

Magnetic anisotropy and spin-spiral wave in V, Cr and Mn atomic chains on Cu(001) surface:
first principles calculations

This article has been downloaded from IOPscience. Please scroll down to see the full text article.

2011 J. Phys. D: Appl. Phys. 44 205003

(<http://iopscience.iop.org/0022-3727/44/20/205003>)

View [the table of contents for this issue](#), or go to the [journal homepage](#) for more

Download details:

IP Address: 140.116.46.82

The article was downloaded on 19/05/2013 at 03:30

Please note that [terms and conditions apply](#).

Magnetic anisotropy and spin-spiral wave in V, Cr and Mn atomic chains on Cu(001) surface: first principles calculations

J C Tung¹, Y K Wang¹ and G Y Guo^{2,3}

¹ Center for General Education and Department of Physics, National Taiwan Normal University, Taipei 106, Taiwan

² Graduate Institute of Applied Physics, National Chengchi University, Taipei 116, Taiwan

³ Department of Physics and Center for Theoretical Sciences, National Taiwan University, Taipei 106, Taiwan

E-mail: gyguo@phys.ntu.edu.tw

Received 28 January 2011, in final form 6 April 2011

Published 3 May 2011

Online at stacks.iop.org/JPhysD/44/205003

Abstract

Recent *ab initio* studies of the magnetic properties of all 3d transition metal (TM) freestanding atomic chains have predicted that these nanowires could have a giant magnetic anisotropy energy (MAE) and might support a spin-spiral structure, thereby suggesting that these nanowires would have technological applications in, e.g. high-density magnetic data storage. In order to investigate how the substrates may affect the magnetic properties of the nanowires, here we systematically study V, Cr and Mn linear atomic chains on a Cu(001) surface based on the density functional theory with the generalized gradient approximation. We find that V, Cr and Mn linear chains on the Cu(001) surface still have a stable or metastable ferromagnetic state. However, the ferromagnetic state is unstable against the formation of a noncollinear spin-spiral structure in the Mn linear chains and also the V linear chain on the atop sites on the Cu(001) surface, due to the frustrated magnetic interactions in these systems. Nonetheless, the presence of the Cu(001) substrate does destabilize the spin-spiral state already present in the freestanding V linear chain and stabilizes the ferromagnetic state in the V linear chain on the hollow sites on Cu(001). When spin-orbit coupling (SOC) is included, the spin magnetic moments remain almost unchanged due to the weakness of SOC in 3d TM chains. Furthermore, both the orbital magnetic moments and MAEs for V, Cr and Mn are small, in comparison with both the corresponding freestanding nanowires and also the Fe, Co and Ni linear chains on the Cu(001) surface.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

Nanostructured magnetic materials have recently received enormous attention because of their fascinating physical properties and potential applications. Finite freestanding gold atomic chains in break-junction experiments were first reported in 1998 [1, 2]. However, these freestanding atomic chains are unstable and transient. Physically stable magnetic nanowires deposited on metallic substrates are one of the most important magnetic nanostructures, and many techniques

have been used to prepare and study them. In particular, Gambardella *et al* [3, 4] succeeded in preparing a high density of parallel atomic chains along steps by growing Co on a high-purity Pt(997) vicinal surface in a narrow temperature range, 10–20 K. The magnetism of Co wires was also investigated by x-ray magnetic circular dichroism [4]. Recently, Fe double chains deposited on an Ir(001) surface were prepared [5], and their structures were investigated by both scanning tunnelling microscopy measurements [5] and theoretical calculations [6].

More recently, we have performed systematic *ab initio* studies of magnetic anisotropy [7] and spin-spiral wave in all 3d transition metal (TM) freestanding linear chains. Interestingly, we found that Fe and Ni freestanding linear chains have a gigantic magnetic anisotropy energy (MAE) [7], and that the magnetic couplings in V, Mn and Fe linear chains are frustrated, resulting in the formation of stable spin-spiral structures [8]. Saubanere *et al* also found a stable spiral magnetic order in a freestanding V atomic chain in their recent *ab initio* theoretical study of TM nanowires [9]. Experimentally, copper and tungsten are excellent substrates for growth of Fe thin films [10, 11] because of the small lattice constant mismatch between Fe and Cu (3.61 Å) as well as W (3.61 Å). This stimulated, e.g. a recent theoretical study of the magnetic order and exchange interactions of 3d TM monoatomic chains on the (1 1 0) surface of Cu, Pd, Ag and NiAl [12]. Here in this paper, we perform first principles calculations for magnetic moments, MAEs and spin-spiral wave energies of V, Cr and Mn linear chains deposited on a Cu(001) surface, in order to study how the presence of the substrate would modify the magnetic properties of the V, Cr and Mn nanowires.

