms inside the C4 chain is $0.96\mu_B$ and the deviation between the Korringa-Kohn-Rostoker (KKR) and TB results is less than 3%. Although our result agrees well with the *ab initio* result for the adsorbed chain, larger deviations are found for the embedded chain.

TABLE II. The magnetic moment of the investigated Rh structures.

Configuration		Magnetic moment (μ_B) ⟨010⟩	⟨110⟩
Adchain		1.325	0.990
Embedded chain		0.960	0.916
Two chains		1.241	0.706
Three chains	(1,3)	0.833	0.852
	(2)	0.849	0.769
Four chains	(1,4)	1.001	0.882
	(2,3)	0.922	0.835
Monolayer (TB)		0.990	
Monolayer (*ab initio*)		1.040	

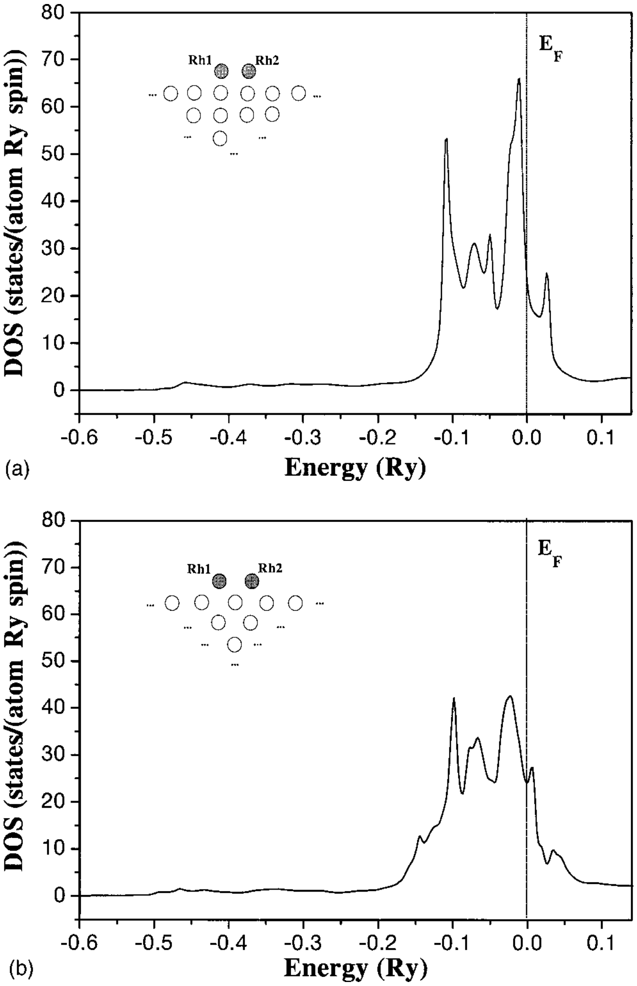

FIG. 3. The paramagnetic density of states of the pair of Rh chains in the ⟨010⟩ (a) and ⟨110⟩ (b) directions (70 **k** points in 1D BZ, 260 chains in cluster).

B. Cluster of chains

We have also studied clusters of chains on the Ag(001) surface. For all configurations the Ag environment is the same for each Rh atom (cf. Table I), but the number of Rh neighbors varies from 4 to 8 (monolayer environment). Figure 3 shows the paramagnetic DOS for a pair of Rh chains along the ⟨010⟩ and the ⟨110⟩ direction. For both directions the number of Rh neighbors increases with respect to the single chain so that the magnetic moment decreases (cf. Table II). A Rh atom in a pair of chains in the ⟨110⟩ direction has more nearest Rh neighbors than in the ⟨010⟩ direction. This leads to a slightly broader DOS and a reduced magnetic moment.

The results show that magnetism for the pair of Rh chains obeys the conventional understanding of low-dimensional

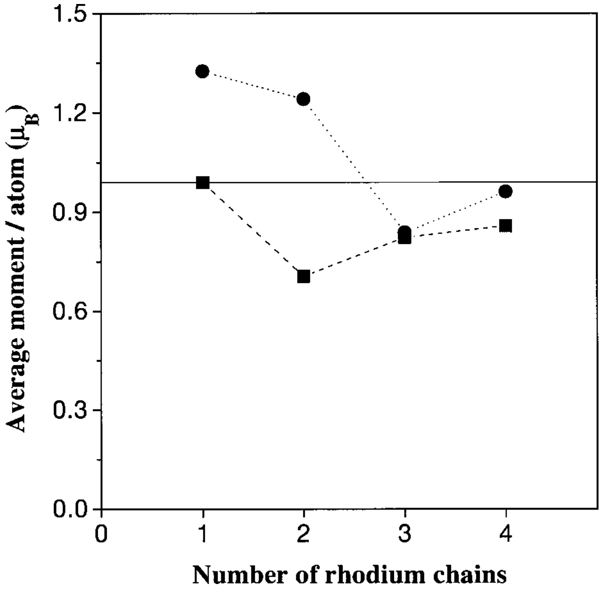

FIG. 4. The average magnetic moment of the Rh wire as a function of the number of chains in the wire.

