Structure and magnetic properties of Co chains on a stepped Cu surface

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Abstract
Magnetic moments and the magnetic anisotropy energy (MAE) are calculated for Co chains on a stepped Cu(111) surface in a fully relaxed geometry. The Korringa–Kohn–Rostoker Green's function method is used to determine parameters of N-body interatomic potentials and to fit the semi-empirical tight-binding electronic Hamiltonian. The strain relief at steps and in the Co chains is demonstrated to have a profound effect on the morphology of the substrate. Atomic relaxations are shown to decrease the magnetic moments and the MAE. The MAE and orbital moments are found to exhibit an oscillatory behavior with increasing size of the chains.

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

1. Introduction

Since the pioneering work of Elmers *et al* [1] on Fe nanostripes on a W(110) surface, a large number of experimental and theoretical studies have been devoted to quasi-one-dimensional (1D) systems on different substrates [2–16]. A question of primary interest is related to the magnetic properties of low-dimensional systems. Such nanostructures are considered as possible candidates for future magnetoelectronic device use: magnetic properties of low-dimensional systems can be very much different from properties of bulk materials. For example, the orbital contribution to magnetism can be strongly enhanced at surfaces as was shown by Ticher *et al* for Co on Cu(001) [14]. According to their experimental and theoretical studies, the orbital moment of the first Co layer was twice larger than in the bulk. The enhanced

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spin magnetic moment in the surface layer and reduced spin magnetic moment in a subsurface layer of 2Co/Cu(001) have been obtained in *ab initio* calculations of Pentcheva *et al* [17]. Strong relaxation of the interlayer spacing has been shown to affect magnetic moments. Felix-Medina *et al* [15] performed tight-binding (TB) calculations which revealed remarkably large total magnetic moment of Co wires on Pd(110). They have shown that the orbital moment per Co atom in wires is almost three times larger than the Co bulk orbital moment. Dürr *et al* [18] reported on similar results for Co films on a stepped Cu(1 1 13) surface. TB calculations of Dorantes-Dávila and Pastor [5] have predicted that the MAE of 3d transition metal wires can be an order of magnitude larger than in two-dimensional thin films [5]. Experiments revealed extremely large MAE values for Co adatoms, nanoparticles and Co wires on Pt(111) [4, 19, 20]. On the other hand, the full-potential linearized augmented plane wave (FLAPW) calculations performed by Hong and Wu [8, 9] revealed no obvious MAE enhancement in Co chains in comparison to Co thin films. The MAE and orbital magnetic moments were found to exhibit an oscillatory behavior with increasing size of the chains. Magnetic moments of supported monatomic Co chains on Cu(001) and Pt(001) were found to align along the chain, contrary to the perpendicular alignment of the magnetic moment of the same free-standing chains. Calculations for spin and orbital moments of finite Co nanowires on Cu(001) performed by Klautau and Frota-Pessôa [21] by means of the linear muffin tin orbital atomic approximation (LMTO) method have predicted orbital moments of 0.7 μ_B for the Co sites at the end of a Co nanowire on Cu(001), and 0.3 μ_B per atom in the infinite Co wire on Cu(001). These values should be experimentally observable. Lazarovits *et al* [12, 13, 22] have studied magnetic properties of finite monatomic Fe chains on Cu(001) and Cu(111) by means of Korringa–Kohn–Rostoker (KKR) Green's function method. They have found that spin and orbital moments in the chains are larger than those in the monolayer. A strong out-of-plane easy axis of magnetization was found for chains on Cu(001) and Cu(111).

Stepped surfaces bring an additional magnetic anisotropy within the surface plane since the direction parallel and perpendicular to the step edge are no longer equivalent [23]. Dhesi *et al* [24] have found by means of x-ray magnetic linear dichroism measurements that the spin–orbit coupling parallel to the step is larger than that perpendicular to the step. Weber *et al* [25] have reported on the adatom-induced reorientation of spins in Co on a stepped Cu surface from the direction parallel to steps to the perpendicular one. Hahlin *et al* [26] have performed x-ray magnetic circular dichroism (XMCD) and x-ray reflectivity measurements on Co deposited on vicinal and flat Cu(111). They have revealed that the orbital moment and the spin moment for the vicinal surface are enhanced by 25% for the thickness range 1–25 monolayers as compared to those found for Co on the flat surface. The first-principles investigation of Shick *et al* [27] of the anomalous ferromagnetism of a quasi-one-dimensional Co chains at the Pt(111) step edge has shown that the symmetry breaking at the step leads to an easy magnetization axis at an odd angle of about 20° towards the Pt step.