2. Theory and computational method

The present calculations are based on density functional theory with the generalized gradient approximation (GGA) [13]. The accurate frozen-core full-potential projector augmented-wave (PAW) method [14], as implemented in the Vienna Ab-initio Simulation Package (VASP) [15, 16], is used. A large plane-wave cutoff energy of 350 eV is used for all the systems considered. The V, Cr and Mn linear atomic chains along the x direction on the Cu(001) surface are modelled by a nanowire attached to both sides of a seven-layer-thick Cu(001) slab, as plotted in figure 1. The TM atoms on the nanowires are placed either on the top of the surface Cu atoms (denoted here as the atop (A) site) or at the hollow position on the Cu surface (called here the hollow (H) site). The two-dimensional unit cell is chosen to be of $p(1 \times 4)$ structure. The nearest in-plane (out-of-plane) wire–wire distance is larger than 10 Å (11 Å) which is sufficiently wide to decouple the neighbouring wires. The theoretical lattice constant (3.60 Å) of bulk copper, which is in good agreement with the experimental Cu lattice constant of 3.61 Å, is used as the fixed in-plane lattice constant of the Cu slab. However, the atoms are allowed to move in the surface-normal direction, and structural relaxations are performed using the conjugate gradient method. We focus on the nonmagnetic (NM) and ferromagnetic (FM) states of the V, Cr and Mn linear chains on the Cu(001) surface. The equilibrium structure is obtained when all the forces acting on the atoms are less than 0.02 eV \AA^{-1} . The Γ -centred Monkhorst–Pack scheme with a k -mesh of $20 \times 5 \times 1$ in the full Brillouin zone (BZ), in conjunction with the Fermi–Dirac smearing method with $\sigma = 0.2 \text{ eV}$, is used for BZ integration.

We also consider the transverse spin-spiral states where all the spins rotate in a plane perpendicular to the atomic chain axis. The generalized Bloch theorem [17, 18] is used to calculate self-consistently the total energies of the transverse

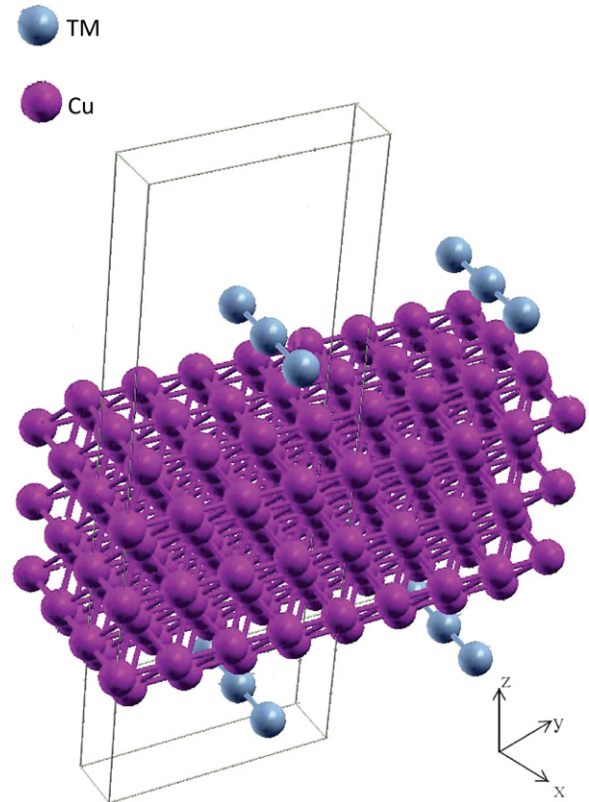


Figure 1. Theoretical atomic structure used for the present slab supercell modelling of the 3d TM V, Cr and Mn linear chains on the hollow sites of the Cu(001) surface. The rectangular box frame represents the primitive cell of the three-dimensional periodic slab supercell structure.

spin spirals as a function of the spin-spiral wave vector. Therefore, the relativistic spin–orbit coupling (SOC) is not included in these calculations. A denser $25 \times 5 \times 1$ k -point mesh is used for the V and Mn chains, in order to ensure that the calculated spin wave excitation energies (see figure 3(a)) and also the first and second near-neighbour exchange interaction parameters (i.e. J_{01} and J_{02} in table 2) are converged to within a few per cent.

Ab initio calculation of the MAE is computationally very demanding because of the smallness of MAE, and thus needs to be carefully carried out [19]. Here we use the total energy difference approach rather than the widely used force theorem to determine the MAE, i.e. the MAE is calculated as the difference between the full self-consistent total energies for the two different magnetization directions concerned. The total energy convergence criterion is 10^{-8} eV/atom . The same k -point mesh is used for the density of states (DOS) calculations. The MAEs calculated with a denser $32 \times 6 \times 1$ k -point mesh hardly differ from that obtained with the $20 \times 5 \times 1$ k -point mesh (within 0.01 meV per magnetic atom).

