Structural relaxation effects in nanomagnetism

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In viewing layer-resolved components of physical properties as a function of multiples of the interlayer spacing and by using a Taylor expansion structural relaxation effects can be described not only for the free-energy part of the magnetic anisotropy energy but directly also for electric and magneto-optical transport properties. Examples for such a procedure are shown for the anisotropy energy of free surfaces and magnetic tunneling junctions, for tunneling currents and for permittivities, which in turn determine Kerr angles. Considered as a test case, the already well-studied magnetic anisotropy energy of $Co_2/Cu(111)$ turns out to be in excellent agreement with very recent experiment data.

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I. INTRODUCTION

In nanoscience, in particular, in nanomagnetism, "relaxation effects" are apodictically said to be important. Unfortunately, before confirming or refuting such a statement, it needs a proper definition of what actually is meant by the term "relaxation effects." Assuming three-dimensional cyclic boundary conditions, i.e., the "bulk" case, which is rather uninteresting in the context of nanomagnetism, relaxation effects are easy to deal with, since only scaling of the lattice constant(s) is required. The ground state of a bulk system is then defined by the minimum of the total energy with respect to the lattice spacing. There are quite a few density-functional-theory (DFT) approaches specialized to find this minimum very accurately. Whether or not to be in the neighborhood of the theoretically found equilibrium spacing is important for particular physical properties has then to be found out in separate investigations.

Is only two-dimensional translational symmetry present such as in layered systems then by the term "relaxation effects" usually only changes in the interlayer distances are meant. The reason for this restriction is quite clear: if translational symmetry is used for computational reasons (Brillouin zone integrals or sums) then one and the same translational group has to apply for all layers in such a system.[1] There is no way to keep the condition of a single translation group common to all layers and concomitantly relax individual in-plane lattice constants. Of course the seemingly easiest way out in order to relax also in-plane spacings would be to abandon translational symmetry completely and move into real space. Unfortunately then essential parts of a nanosystem, namely, substrates and/or leads no longer can be treated properly: the total energy is a function of (arbitrarily) chosen outer boundaries.

Since the total energy is not an observable the question arises whether there are ways by which relaxation effects for particular physical properties can at least be estimated directly, in particular, since for many systems of technological interest proper total energy calculations as a function of all relevant interlayer spacings are simply prohibitive or become meaningless. Imagine a typical spin valve or tunneling junction. It is virtually impossible to vary all interlayer distances in such system in order to find the minimum in the total energy. Assume for matters of illustration an average contribution per atomic layer to the total energy on the order of 10^4 Ry. For (typically) a hundred relevant layers in a tunneling junction the total energy then amounts to 10^6 Ry implying that even the third decimal place will be rather shaky, i.e., the accuracy will be confined at best to a few millirydberg.

Furthermore, it seems to be rather unclear when in the course of evaluating total energy differences as is necessary, for example, to compute free energies that relaxation plays an important role. Also open remains the question of the sensitivity of electric or (magneto-) optical transport properties with respect to relaxation effects. Can they be estimated for realistically large systems? Clearly, electric or optical properties are of primary interest in spintronics, since they are actually measured, and not total energies; since they are at the very heart of any switching device.

In the present paper an attempt is made to address the above problems by making use of two-dimensional translational symmetry by which so-called layer-projected (or layer-resolved) properties can be defined. This approach is then applied to discuss possible relaxation effects for the free-energy (band-energy) contribution to the anisotropy energy and then to electric and magneto-optical properties. As a final example the switching mechanism in an almost technological system is considered.

II. TRANSLATIONAL INVARIANCE AND MAGNETIC CONFIGURATIONS

As follows directly from the condition of translational invariance for the Dirac equation[1] magnetic configurations of layered system (two-dimensional translational symmetry) corresponding to a simple parent lattice can be defined unambiguously by assigning to each atomic layer a particular orientation of the magnetization.[2,3] For a free surface, spin valve or tunneling junction such a magnetic configuration is of the following form:

$$\mathcal{C}_\alpha = \{\vec{n}_l;\vec{n}_1,\vec{n}_2,\ldots,\vec{n}_N;\vec{n}_r\}, \quad (1)$$

$$\mathcal{C}_0 = \{\vec{z}_l; \vec{z}_k; \vec{z}_r = \vec{z}, \forall\, k\}, \tag{2}$$