Still little attention has been paid so far to the effect of strain relaxations at steps on structure and magnetic properties of chains. There have been only a few investigations, to our knowledge, which have addressed this problem for infinite chains. *Ab initio* calculations of Máca *et al* [28] have indicated that the effect of structural relaxations on magnetic properties of infinite Co wires on a stepped Pt surface could be important to correctly describe the MAE on stepped surfaces [28]. Spišák and Hafner [10, 11] have found by use of a PAW package that the equilibrium bond length of a free-standing straight wire is smaller by 12% than the corresponding bond length of a wire on a Cu substrate. These results indicate that wires on a surface are under a strong tensile stress. The aim of our work is to study the strain relaxations in finite atomic chains at stepped surfaces and their effect on magnetic properties. Performing *ab initio* and TB calculations, we concentrate on Co chains on a stepped Cu(111) surface.

2. Computational methods

Ab initio calculations for ideal Co chains on a stepped Cu(111) surface are performed by KKR and Screened KKR Green's function method (SKKR) [29, 30] in the framework of the density functional theory (DFT) in the local spin density approximation (LSDA). Up to several hundreds of inequivalent atoms can be involved in self-consistent calculations. The concept of a vicinal surface is applied to simulate a superlattice of regularly separated steps of monatomic height [31, 32]. A stepped surface is treated as a two-dimensional perturbation of the infinite bulk. The Dyson equation for stepped surfaces is solved in $k_{\parallel}$ representation, where $k_{\parallel}$ belongs to 2D Brillouin zone. Finite chains adsorbed at the step edges destroy the 2D periodicity. Therefore, we calculate electronic and magnetic properties of chains in a real-space representation. In this case, the Green's function of a stepped surface (we have chosen Cu(554) surface) calculated by means of the SKKR method is used in the Dyson equation as the reference Green's function. Details of our approach can be found elsewhere [29–31].

The relaxed atomic geometries have been obtained by means of *ab initio* fitted many-body potentials formulated in the second moment approximation of the TB theory [33–35]. The KKR Green's function method [29, 30] is used to create an *ab initio* data pool to fit the parameters of the potentials. Surface (binding energies of supported Co clusters of different sizes, the Hellmann–Feynman forces acting on the Co adatom for different positions above the surface) and bulk properties (bulk modulus, lattice constants, cohesive energies, and elastic constants) are included in the data pool. The reliability of such potentials for different atomic configurations has been demonstrated [36–42]. Recent studies [43] have shown that our method describes atomic relaxations in nanostructures in very good agreement with fully *ab initio* calculations. Note, a full optimization of the structure of chains, steps and the substrate by *ab initio* methods is still beyond the accessible computation time. For technical details we refer to our former studies [35].

In order to avoid tedious first-principles electronic structure calculations for *relaxed* atomic geometries and to include spin–orbit coupling we apply the TB method for relaxed chains. To make the extensive calculations feasible, only the changes introduced by the geometry relaxation of the Co atoms and their nearest neighbors are taken into account. It has been demonstrated in our previous studies [38, 44] that moderate perturbation of more distant Cu atom can be safely neglected. The parameters of a semi-empirical TB Hamiltonian are fitted to reproduce closely the *ab initio* KKR results for ideal chains at the step (atomically resolved local density of states (LDOS) and magnetic moments). TB calculations are performed self-consistently with commonly used conditions: the local charge neutrality and linear dependence of the exchange splitting on the spin magnetic moment [45]. The local densities of states (LDOS) and electronic properties of interest are calculated with the help of the recursion method technique (continued fraction with large number of levels) [46, 47]. Actually, the method is essentially the same as in our previous investigations [38, 44]. In order to avoid too sharp peaks near E_F we have changed the small $dd\delta$ parameter of Co [48] to fulfill the canonical prescription [49] $dd\sigma{:}dd\delta = 6{:}1$. This minor change in the parameterization seems to have no effect on the results.