3. Results and discussion

3.1. Formation energy and spin magnetic moment

To see how the Cu substrate interacts with the V, Cr and Mn chains, we first study the chain formation energy. The

Table 1. Calculated formation energy E^f , equilibrium interlayer distance d_{eq} , spin magnetic moment per magnetic atom, m_s , and magnetization energy per magnetic atom $E^{\text{mag}} = E^{\text{FM}} - E^{\text{NM}}$ of the 3d TM nanowires on both the hollow (H) and atop (A) sites of the Cu(001) surface. Here superscripts FM and NM denote the ferromagnetic and nonmagnetic states, respectively.

		E^f (eV/u.c.)	$d_{\text{eq}}^{\text{NM}}$ (Å)	$d_{\text{eq}}^{\text{FM}}$ (Å)	m_s (μ_B)	E^{mag} (eV)
V	H	-1.29	1.64	1.70	2.11	-0.559
	A	-0.01	1.83	2.03	3.30	-0.727
Cr	H	-1.56	1.56	1.80	4.23	-0.769
	A	-0.86	1.70	2.18	4.60	-1.222
Mn	H	-0.52	1.49	1.73	4.14	-0.613
	A	-0.25	2.25	2.37	4.53	-0.458
Fe ^a	H	-2.14	1.51	1.64	3.07	-0.337
	A	-0.31	1.79	2.31	3.29	-0.444
Co ^a	H	-2.15	1.50	1.57	1.79	-0.130
	A	-1.19	1.80	2.27	1.99	-0.205
Ni ^a	H	-2.26	1.55	1.55	0.00	0.000
	A	-1.32	1.96	2.26	0.65	-0.032

^a Theoretical calculations ([20]).

chain formation energy E^f describes the difference in the total energy of the combined system of the Cu substrate and a TM chain before and after the TM chain is deposited on the substrate. As in [8], we introduce the chain formation energy as $E^f = \frac{1}{2}(E_t - nE_{\text{Cu}}^{\text{bulk}} - mE_{\text{TM}}^{\text{chain}})$ where E_t is the total energy of the system in the FM state, $E_{\text{Cu}}^{\text{bulk}}$ is the total energy of the bulk Cu and $E_{\text{TM}}^{\text{chain}}$ is the total energy of the freestanding TM nanowires in the FM state. n and m are the numbers of Cu and TM atoms in the system, respectively. It should be noted that there is no universal definition for the chain formation energy. The calculated formation energies of all the V, Cr and Mn nanowires are listed in table 1. The formation energies for the Fe, Co and Ni linear chains on the Cu(001) surface, reported recently [20], are also listed in table 1 for comparison. It is clear from table 1 that it is more energetically favourable when the TM atoms are placed on the hollow sites, as might be expected because the hollow site has a higher coordination number. Among all the 3d TM nanowires, Ni nanowire is the most energetically favourable on both the hollow and atop sites. Generally, the V, Cr and Mn chains are less energetically favourable than the corresponding Fe, Co and Ni chains (table 1). Interestingly, the formation energy of the V chain on the atop site is almost zero, thereby suggesting that this chain would not be stable.

Table 1 shows that the interlayer distance between the V, Cr and Mn nanowires on the hollow (atop) site and the Cu substrate is 1.70 (2.03) Å, 1.80 (2.18) Å and 1.73 (2.37) Å, respectively. The ideal interlayer distance for the Cu substrate is 1.81 Å. Therefore, the copper substrate seems to pull (push) the TM nanowires when deposited on the hollow (atop) site. In all the cases considered here, the equilibrium interlayer distance is larger in the FM state than in the NM state. This is due to the larger kinetic energy in a magnetic state which makes the magnetic materials softer and larger in size (see table 1). Table 1 also shows that when the interlayer distance changes, the spin magnetic moment changes as well. In general, for all the 3d TM nanowires considered, an increase in interlayer

distance will result in an increase in the spin moment. This is because the stronger overlap between TM 3d orbitals and the Cu substrate would result in a decrease in the magnetic moment. The interatomic distance between the deposited TM atoms in all the cases considered here is 2.55 Å. The calculated spin moments of the V, Cr and Mn atoms on the hollow (atop) sites are 2.11 (3.30) μ_B /atom, 4.23 (4.60) μ_B /atom and 4.14 (4.53) μ_B /atom, respectively. In comparison, the calculated spin moments at the same bond length (2.55 Å) of the freestanding V, Cr, Mn, Fe, Co and Ni nanowires, reported recently [7], are 4.07 μ_B /atom, 5.06 μ_B /atom, 4.53 μ_B /atom, 3.30 μ_B /atom, 2.30 μ_B /atom and 1.14 μ_B /atom, respectively. Clearly, placing the 3d TM nanowires on the hollow sites significantly reduces or even quenches the spin moments on the nanowires, whilst the spin moments are much less affected when the nanowires are deposited on the atop sites.