itinerant magnetism: increasing the coordination number leads to the reduction of magnetic properties.[13,16,43,44] Let us note also that the magnetic moment for the 2 Rh ⟨010⟩ chains is practically unchanged (less than 6%) with respect to the single Rh chain. Nearest-neighbor interaction does not exist in chain direction in this case. Nearest-neighbor interaction between the chains is introduced by the second chain. The single chain in ⟨110⟩ has a lower magnetic moment than the chain in the ⟨010⟩ direction because of the nearest-neighbor interactions in chain direction. The second ⟨110⟩ chain increases the nearest-neighbor interaction further and leads also to next-nearest-neighbor interactions (cf. Table I). This all together leads to a stronger decrease of the magnetic moment compared to a couple of ⟨010⟩ chains.

If one increases the number of Rh chains in the cluster on the surface the monolayer limit should be reached. It can be seen from Table II that two chains in the ⟨110⟩ direction show a magnetic moment clearly below the monolayer limit of $1\mu_B$. Therefore we increased the number of chains to 3 and 4. In Fig. 4 we show the evolution of the average magnetic moment $\overline{\mu_N}$ as a function of the number of chains and their direction. The nonmonotoneous behavior of $\overline{\mu_N}$ with the number of Rh chains in both directions can be clearly seen. Moreover, the gradual convergency of the average magnetic moment $\overline{\mu_N}$ to its boundary value μ_N^{layer} is also discernible.

The results for the magnetic properties of three Rh ⟨010⟩ and ⟨110⟩ chains can be compared with the results of the first-principles calculation[7] of small compact Rh clusters on Ag(001).[45] Islands in ideal adatom position consisting of five atoms (I5) or 9 atoms (I9) are investigated (cf. Fig. 5). The packing of the atoms in the I5 and I9 islands is similar to the structure of the three Rh chains in the ⟨010⟩ and ⟨110⟩ directions, respectively. First-principles investigations[7] show that for the I5 island the inner moment ($1.00\mu_B$) is larger than the outer one ($0.66\mu_B$), while the central atom in the I9 cluster has a rather small moment of $0.16\mu_B$ compared to the moments of the outer atoms ($0.62\mu_B$ and $0.64\mu_B$). The central chain of the ⟨010⟩ cluster has a slightly higher moment than the outermost chains, whereas the central chain of the ⟨110⟩ cluster has a significantly lower moment than the outermost chains. This corresponds nicely to KKR-GF calculations.

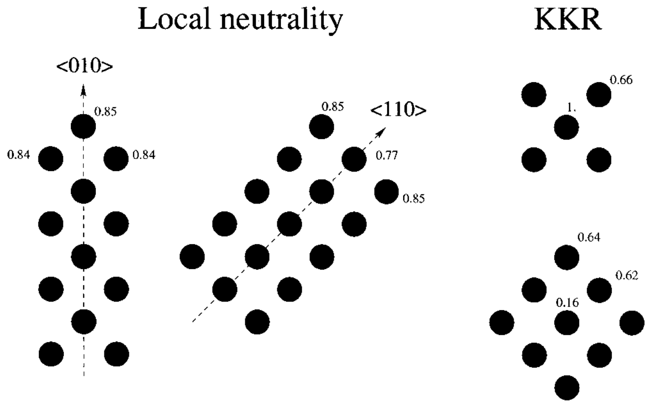

FIG. 5. The top view of the wires of three Rh chains and the five and nine atoms Rh clusters.

IV. CONCLUSIONS

We have shown that one-dimensional *ideal* Rh nanostructures on Ag(001) are clearly magnetic and that the magnetic moment corresponds roughly to the moment of a perfect ferromagnetic Rh monolayer on Ag(001). Our results show that not only Rh monolayers and small Rh clusters on the Ag surface but also one-dmensional structures show a considerable magnetic moment. The average magnetic moment of Rh atoms in ferromagnetic chains is found to depend on chain direction. The magnetic moment of Rh atoms depends nonmonotonously on the number of Rh chains supported on the ideal Ag(001) surface.

These results demonstrate clearly that the magnetic structure of Rh chains is defined not only by intra and interatomic interaction among nearest neighbors, but local coordination number as well. Due to the interchain interaction, it was found for one to three Rh chains, that the local magnetic moments of Rh atoms on silver surface are defined not only by Rh-Rh interaction. The essential contribution to the formation of magnetic properties of Rh atoms on Ag comes from interaction between their electronic subsystems. The self-consistent calculations of partial densities of states notified the crucial role of *sp-d* and *d-d* hybridizations in Rh-Rh, Rh-Ag interfaces in the formation of magnetic properties for transition metals. The numerical scheme developed in this paper can be applied in the future to more complicated structures.

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