3. Results and discussion

Relaxation of short Co chains placed at the Cu(111) vicinal surface step edge would differ significantly from the case of the flat Cu(111) substrate due to interactions of Co atoms with the Cu atoms of the step. We calculated relaxations of short Co_2–Co_7 chains at the step edge

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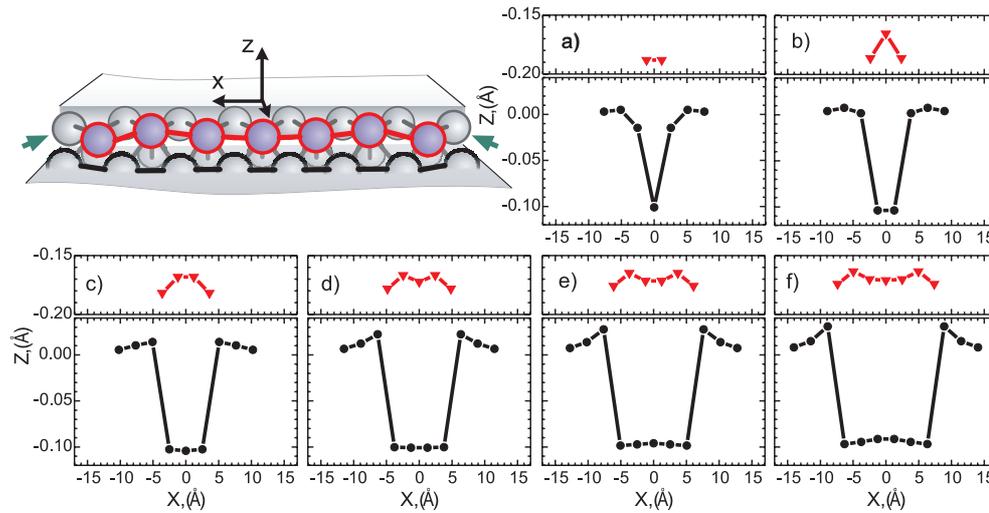
Figure 1. Strain relaxations in short Co chains placed at the Cu(111) vicinal surface step edge. The upper panels of all the figures demonstrate displacements of Co atoms in (a) Co_2, (b) Co_3, (c) Co_4, (d) Co_5, (e) Co_6, (f) Co_7 chains. The corresponding relaxation profiles of underlying substrate atoms are shown in lower panes. Coordinate origins coincide with the geometrical centers of corresponding unrelaxed structures.