The obtained magnetic moments of the V, Cr and Mn nanowires can be understood in terms of the calculated spin-polarized DOS, as displayed in figure 2. In figure 2, the Fermi level is set to be zero, the DOS spectra for the minority spin are multiplied by -1 , and the sp orbital decomposed DOS are scaled up by a factor of 10 for clarity. Clearly, the d orbitals of the V, Cr and Mn nanowires on both sites are significantly localized due to the reduction in the coordination number whilst the sp orbitals are more dispersive. The reduction in coordination number thus induces considerable enhancement in the spin splitting of the V, Cr and Mn 3d bands. The spin splitting values of the V, Cr and Mn 3d bands for the hollow (atop) site are 1.48 (2.01) eV, 2.65 (2.93) eV and 2.98 (3.30) eV, respectively. The interlayer distance between the TM nanowires and Cu substrate is larger on the atop site. This indicates that the overlaps between the TM and substrates are smaller, and hence the spin magnetic moments are larger. The splitting of the 3d band is approximately proportional to the spin moment.

3.2. Spin-spiral wave and exchange interaction

In our recent study of noncollinear magnetism in freestanding 3d TM nanowires [8], V, Mn and Fe chains were found to have a stable noncollinear spin-spiral structure due to the frustrated exchange interactions in these systems whilst Cr chain was found to have an antiferromagnetic (AF) ground state. Therefore, here we perform total energy calculations for the spin-spiral structure in V, Cr and Mn chains on Cu(001) to examine how these interesting magnetic properties would be modified in the presence of the Cu substrate. The calculated total energies $[E(\mathbf{q}, \theta)]$ of the V, Cr and Mn linear chains on Cu(001) are plotted as a function of the spin-spiral wave vector q in figure 3(a). Since here only the transverse spin-spiral waves along the chain direction (i.e. x -axis) are considered, the angle between the chain axis and the magnetization direction $\theta = \pi/2$, and hence we simply write $E(\mathbf{q}, \theta = \pi/2) = E(q)$. The spin-spiral structure at $q = 0$ corresponds to the collinear FM state, whilst the state at $q = 0.5 (2\pi/d)$ corresponds to the AF state. Figure 3(a) shows that the FM state in all the 3d TM chains considered here, except the hollow-site V chain, is unstable against the formation of a spin-spiral

