Magnetic properties of 3d transition metal wires on vicinal Cu(111) surfaces at finite temperature

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One-dimensional transition metal (TM) nanowires can be formed on a stepped Cu(111) surface. The basic template is an embedded Fe chain at one-atom distance away from the upper edge of the monoatomic surface step, supply the deposition of 3d TM chains from V to Co to form on top of the Fe chain. Density functional theory (DFT) is applied to calculate the magnetic properties of these TM-Fe wires. Exchange parameters are extracted from the DFT calculations. A classical Heisenberg model is used in Monte Carlo simulations to study finite temperature effects. © 2010 American Institute of Physics. [doi:10.1063/1.3368794]

I. INTRODUCTION

Magnetic nanostructures on surfaces are of great interest for modern nanoscience due to their potential application as atomic-scale magnetic devices.1,2 Therefore, nanoscale clusters, monoatomic wires, or quasi-one-dimensional stripes have been investigated from experimental3–8 and theoretical points of view.9–16 The lower coordination of the magnetic atoms in such systems located on a metallic surface compared to bulk leads to an enhancement of the moments, and a large magnetocrystalline anisotropy energy (MAE) can help to stabilize the direction of the magnetic moments. The Cu(111) stepped surface with an embedded Fe chain can be considered as an exemplary template for the deposition of other 3d transition metal (TM) atoms to form a chain on top of this embedded Fe chain (cf. Fig. 1). The growth mechanism of such templates was investigated by Guo et al.15 and Mo et al.16 by means of DFT calculations and by scanning tunnelling microscopy. To use a clear notation, a single linear periodic arrangement of atoms will be called a chain in the following investigation, while a system consisting of two parallel chains, either isolated or embedded in the Cu(111) surface, will be named wire.

We will focus our discussion on the magnetic properties of the wires. Detailed information on the real structure of such systems is given elsewhere.17 We present a systematic investigation of the magnetic ground states and the magnetic coupling in TM-Fe wires. The analysis of the exchange coupling and of the MAE allows to set up a classical Heisenberg model to study finite temperature effects.

II. COMPUTATIONAL DETAILS

The calculations are performed within the framework of spin-polarized density functional theory using the Vienna ab initio simulation package.18,19 The frozen-core full-potential projector augmented-wave method (PAW) is used applying the generalized gradient approximation of Perdew and Wang (PW91-GGA).20 Computational details and convergence checks are the same as those in Ref. 17 and 22. The isolated chains and wires are modeled as a two-dimensional array of infinitely long units, keeping the distance to be at least 13 Å. A large plane-wave cutoff energy of 350 eV is used for all 3d TM chains. 25 k-points are used to sample the one-dimensional Brillouin zone. A supercell containing six Cu layers, which corresponds to 60 Cu atoms, is constructed to model the Cu(111) stepped surface (cf. Fig. 1). The same construction was used by Mo et al.14

For the Monte Carlo (MC) simulations, lattices of the size of 5200 sites representing the atoms of the single wire are used. Nearest-neighbor exchange interaction is assumed to define the classical Heisenberg Hamiltonian $H = -\sum_{i,j} J_{ij} \vec{e}_i \cdot \vec{e}_j - \sum_i \Delta e_i^2$, where $(i,j)$ denotes summation over pairs of classical unit spinvectors $\vec{e}_i$, interacting via $J_{ij}$. Anisotropy effects are taken into account by taking the MAE $\Delta$ to be 0, 0.01, 0.03, 0.10, 0.30, 1, 3, or 9 meV per site. By doing so, it is assumed that the MAE of Fe and the TM sublattices are equal. Periodic boundary conditions in direction of the wire are applied. To find the critical temperature...
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spin-polarized DFT calculations. The magnetic groundstates
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bor interactions only. Noncollinear configurations used to
Therefore, we restrict the Heisenberg model to nearest neigh-
neighbor interaction is already an order of magnitude smaller.
force theorem reveal that the nearest neighbor exchange in-
TABLE I. Exchange constants for the freestanding TM chain, freestanding
TM-TM chains, and between Fe and TM chain (yellow) cancel out in the Heisenberg Hamiltonian. $J_{TM,Fe}$ can be calculated. [(c) and (d)] Configurations that allow to calculate the interaction $J_{TM,Fe}$ between the chains.

III. DISCUSSION
Three systems are investigated. In freestanding TM
chains, the atomic distance is constrained to the Cu bond
length $d_{Cu}$ of the Cu(111) substrate in order to simulate a
freestanding equivalent to the TM chain in the TM-Fe wire
on the substrate. A freestanding wire is studied as an equiva-
lent to the one embedded into the Cu(111) surface (cf. Fig.
1). All interatomic distances correspond to the Cu bond
length of the substrate in this case. The structure of the em-
bedded TM-Fe wire is fully relaxed. The main effect of
structural relaxations is an inward relaxation of the TM at-
oms relative to their ideal positions. For Mn–Fe, the inward
relaxation of Mn is 16% (related to Cu lattice plane dis-
tance). The Fe chain also shows an inward relaxation of 7%,
respectively. Details of the relaxations for all 3d TM-Fe
wires are given in Ref. 17.