of Cu(554) vicinal surface. The coordinate frame used is drawn in the inset of figure 1. The x-axis is parallel to the step, the z-axis direction matches the surface terrace normal and the y axis points from the step. Projections of relaxed atomic positions of the Co chains and underlying substrate atoms on xz plane are plotted respectively in upper and lower panels of figures 1(a)–(f). Vertical displacements of Co atoms strongly depend on the chain length. To rationalize such a difference and to find common features in Co chain relaxations, we should stress that the edge atoms of Co chains due to lower coordination number, exhibit the strongest relaxations towards the substrate, towards the step and towards the adjacent Co atom. The positions of Cu atoms in the step remain practically the same except when at the chain edges (they are marked with green arrows in the inset of figure 1). These atoms move out from the step to the terrace. The picture described above remains valid for all the considered Co chains (see upper panels of figures 1(a)–(f)). Such a displacement of the edge Co atoms hinders the relaxation of the second atom in the chain towards the substrate. As a result, the second Co atoms are situated remarkably higher than the edge ones. This 'edge effect' completely explains the arched relaxations profiles of Co_3 and Co_4 chains. The longer Co_5, Co_6 and Co_7 chains have the 'letter M-like' shape when three outermost Co atoms form two arches at each edge of the chain and the remaining Co atoms in the center exhibit similar relaxations forming steady central region. The description of the atomic relaxations in the Co chains can be summarized in the 3D illustration as it is plotted in figure 2 for the Co_7 chain. All the considered Co chains push underlying substrate atoms downwards, but the outer substrate atoms exhibit upward vertical relaxations due to the shift of the edge Co atoms towards the chain center. The relative changes of Co–Co and Co–Cu bonds in Co_7 chain caused by relaxation are listed in table 1. The Co atoms' enumeration is explained in figure 3. Because of the reflection symmetry $x \to -x$ only the first four Co atoms are considered in table 1. The zoomed view in figure 3 clarifies the bond notation. To illustrate the effect of relaxations on the electronic structure of the Co_7 chain we also put in table 1 values of spin magnetic moments for ideal and relaxed configurations. In both cases
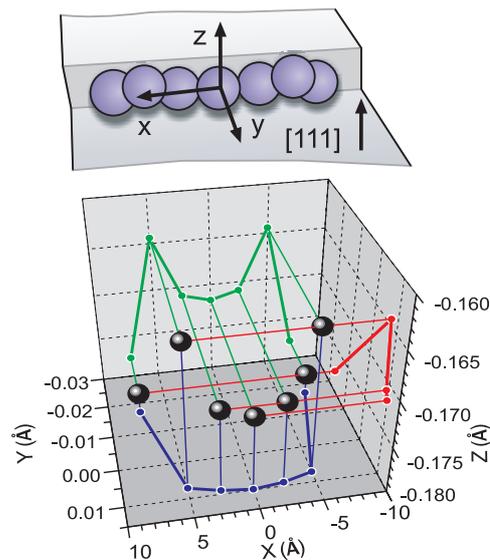
Figure 2. The three-dimensional relaxation profile in the Co_7 chain. Edge atoms are strongly attracted to the step due to the lower coordination number. The second atoms from the edge are shifted from the step. Atoms in the middle of the chain lie approximately in a straight line.

Table 1. Effect of atomic relaxations on structural and magnetic properties of the Co_7 chain. Values of Co–Co and Co–Cu bonds length changes are listed in per cents relative to the unrelaxed bond length. Order of the Co atoms and bonds notation are illustrated in figure 3.

	Co atom			
Bonds	1	2	3	4
1	—	−6.2	−3.2	−2.3
2	−6.2	−3.2	−2.3	−2.3
3	0.3	0.6	−0.8	−1.5
4	−5.2	−2.6	−2.0	−1.5
5	−0.8	−0.4	−1.9	−2.6
6	−6.1	−3.8	−3.2	−2.6
7	−3.5	−3.3	−3.3	−3.3
	Magnetic moments (μ_B)			
Ideal	1.71	1.68	1.64	1.66
Relaxed	1.59	1.52	1.53	1.50

edge Co atoms have the maximum magnetic moment in the chain. Atomic relaxations reduce magnetic moments of all the atoms.

Some general discussion on the symmetries in the considered systems is required. The presence of the reflection symmetry $x \rightarrow -x$ fixes the x-direction (parallel to the chain) for the magnetic anisotropy and therefore the corresponding orbital and spin moments are parallel. But it is still necessary to perform a complete analysis of the magnetic anisotropy in yz plane. Strictly speaking, the magnetic spin[5] and the orbital moments need not to be

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[5] We identify the spin moment by the direction **n** included in the part of the TB Hamiltonian $0.5\Delta(\mathbf{n}\sigma)$ introducing the exchange splitting Δ.
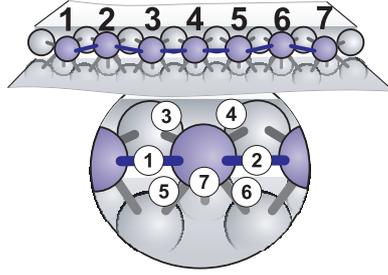
Figure 3. Sketch of the Cu(111) vicinal surface step with the Co_7 chain. Substrate Cu atoms are drawn with grey colour; the Co chain is light blue. The top view illustrates the Co atoms' enumeration order used in table 1. The bottom zoomed view is designed to clarify the bond notation used in table 1.

mutually parallel [50], so we vary the orientation of the spin moment in the yz plane and for each spin moment orientation we calculate the orbital moment projections onto y and z axes. The obtained orbital moments and anisotropy energies are fitted by the formula

$$A + B \cos(2(\phi - \phi_0)), \tag{1}$$

where ϕ is the angle between the spin moment in the yz plane and the (111) normal. It is positive (negative) for a magnetic moment tilted above the upper (lower) terrace. The coefficients A, B and ϕ_0 are found by the usual Fourier-series technique.