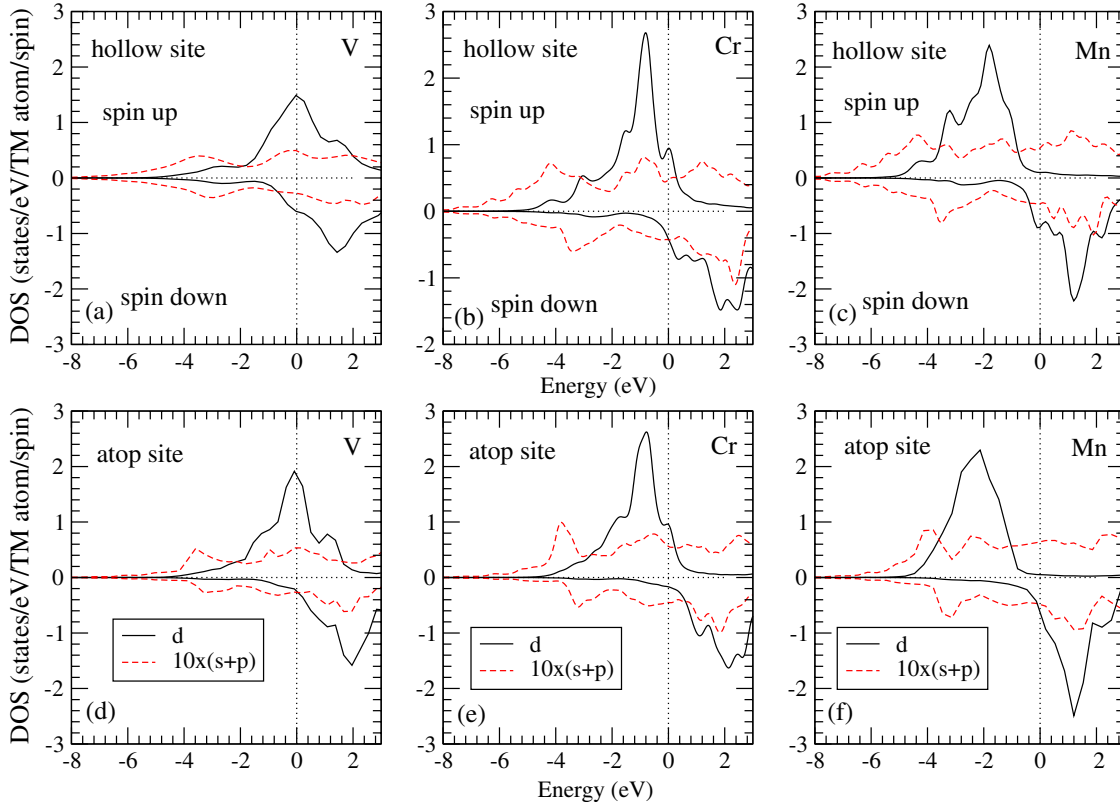


Figure 2. Spin-polarized DOS of the V, Cr and Mn nanowires on Cu(00 1). the Fermi level is at 0.0 eV. The DOS spectra for the minority spin are multiplied by -1 , and the sp orbital decomposed DOS are scaled up by a factor of 10 for clarity.

structure. In the Cr chains on Cu(00 1), the lowest energy spin-spiral state corresponds to the AF state (i.e. $q = 0.5$), being the same as in the freestanding Cr chain case [8]. For comparison, we note that in previous GGA calculations [21], the FM state could not be stabilized in bulk Cr metal, whilst the magnetization energy of the AF state is rather small (~ 0.016 eV/atom). The genuine stable spin-spiral state occurs in the atop-site V chain and hollow-site (atop-site) Mn chain on Cu(00 1) with $q = 0.15$ and $q = 0.15$ (0.40), respectively. We note that the freestanding V and Mn linear chains at equilibrium bond length has a stable spin-spiral state with $q = 0.25$ and $q = 0.33$, respectively [8]. Therefore, it appears that depositing the V chain on the hollow sites would destabilize the noncollinear spin-spiral state and stabilize the FM state.

The energy of a spin-wave excitation (i.e. the magnon dispersion relation) $\varepsilon(q)$ (or $\hbar\omega(q)$) can be related to the calculated total energy of the spin-spiral state as [8, 22, 23]

$$\varepsilon(q) = \frac{4\mu_B}{m_{s0}} [E(q) - E(0)], \quad (1)$$

where m_{s0} is the spin magnetic moment per site at $q = 0$. In the range of small q , $\varepsilon(q) = Dq^2$, where the spin-wave stiffness constant D relates the spin-wave energy $\varepsilon(q)$ to the wave vector q in the long wavelength limit. The spin-wave stiffness constant D of an atomic chain can be estimated by fitting an even order polynomial to the corresponding spin-wave spectrum shown in figure 3(a). The spin-wave stiffness constant D obtained in this way for the V, Cr and Mn linear

Table 2. Calculated exchange interaction parameters (J_{0j}) (meV) between two j th near neighbours ($j = 1, 2, 3, 4, 5$) and spin-wave stiffness constant D (meV \AA^2) as well as ground state spin-spiral wave vector q ($2\pi/d$) ($d = 2.55$ \AA is the interatomic distance along the chain) in the V, Cr and Mn atomic chains on Cu(00 1).

	J_{01}	J_{02}	J_{03}	J_{04}	J_{05}	D	q
H-site							
V	105.2	-30.6	17.8	-11.6	8.4	345	0.00
Cr	-154.0	12.8	-3.2	2.0	-1.8	-363	0.50
Mn	57.6	-38.6	17.0	-9.2	6.0	~ 0	~ 0.15
A-site							
V	24.2	-25.2	3.8	-10.4	10.8	-379	0.20
Cr	-174.6	15.0	-6.4	4.6	-3.8	-399	0.50
Mn	-59.4	-18.2	-7.6	-5.0	2.2	-683	0.40

chains on Cu(00 1) are listed in table 2. A negative value of D means that the FM state is not stable against a spin-spiral wave excitation. As mentioned above, the FM state in all the atop-site TM chains and also in the hollow-site Cr chain is unstable and hence D for these nanowires is negative (table 2). Interestingly, D for the hollow-site Mn chain is nearly zero and this is because the $E(q)$ curve is very flat in the range $0 < q < 0.2$ (figure 3(a)). Furthermore, when deposited on the hollow sites on Cu(00 1), the spin-wave stiffness D of the V chain changes from -424 meV \AA^2 (freestanding chain) [8] to 345 meV \AA^2 .