Central task for the mapping onto a classical Heisenberg
model is the determination of exchange constants and the
MAE. The former can, for example, be extracted from DFT
calculations either by the comparison of total energy of several
artificial collinear magnetic structures or by applying the
magnetic force theorem in the framework of the
Korringa–Kohn–Rostoker Green’s function method. In
this work, artificial noncollinear structures are used. The idea
is to choose such noncollinear states that exchange inter-
actions in the Heisenberg model can be switched on or off in a
controlled manner. Investigations of the freestanding TM
chains by means of total energy considerations and magnetic
force theorem reveal that the nearest neighbor exchange in-
teraction is the most important one. The next-nearest neigh-
bor interaction is already an order of magnitude smaller.
Therefore, we restrict the Heisenberg model to nearest neigh-
bor interactions only. Noncollinear configurations used to
calculate the exchange parameters for freestanding and em-
bedded wires are given in Fig. 2. It is checked that the mag-
netic moments are constant for the different noncollinear
configurations used for a specific system. Noncollinear ar-
rangements being equivalent by symmetry lead to the same
exchange parameters. The exchange parameters for all sys-
tems calculated by such a procedure are given in Table I. The
discussion is restricted to the TM elements from V to Co
because it is not possible to stabilize all necessary magnetic
configurations for the other elements. In Ref. 17, the
magnetic groundstates of such freestanding and embedded wires
were investigated for ideal structures by means of collinear
spin-polarized DFT calculations. The magnetic groundstates
for the free chains are in agreement with the results of Tung
and Guo for the relaxed chains with V as an exception.
This can be understood easily because the relaxed bond
length in the ferromagnetic state is close to the Cu bond
length, whereas in the antiferromagnetic ground state the
bond length is 20.2% smaller than $d_{Cu}$. The exchange con-
stants reflect the antiferromagnetic groundstates of Cr and
Mn chains. Noncollinear calculations for such 3d-TM chains
reveal that the easy axis is in chain direction with Mn as an
exception having the easy axis perpendicular to the chain.
The MAE of the chains is in the order of a few meV. We take
it as a parameter in the MC calculations.

Some general conclusions can be drawn from Table I.
The exchange constants reflect the result that Fe–Fe and
Co–Fe wires have a ferromagnetic groundstate in collinear
calculations. Antiferromagnetic couplings are present at the
beginning of the series. For the freestanding wires, $J_{Fe-Fe}$ is
roughly constant through the series. Cr shows a strong anti-
ferromagnetic intrachain coupling, whereas in V–Fe a strong
antiferromagnetic interchain coupling is present. Of course,
relaxation effects are reflected in the exchange constants of
the embedded systems. The stronger hybridization due to the
inward relaxation of the TM chains leads to a decrease of the
interchain exchange constants.

TABLE I. Exchange constants for the freestanding TM chain, freestanding
TM-Fe wires, and the embedded TM-Fe wires. The definition of the con-
stants in the Heisenberg model incorporates the magnetic spin moments.

![Graph](image_url)
Figure 3 shows the susceptibility for an embedded Mn–Fe wire calculated for different MAE values. It can be seen that, in agreement with the Mermin–Wagner theorem, there is no magnetic ordering for a vanishing MAE. But for small values, a phase transition can be observed. An increasing anisotropy stabilizes the moments against thermal fluctuation and, thus, leads to an increase of the $T_C$. Furthermore, the phase transition is broadened. The latter and the relative increase of $T_C$ with respect to the MAE, as shown in Fig. 3, are very similar for the other TMs. All calculated $T_C$’s are well below room temperature for all systems. A summary of the $T_C$’s of all systems for MAE=1.00 meV can be found in Table II.

**IV. CONCLUSIONS**

*Ab initio* DFT calculations are used to set up Heisenberg models to study finite temperature properties of TM-Fe wires.

<table>
<thead>
<tr>
<th>$T_C$</th>
<th>V (K)</th>
<th>Cr (K)</th>
<th>Mn (K)</th>
<th>Fe (K)</th>
<th>Co (K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Freestanding wire</td>
<td>100</td>
<td>20</td>
<td>132</td>
<td>68</td>
<td>75</td>
</tr>
<tr>
<td>Embedded wire</td>
<td>88</td>
<td>41</td>
<td>63</td>
<td>122</td>
<td>94</td>
</tr>
</tbody>
</table>

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