where $\vec{n}_l$ is the uniform orientation of the "left" semi-infinite system (substrate, lead), $\vec{n}_r$ that of the "right" semi-infinite system (vacuum, lead), and $\vec{n}_k$ refer to the orientations of the magnetization in all (remaining) layers between the two semi-infinite systems. These layers consist of magnetic overlayers (free surface), a spacer (spin valve, tunneling junction), or magnetic overlayers plus vacuum and a tip in the case of spin-polarized scanning tunneling microscopy (STM), see Table I.[4,5] Clearly in Eq. (1) N has to comprise also a sufficiently large number of atomic layers of the material of the left and the right semi-infinite systems to be determined self-consistently in order to guarantee a smooth transition to the respective bulk properties, i.e., to take care of occurring Friedel oscillations.[7] All data referenced and used in here were originally obtained by means of the fully relativistic screened Korringa-Kohn-Rostoker method[3] with a minimum of 12 atomic layers in the transitional regime to the substrate or leads.

III. STRUCTURAL RELAXATION EFFECTS FOR THE FREE ENERGY AT 0 K

In order to evaluate energy differences between magnetic configurations it is useful to define a reference configuration such as for example $\mathcal{C}_0$ in Eq. (2), in which the orientation of the magnetization points uniformly along $\vec{z}$ (surface normal). The free energy at 0 K, the so-called band-energy contribution to a particular anisotropy energy, is then defined as[3]

$$\Delta E(\mathcal{C}_\alpha) = E(\mathcal{C}_\alpha) - E(\mathcal{C}_0), \tag{3}$$

where the $E(\mathcal{C}_\alpha)$ refer to sums over layer-wise contributions $E^k(\mathcal{C}_\alpha)$

$$\Delta E(\mathcal{C}_\alpha) = \sum_{k=1,N} [E^k(\mathcal{C}_\alpha) - E^k(\mathcal{C}_0)], \tag{4}$$

which in turn are given by

$$E^k(\mathcal{C}_\alpha) = \int_{E_b}^{E_F} n^k(\mathcal{C}_\alpha; \epsilon)(\epsilon - E_F) d\epsilon. \tag{5}$$

In Eq. (5) E_b is the (valence) band bottom, E_F the Fermi energy, and $n^k(\mathcal{C}_\alpha; \epsilon)$ refers to the density of states of the kth atomic layer and configuration $\mathcal{C}_\alpha$. If in Eq. (1)

$$\mathcal{C}_\alpha = \{\vec{n}_l; \vec{n}_k; \vec{n}_r = \vec{x}, \forall\, k\} \tag{6}$$

then $\Delta E(\mathcal{C}_\alpha)$ is the free-energy or band-energy contribution to the anisotropy energy in the "usual sense:" the transition from a uniform perpendicular to a uniform in-plane orientation of the magnetization is usually called "reorientation transition."

Consider now a Taylor-series expansion

$$f(u) = \sum_{n=0,P} \frac{f^{(n)}(u_0)}{n!}(u - u_0)^n, \quad f^{(n)} = \frac{d^{(n)}}{du^n} \tag{7}$$

for the layer-resolved band energies, see Eq. (5), reformulated in Eq. (8) for matters of clarity such that the layer index can be associated with multiples of the interlayer distance $d_\perp$ of the parent lattice used

$$f{:}\{x_k = kd_\perp\} \rightarrow \{\Delta E^k(\mathcal{C}_\alpha)\} \equiv \{\Delta E^k(\mathcal{C}_\alpha; x_k)\}. \tag{8}$$

In defining a set U of displacement vectors $\vec{u}_k = (0,0,u_k)$, $u_k = x'_k - x_k$, in direction of the surface normal (layer relaxation), it is easy to see that layer-resolved band energies shifted along the surface normal can be written as

$$\Delta E^k(\mathcal{C}_\alpha; x'_k) = \Delta E^k(\mathcal{C}_\alpha; x_k) + \alpha_k u_k + \beta_k u_k^2 + \gamma_k u_k^3 + \cdots, \quad k = 1,N. \tag{9}$$