In the frozen magnon approach, the exchange interaction parameters J_{ij} between atom i and atom j on a TM chain

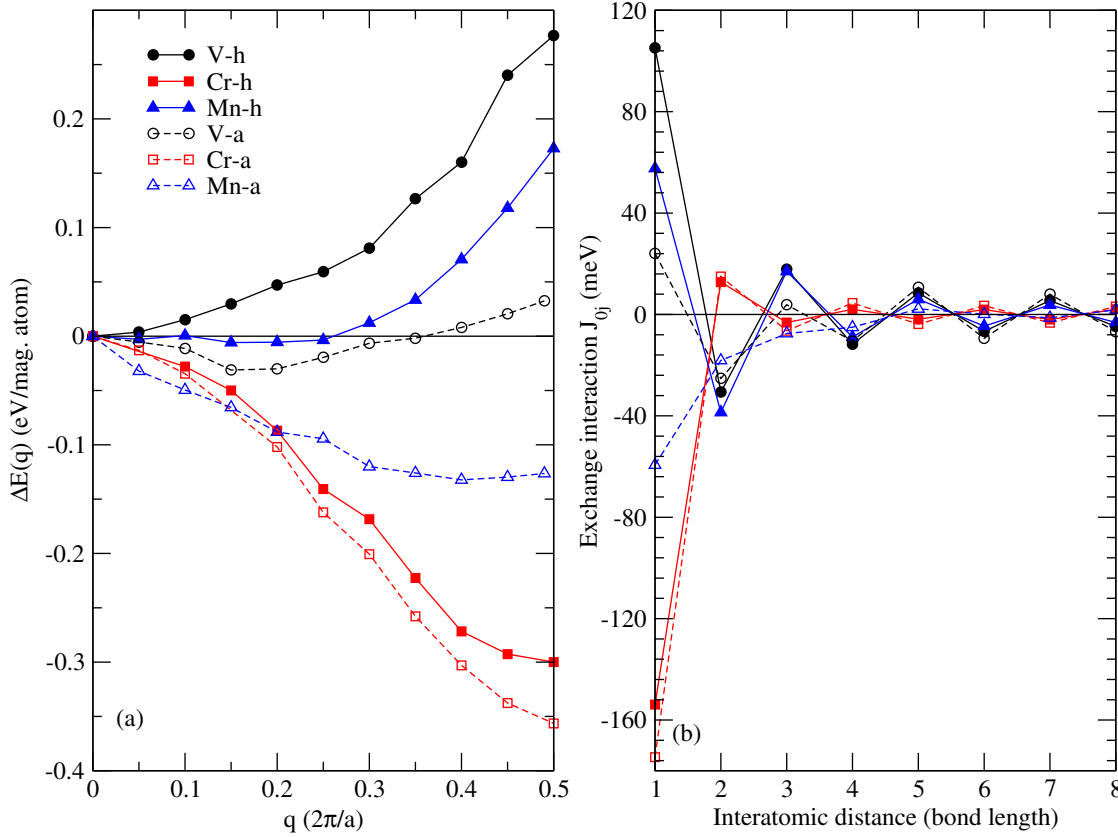


Figure 3. (a) Calculated total energies $\Delta E(q)$ (relative to the total energy of the FM state $E(0)$, i.e. $\Delta E(q) = E(q) - E(0)$) of the V, Cr and Mn linear chains on the Cu(001) surface as a function of spin-spiral wave vector q ($2\pi/a$). (b) Exchange interaction parameters J_{0j} in the V, Cr and Mn linear chains on Cu(001) derived from (a) (see text).

are related to the magnon excitation energy $\varepsilon(q)$ by a Fourier transformation:

$$J_{0j} = \frac{1}{N_q} \sum_q e^{-iq \cdot R} J(q), \quad (2)$$

where N_q is the number of q points in the BZ included in the summation. $J(q)$ is the Fourier transformation of the exchange parameters J_{ij} and is related to the magnon excitation energy $\varepsilon(q)$ by

$$\varepsilon(q) = -\frac{2\mu_B}{m_{so}} J(q). \quad (3)$$

Here the negligible induced magnetization on all the Cu atoms is neglected and hence only the TM atoms on the deposited chain are considered in the summation. The calculated exchange parameters J_{ij} are plotted in figure 3(b) and also listed in table 2. The magnetic coupling between two first near neighbours in the V chains and also the hollow-site Mn chain is FM ($J_{01} > 0$), whilst it is AF ($J_{01} < 0$) in the rest of the Cr and Mn chains (figure 3(b) and table 2). Interestingly, the magnetic coupling between two second near neighbours in the V and Mn chains is AF ($J_{02} < 0$), whilst it is FM ($J_{02} > 0$) in the Cr chains, i.e. the second near-neighbour magnetic coupling is opposite to the first near-neighbour magnetic coupling in all the nanowires considered here except for the atop-site Mn chain.