The common property of all studied cases is that the energetically preferred easy axis of the magnetization is found to be parallel to the x-axis of the coordinate frame drawn in figure 2, similar to the *ab initio* results of Hong and Wu [8, 9]. To illustrate the physics behind this, let us consider an infinite free-standing Co chain oriented along the z-axis. The minority-spin electrons form a wide σ-band ($3z^2 - r^2$ orbitals), doubly degenerate π-band (xz, yz) and a narrow doubly degenerate δ-band (xy, $x^2 - y^2$) [51–53]. Analogous features in the local density of states at the third Co atom in the Co_7 chain are drawn in figure 4(a). E_F falls well inside a high-density peak in LDOS stemming from the δ-orbitals with the magnetic orbital numbers $m = \pm 2$ and therefore an effective spin–orbit coupling is possible. LDOSs calculated with spin–orbit coupling are drawn in figure 4(b). The effect of spin–orbit coupling on the δ-band is obvious.

Before proceeding to the discussion on the hard axis orientation, let us clarify the following point. The hard axis lying in the xy plane and providing most of the energy for the whole system is determined by the Fourier fit of the MAE of the whole system. The angles found by an analogous fit of *local* MAE contributions from particular atoms need not coincide with the system hard axis direction. It is also true for extrema of angular moments on particular atoms [50]. This misorientation varies in a range from negligibly small values up to several degrees. Larger differences are possible due to numerical errors in fitting if the B parameter in equation (1) is very small. The orientations of the hard axis in the yz plane both for ideal and relaxed Co_2–Co_7 chains are demonstrated in figure 5. Relaxation has no significant effect on Co_2 dimer. In both cases the angle between the hard axis and (111) normal is approximately $40°$. Calculations performed for Co dimer on Cu(111) revealed an in-plane hard axis. A similar result was obtained by Lazarovits *et al* [54] for Co on Ag(001). The difference between the orientations of the hard axis of the Co dimer adsorbed at the step and on the flat surface is definitely the effect of the step Cu atoms. The effect of relaxation becomes very significant for the Co trimer. The hard axis orientation of the unrelaxed trimer is almost in-plane, but strong relaxation disturbs linear shape of the trimer (see figure 1) and makes hard axis to be almost
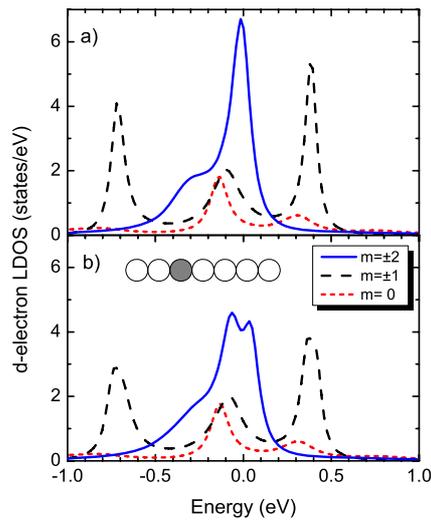
Figure 4. The effect of spin–orbit coupling on the d-electron LDOS at the third Co atom in the Co_7 chain adsorbed at the step. (a) Spin–orbit coupling is neglected, (b) it is taken into account. The Fermi level coincides with the energy zero. Solid, long-dashed and short-dashed) curves correspond to the orbital moment eigenvalues $m = \pm 2, \pm 1, 0$ with the quantization axis parallel to the x-axis of the coordinate frame drawn in figure 2.
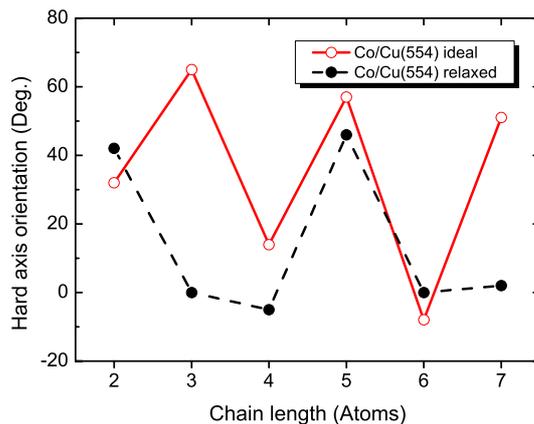
Figure 5. Orientation of the hard axis in the yz plane for Co_2–Co_7 chains. Empty (full) circles correspond to ideal (relaxed) chains at the step. See the text for details.