In Eq. (9) the coefficients α_k, β_k,... denote in turn the first, second, and so on derivative in Eq. (7). In defining U_0 for a moment as

$$U_0 = \{\vec{u}_k | \vec{u}_k = (0,0,0), \forall\, k \leq N\} \tag{10}$$

then the band energy that belongs to the original spacing of layers is given by

$$\Delta E(\mathcal{C}_\alpha, U_0) = \sum_{k=1,N} \Delta E^k(\mathcal{C}_\alpha, x_k) \tag{11}$$

and that corresponding to the system with the displaced layers by

$$\Delta E(\mathcal{C}_\alpha, U) = \sum_{k=1,N} \Delta E^k(\mathcal{C}_\alpha, x'_k). \tag{12}$$

Clearly, the set U can consist of an arbitrary number $M \leq N$ of nonvanishing displacements. Note that since the u_k are the z components of vectors in coordinate space and not in function space, $\vec{u}_k = (0,0,u_k)$, a particular vector $\vec{u}_k/|\vec{u}_k| < 0$ moves the kth atomic layer in direction of the surface normal, while for $\vec{u}_k/|\vec{u}_k| \geq 0$ this layer is moved antiparallel with respect to the surface normal. If a uniform relaxation is performed, then per definition there are no changes in the free energy, i.e.,

$$\Delta E(\mathcal{C}_\alpha, U) = \Delta E(\mathcal{C}_\alpha, U_0), \quad U = \{\vec{u}_k | \vec{u}_k = (0,0,u), \forall\, k\}. \tag{13}$$

Furthermore, if $u_k = d_\perp, \forall\, k$, then a simple reindexing of atomic layers takes place, i.e.,

$$\mathcal{C}_\alpha = \{\vec{n}_l; \vec{n}_2, \vec{n}_3, \ldots, \vec{n}_{N+1}; \vec{n}_r\} \equiv \mathcal{C}_0$$

since, as follows immediately from the definitions of $\vec{n}_l$ and $\vec{n}_r$, the origin of counting is irrelevant. Clearly, Eq. (13) offers a unique condition for the numerical procedures that have to be performed. It should be noted that the manifold $\{\Delta E(\mathcal{C}_\alpha, U)\}$ forms a hypersurface in the space of all possible relaxations that can occur. For a given U in switching on a current or an external magnetic field the path of minimal changes on this surface is taken. It is therefore in many cases, e.g., when trying to compare theoretical results with experimental data, more important to explore the dependence of this path on U than to know structural details of the ground state. In the following for all data shown a fifth order Taylor expansion, see Eq. (7), was used. In all figures the term "relaxation (%)" means $(d_\perp + u)/d_\perp$ expressed in per-

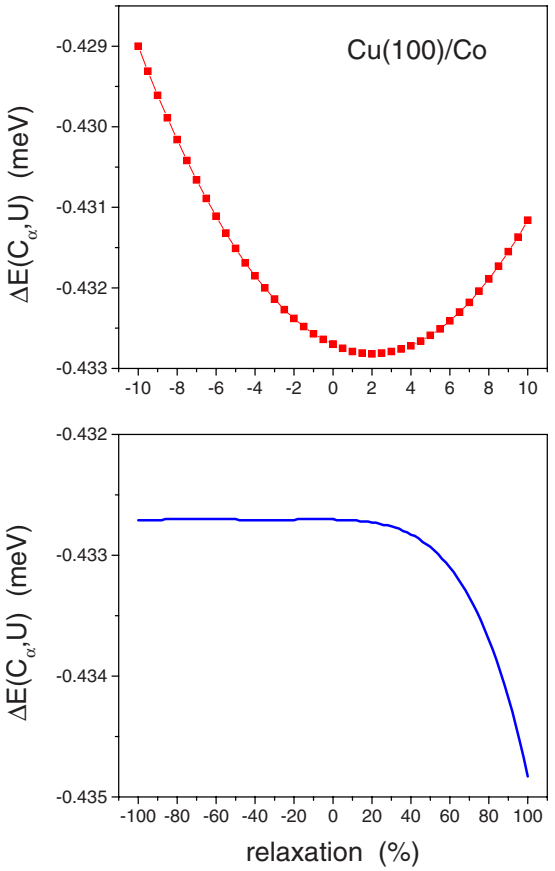

FIG. 1. (Color online) $\Delta E(\mathcal{C}_\alpha, U)$ for Cu(100)/Co. Top: only the Co layer is relaxed and bottom: uniform relaxation in all atomic layers with respect to the interlayer distance in fcc Cu(100). $\mathcal{C}_o$ refers to Eq. (2) and $\mathcal{C}_\alpha$ to Eq. (6). The unrelaxed results are from Ref. 7.

cent, where $d_\perp$ is the unperturbed interlayer distance of the semi-infinite system.