3.3. Magnetic anisotropy energy

Relativistic SOC is essential for orbital magnetization and magnetocrystalline anisotropy in solids, although it may be weak in 3d TM systems. Therefore, we perform further self-consistent calculations with SOC included in order to study the magnetic anisotropy and also orbital magnetization of the V, Cr and Mn nanowires on Cu(001), and the results are summarized in table 3. For comparison, the same results for the Fe, Co and Ni linear chains on Cu(001) reported recently [20] are also listed in table 3. First, when the SOC is taken into account, the spin magnetic moments for the V, Cr and Mn TM nanowires on the hollow (atop) site are 2.11 (3.30), 4.23 (4.60) and 4.14 (4.53) μ_B /magnetic atom, being almost identical to the corresponding one obtained without SOC. This is due to the weakness of the SOC in the 3d TMs. Nevertheless, including the SOC gives rise to orbital magnetic moments in the 3d TM nanowires and, importantly, allows us to determine the easy magnetization axis in the nanowires. If the magnetization lies along the chain direction (i.e. the x -axis) and the chain is on the hollow (atop) site, the calculated orbital moments for the V, Cr and Mn atoms are 0.01 (-0.06) μ_B /magnetic atom, -0.01 (0.01) μ_B /magnetic atom and 0.02 (0.02) μ_B /magnetic atom (see table 3), respectively, being small when compared with the Fe, Co and Ni chains. For comparison, we note that the corresponding orbital moments in the freestanding V, Cr and Mn nanowires are $-0.16 \mu_B$ /magnetic atom, $0.04 \mu_B$ /magnetic atom, $0.02 \mu_B$ /magnetic atom, respectively [7]. In [7], it

Table 3. Calculated spin magnetic moment per atom, m_s , orbital magnetic moment per magnetic atom, m_o , along three different directions and MAE per magnetic atom of V, Cr, Mn, Fe, Co and Ni chains on Cu(001). The chain direction is along (100), and the (010) [(001)] direction is in plane (out of plane) but perpendicular to the chain direction. The MAE E^1 is defined as $E^{100} - E^{001}$ and E^2 is $E^{100} - E^{010}$. The calculated MAE values are converged to within 0.01 meV per magnetic atom with respect to the k -points used.

	m_s (μ_B)	m_o (μ_B)			MAE (meV)	
		100	010	001	E^1	E^2
H-site						
V	2.11	0.01	0.01	0.01	0.00	0.00
Cr	4.23	-0.01	-0.01	-0.01	-0.01	0.01
Mn	4.14	0.02	0.02	0.03	-0.01	0.01
Fe ^a	3.07	0.10	0.09	0.10	0.32	0.25
Co ^a	1.78	0.27	0.18	0.17	-1.17	-1.16
Ni ^a	0.02	0.02	0.00	0.00	-0.53	0.01
A-site						
V	3.30	-0.06	0.18	-0.03	0.00	0.00
Cr	4.60	0.01	0.09	-0.01	-0.01	0.01
Mn	4.53	0.02	0.21	0.03	-0.01	0.01
Fe ^a	3.28	0.12	0.11	0.13	0.38	0.29
Co ^a	1.99	0.19	0.25	0.12	-0.40	-1.51
Ni ^a	0.64	0.13	0.27	0.11	-0.05	-0.32

^a Theoretical calculations ([20]).

was also found that the magnetization of the freestanding 3d TM nanowires has a strong directional dependence, and that the orbital moment is larger when the magnetization lies along the chain direction. Table 3 shows that the directional dependence of the orbital moment is weak in the on-hollow-site V, Cr and Mn chains but is rather significant when the V, Cr and Mn chains are on the atop sites.

The calculated MAEs of the V, Cr, Mn, Fe, Co and Ni nanowires are listed in table 3. The MAEs E^1 and E^2 are defined as the energy differences $E^1 = E^{100} - E^{001}$ and $E^2 = E^{100} - E^{010}$, where the E^{100} is the calculated total energy when the magnetization lies along the x direction. If both the E^1 and E^2 are negative, the magnetization prefers to lie along the chain (x -axis) direction. The MAEs of the V, Cr and Mn nanowires on both hollow and atop sites are quite small. In contrast, the MAEs E_1 of the freestanding V, Cr and Mn chains are -0.45 meV/magnetic atom, -0.07 meV/magnetic atom and 0.28 meV/magnetic atom, respectively, with $E^2 = 0$ [7]. In [20], it was found that the Fe chain on Cu(001) has an out-of-plane anisotropy while the Co and Ni chains on Cu(001) have an in-plane anisotropy (table 3). In contrast, here we find that the Cr and Mn chains on Cu(001) have an in-plane anisotropy, however, with the total energy changes due to the magnetization rotation from the x -, through y -, to z -axes being very small. Clearly, when the 3d TM chains are deposited on Cu(001), the MAEs generally become smaller due to the overlap of the wave functions between the TM nanowires and substrate (table 3). In particular, the MAEs of the V, Cr and Mn chains become very small when they are deposited on the Cu(001) substrate.