parallel to the (111) normal. We check the direction of the hard axis of the Co trimer on the flat Cu(111) surface and found that it also points out-of-plane. The same result was obtained for Co trimer on Ag(001) [54]. The hard axis orientation of the Co_4, Co_5, Co_6 are very similar for relaxed and ideal atomic positions but for the Co_7 chain its orientation changes. Such a large difference between the relaxed and ideal Co_7 can be explained by the very low anisotropy in the yz plane for the relaxed chain.

Now we focus on the distribution of the magnetic properties along the chain and their averages. The total spin magnetic moments in the Co_7 chain calculated by means of KKR Green's function can be found in table 1. The exhaustive information on MAE and orbital

Table 2. MAE and magnetic orbital moments L^m calculated for the ideal Co_7 chain for the magnetization orientations along the easy, hard, and intermediate axis, respectively. Zero energy is chosen for magnetization orientation parallel to the surface (111) normal. Negative energy means that corresponding magnetization orientation is more energetically preferable. Easy magnetization axis (corresponding to the ground state) is oriented along the chain. Order of the Co atoms is illustrated in figure 3. Average values ⟨·⟩ per atom in the chain are also shown.

|		Co atom				
	Magn. orient.	1	2	3	4	⟨·⟩
MAE	Along the chain	−3.59	−3.72	−4.88	−2.89	−3.90
(meV)	$\phi = 51°$	0.14	0.11	0.31	0.06	0.17
	$\phi = -39°$	−0.11	−0.10	−0.13	−0.07	−0.11
L^m	Along the chain	0.55	0.47	0.63	0.42	0.53
(μ_B)	$\phi = 51°$	0.28	0.22	0.19	0.27	0.23
	$\phi = -39°$	0.29	0.24	0.22	0.27	0.25

Table 3. MAE and magnetic orbital moments L^m calculated for the relaxed Co_7 chain. For details see description of table 2.

		Co atom				
	Magn. orient.	1	2	3	4	⟨·⟩
MAE	Along the chain	−3.23	−3.80	−5.05	−2.54	−3.81
(meV)	$\phi = 2°$	0.00	0.00	0.00	0.00	0.00
	$\phi = -88°$	0.05	0.02	−0.17	−0.41	−0.09
L^m	Along the chain	0.48	0.40	0.59	0.39	0.47
(μ_B)	$\phi = 2°$	0.25	0.18	0.24	0.19	0.22
	$\phi = -88°$	0.25	0.18	0.25	0.24	0.23

moments for the same chain in ideal and relaxed configurations is listed in tables 2 and 3 respectively. The MAE and the orbital moments of the relaxed Co_7 chain drop in comparison to the ideal system. We expect that the properties of chains will converge with damped oscillations as the chain length increases. Actually, we did some tests that allow us to compare *unrelaxed* infinite and Co_7 chains on the ideal or stepped Cu(111) surface, respectively. The corresponding differences of the MAE, orbital moment or the hard axis orientation do not exceed several per cents. Orientation of hard axes is shown in figure 5. Stabilizations of the intermediate magnetization axis and easy axis with respect to the hard axis are demonstrated in figure 6. For ideal chains the tendency towards stabilization is visible starting from Co_4. The same trend is obtained for magnetic orbital moments (see figure 7). For relaxed chains a similar comparison is problematic since there is no effective way of Co–Co distance relaxation for very long but finite chains. For example, for the Co_7 chain, the Co–Co bond length at the central part of the chain is relaxed only by 2%. Naturally, broken-symmetry geometries should be checked for very long chains [51].