A. Free surfaces

In the top part of Fig. 1 the band energy as a function of the relaxation (contraction) of the top (Co) layer is displayed for a free surface of a single Co overlayer on Cu(100). Relaxing also adjacent Cu or vacuum layers has no further effect.[6] The bottom entry of this figure looks at the first glance a bit boring. However, it is not. In this part of the figure the accuracy of the numerical procedure in Eq. (9) is checked by relaxing uniformly between −100% and 100%. As can be seen between about ±30% the numerical scheme seems to be most reliable. It should be noted that ±30% for a relaxation is rather very big: the interlayer spacing in fcc Pt, for example, is only by about 8% larger than the one in fcc Cu.

In Fig. 2 relaxation effects for a single layer of Co on Pt(111) (Ref. 7) are displayed. Two cases are shown in this figure, namely, when only the Co layer is relaxed and also when the Co layer and the adjacent vacuum layer are moved. Other combinations of layer relaxations fall on top on these two cases. While a variation in the spacing of the Co layer

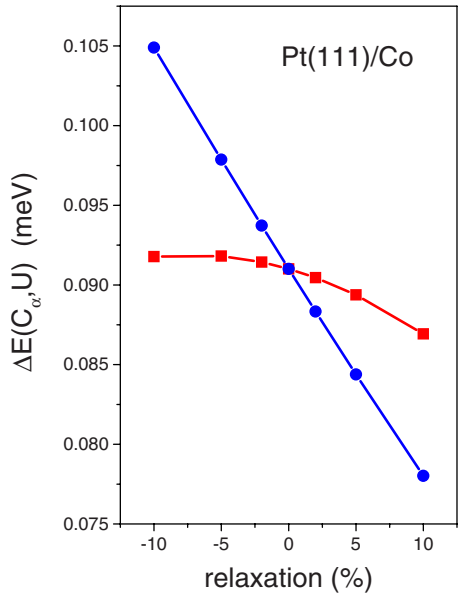

FIG. 2. (Color online) $\Delta E(\mathcal{C}_\alpha, U)$ for Pt(111)/Co when only the Co layer (squares) and when the Co and the adjacent vacuum layer (circles) are relaxed with respect to the interlayer distance in fcc Pt(111). $\mathcal{C}_0$ refers to Eq. (2) and $\mathcal{C}_\alpha$ to Eq. (6). The unrelaxed results are from Ref. 7.

with respect to that in Pt(111) is rather small, when also the vacuum layer is moved distinctive changes occur. However, in this case one has to keep in mind that the band energy is rather small and an increase or decrease in the interlayer spacing by about 10% only amounts to a change in $\Delta E(\mathcal{C}_\alpha, U)$ of 0.02–0.03 meV.

B. Tunneling junctions

In Fig. 3 effects of interlayer relaxation for two Co layers on top of Cu(111) are shown in systems that recently served to interpret[4,5] spin-polarized STM measurements considering different kinds of tips. It is worthwhile to mention that in the experimental study[9] a value of 0.150 meV for the anisotropy energy is reported for extended Co_2 islands on Cu(111), which agrees very well indeed, in particular, with the values in the fourth row of Table II, namely, for the system with a reasonable thick tip. Whether or not one can conclude from the experimental value and the entries in this row that a contraction of about 2% applies is questionable. It seems that relaxation effects for the anisotropy energy of extended Co_2 islands on Cu(111) are of minor importance.

TABLE I. Systems investigated: systems 1 and 2 correspond to free surfaces and systems 3–5 to tunneling junctions.

	System	Ref.
1	$Cu(100)/Co/Vac_6$	7
2	$Pt(111)/Co/Vac_6$	7
3	$Cu(111)/Co_2Vac_3Cr_3W_7/Cu\text{-lead}$	4
4	$Cu(111)/Co_2Vac_3Cr_{15}W_{22}/Cu\text{-lead}$	4
5	$Cu(111)/Co_2Vac_3Fe_2W_7/Cu\text{-lead}$	5