4. Conclusions

We have performed systematic *ab initio* GGA calculations for V, Cr and Mn linear atomic chains on a Cu(001) surface in order to examine how the substrate would affect the magnetic properties of the nanowires. We found that V, Cr and Mn linear chains on the Cu(001) surface still have a stable or metastable FM state. Nonetheless, we also found that the ferromagnetic state is unstable against the formation of a noncollinear spin-spiral structure in the Mn linear chains and also the V linear chain on the atop sites on the Cu(001) surface, due to the frustrated magnetic interactions in these systems. The presence of the Cu(001) substrate does destabilize the spin-spiral state already present in the freestanding V linear chain and stabilizes the ferromagnetic state in the V linear chain on the hollow sites on Cu(001). When spin-orbit coupling (SOC) is included for the collinear ferromagnetic state, the spin magnetic moments remain unchanged, due to the weakness of SOC in 3d TM chains. Furthermore, both orbital magnetic moments and MAEs (within 0.01 meV/magnetic atom) for V, Cr and Mn are small, in comparison with both the corresponding freestanding nanowires and also the Fe, Co and Ni linear chains on a Cu(001) surface.

Acknowledgments

The authors acknowledge support from the National Science Council and the NCTS of Taiwan as well as the computing time from the National Center for High-performance Computing of Taiwan.

References

- [1] Ohnishi H, Kondo Y and Takayanagi K 1998 *Nature* **395** 780
- [2] Yanson A I, Bollinger G R, van der Brom H E, Agrait N and van Ruitenbeek J M 1998 *Nature* **395** 783
- [3] Gambardella P, Blanc P, Burgi M, Kuhnke L and Kern K 2000 *Surf. Sci.* **449** 93
- [4] Gambardella P, Dallmeyer A, Maiti K, Malagoli M C, Eberhardt W, Kern K and Carbone C 2002 *Nature* **416** 301
- [5] Hammer L, Meier W, Schmidt A and Heinz K 2003 *Phys. Rev. B* **67** 125422
- [6] Mazzarello R and Tosatti E 2009 *Phys. Rev. B* **79** 134402
- [7] Tung J C and Guo G Y 2007 *Phys. Rev. B* **76** 094413
- [8] Tung J C and Guo G Y 2011 *Phys. Rev. B* **83** 144403
- [9] Saubanere M, Tanveer M, Ruiz-Diaz P and Pastor G M 2010 *Phys. Status Solidi b* **247** 2610
- [10] Hauschild J, Elmer H J and Gradmann U 1998 *Phys. Rev. B* **57** R677
- [11] Tian D, Jona F and Marcus P M 1992 *Phys. Rev. B* **45** 11216
- [12] Mokrousov Y, Bihlmayer G, Bluge S and Heinze S 2007 *Phys. Rev. B* **75** 104413
- [13] Wang Y and Perdew J P 1991 *Phys. Rev. B* **44** 13298
Perdew J P and Wang Y 1992 *Phys. Rev. B* **45** 13244
- [14] Blöchl P E 1994 *Phys. Rev. B* **50** 17953
Kresse G and Joubert D 1999 *Phys. Rev. B* **59** 1758
- [15] Kresse G and Hafner J 1993 *Phys. Rev. B* **48** 13115
- [16] Kresse G and Furthmüller J 1996 *Comput. Mater. Sci.* **6** 15
- [17] Herring C 1966 *Magnetism* ed G T Rado and H Suhl (New York: Academic)

- [18] Sandratskii L M 1991 *J. Phys.: Condens. Matter* **3** 8565
Sandratskii L M 1991 *J. Phys.: Condens. Matter* **3** 8587
- [19] Guo G Y, Temmerman W M and Ebert H 1991 *Physica B* **172** 61
- [20] Tung J C and Guo G Y 2011 *Comput. Phys. Commun.* **182** 84
- [21] Guo G Y and Wang H H 2000 *Phys. Rev. B* **62** 5136
- [22] Rosengaard N M and Johansson B 1997 *Phys. Rev. B* **55** 14975
- [23] Niu Q, Wang X, Kleinman L, Liu W-M, Nicholson D M C and Stocks G M 1999 *Phys. Rev. Lett.* **83** 207