For short chains, there are marked oscillations of chain properties in dependence of their length. Such an oscillatory behavior, which has pronouncedly odd–even atomic length character (see figures 5–7), can be understood on intuitive grounds. Let us consider transformation of eigenstate orbital part (i.e. transformation of the spinor is not taken into account) with respect to the symmetry-plane reflection. For antisymmetric states and chains with odd number of atoms, the amplitude of the above two important δ-orbitals (xy, x^2-y^2) is zero on the central atom which has no analogy for even-atom chains.
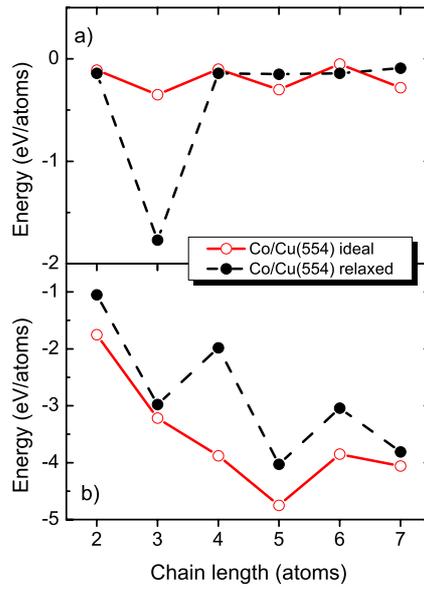
Figure 6. Stabilization of the intermediate magnetization axis (a) and easy axis (b) with respect to the hard axis (energy zero) demonstrated by the electronic part of the average magnetic anisotropy energy in the chain. Both in (a) and (b) panels empty (full) circles correspond to ideal (relaxed) chains at the step.
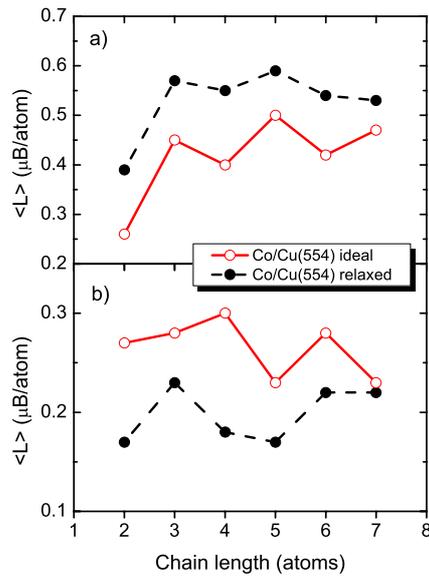
Figure 7. Projections of the magnetic orbital moment L^m on the easy axis (a) and on the hard axis (b) determined by the Fourier fit of the whole chain according equation (1). Both in (a) and (b) panels empty (full) circles correspond to ideal (relaxed) chains at the step.

Finally, the changes of MAE and L^m caused by a switch of magnetization direction can be connected by the approximate relation [55] involving the intra-atomic spin–orbit coupling

parameter ξ:

$$\Delta E \approx -0.25\xi\Delta L^m. \tag{2}$$

We use $\xi = 0.06$ eV as in our previous studies [44]. As a rule, no serious deviations from equation (2) have been found. Equation (2) permits to qualitatively estimate the changes of the MAE.

4. Conclusions

We have demonstrated that the strain relief in the Co chains at a stepped Cu surface significantly affects the atomic structure of the chains and the morphology of the substrate. We have performed extensive calculations of the MAE for ideal and relaxed short Co chains. The easy axis is found to be aligned along the chains and the MAE is determined to be several meV per atom. The magnetic properties of chains exhibit oscillations with increasing chain length. Atomic relaxations are found to affect significantly the direction of the easy axis. We demonstrate also that relaxations reduce the MAE and magnetic moments of Co chains.

Acknowledgments

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