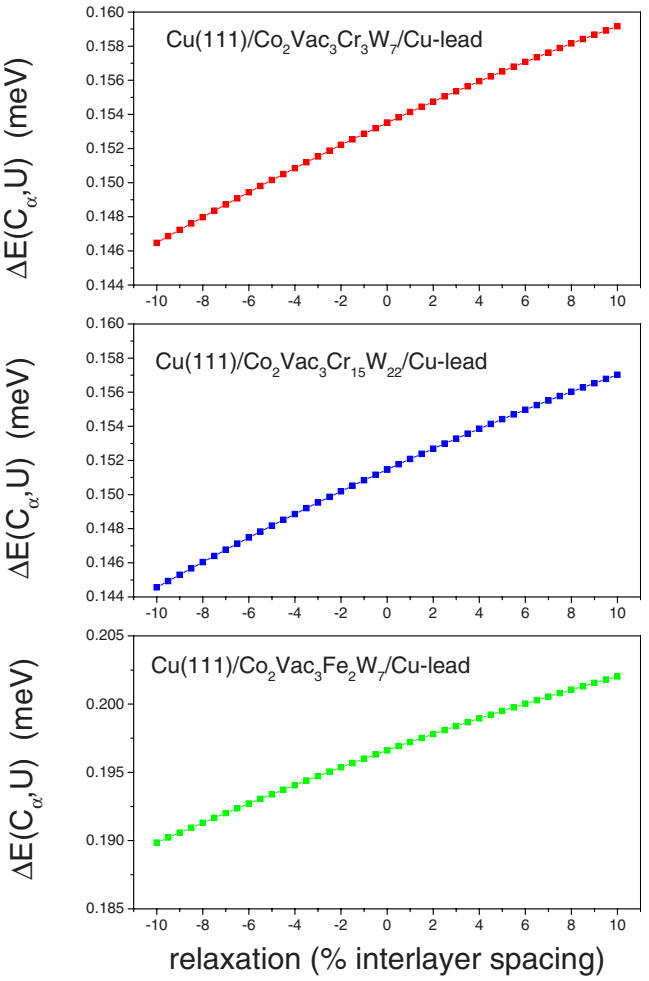

FIG. 3. (Color online) $\Delta E(\mathcal{C}_\alpha, U)$ in $Cu(111)/Co_2Vac_3Cr_3W_7/Cu$-lead (top) (Ref. 4), $Cu(111)/Co_2Vac_3Cr_{15}W_{22}/Cu$ lead (middle) (Ref. 4), and $Cu(111)/Fe_2Vac_3Cr_3W_7/Cu$ lead (bottom) (Ref. 5) as a function of the relaxation of the interlayer spacing in fcc Cu(111). $\mathcal{C}_0$ refers to Eq. (2) and $\mathcal{C}_\alpha$ to Eq. (6).

IV. RELAXATION EFFECTS IN ELECTRIC PROPERTIES

According to the Kubo equation of electric transport the current in a two-dimensional translational invariant system (corresponding to a simple parent lattice) in magnetic configuration $\mathcal{C}_\alpha$ flowing at 0 K in direction of the surface normal is defined by[2]

$$j_z(\mathcal{C}_\alpha) = \sum_{i,j=1,N} \sigma_{zz}^{ij}(\mathcal{C}_\alpha) E_z^j, \tag{14}$$

where the $\sigma_{zz}^{ij}(\mathcal{C}_\alpha)$ are the layer-wise contributions of the zz-like conductivity tensor and the E_z^j the z-like component of the electric field in atomic layer j. Assuming that the electric field remains constant throughout the whole system, local and total current differences between a particular magnetic configuration and the reference configuration $\mathcal{C}_0$ can be specified

$$\Delta j_z(\mathcal{C}_\alpha) = E_z \sum_{i=1,N} \Delta\sigma_{zz}^{i}(\mathcal{C}_\alpha), \tag{15}$$

$$\Delta\sigma_{zz}^{i}(\mathcal{C}_\alpha) = \sum_{j=1,N} [\sigma_{zz}^{ij}(\mathcal{C}_0) - \sigma_{zz}^{ij}(\mathcal{C}_\alpha)], \tag{16}$$

which in turn are important for an interpretation of spin-polarized STM experiments, since they can, for example, be used to point out from which part of a particular system the main contribution in the measured contrast comes from.[4,5]

Applying the same procedure as before, namely, redefining $\Delta j_z(\mathcal{C}_\alpha)$ as

$$\Delta j_z(\mathcal{C}_\alpha) \equiv \Delta j_z(\mathcal{C}_\alpha, U_0) = E_z \sum_{i=1,N} \Delta\sigma_{zz}^{i}(\mathcal{C}_\alpha, x_k), \tag{17}$$

$$\Delta j_z(\mathcal{C}_\alpha, U) = E_z \sum_{i=1,N} \Delta\sigma_{zz}^{i}(\mathcal{C}_\alpha, x_k') \tag{18}$$

then either the change in the current or of a difference current with respect to relaxation effects can be investigated by inspecting the corresponding layer-wise contributions. It should be noted that in Eqs. (17) and (18) the differential conductivity (current) that is measured experimentally is replaced by a finite difference.[5]

In Fig. 4 the value of the peak that corresponds to the top Co layer is displayed versus changes in the interlayer distance. In the inset of this figure the unrelaxed layer-resolved difference conductivities for the system $Cu(111)/Co_2Vac_3Cr_{15}W_{22}/Cu$ lead[4] are displayed. Figure 4 refers to the end point of the so-called reorientation transition of the Co layers in this system. As can be seen, even when the interlayer distance is contracted by about 10%, this peak still remains the dominant contribution to the total difference current. It seems therefore that at least in the case of 2-monolayer- (ML-) high extended islands on Cu(111) relax-

TABLE II. Value of $\Delta E(\mathcal{C}_\alpha, U)$ (meV) for $Cu(111)/Co_2$ as a function of the relaxation of the interlayer spacing (in percent). $\mathcal{C}_0$ refers to Eq. (2), $\mathcal{C}_\alpha$ to Eq. (6). The latest experimental value (Ref. 9) is 0.150 meV. Including a 1% contraction self-consistently a theoretical value for $\Delta E(\mathcal{C}_\alpha, U)$ of 0.1468 meV was reported in Ref. 8 for a free surface of 2 ML Co on Cu(111).

System	−5%	−2%	0%	2%	5%
1	−0.4315	−0.4324	−0.4327	−0.4328	−0.4326
2	0.0918	0.0914	0.0910	0.0905	0.0894
3	0.1502	0.1522	0.1535	0.1548	0.1565
4	0.1482	0.1502	0.1515	0.1527	0.1544
5	0.1502	0.1522	0.1535	0.1548	0.1565

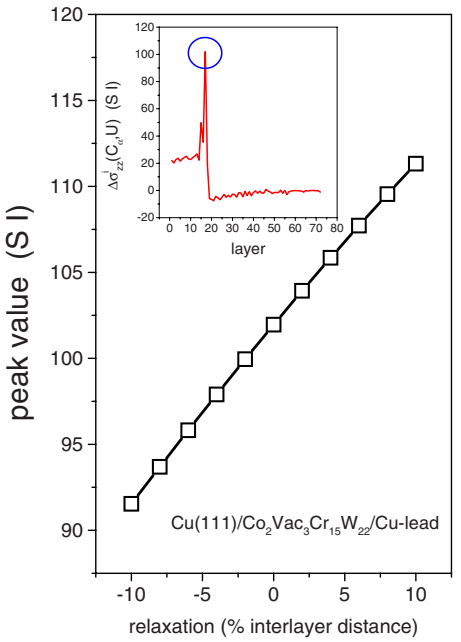

FIG. 4. (Color online) $\Delta\sigma^{j}_{zz}(\mathcal{C}_{\alpha})$ of $Cu(111)/Co_2Vac_3Cr_{15}W_{22}/Cu$ lead: value of the peak corresponding to the top Co layer as a function of the relaxation with respect to the interlayer distance in fcc Cu(111). The inset shows the unrelaxed data (Ref. 4). $\mathcal{C}_0$ refers to Eq. (2) and $\mathcal{C}_{\alpha}$ to Eq. (6).

ation effects do not change the view of spin-polarized STM being a "surface-sensitive" technique: the contrast to be seen arises mostly from the top Co layer,[4,5] independent of relaxation effects.

V. RELAXATION EFFECTS IN MAGNETO-OPTICAL PROPERTIES

By mapping the microscopically (quantum mechanically) well-defined optical conductivity tensor $\boldsymbol{\sigma}(\omega)=\{\sigma_{\mu\nu}(\omega)\mu,\nu=x,y,z\}$ (Ref. 10)

$$\boldsymbol{\sigma}(\omega)=\sum_{p=1,N}\sum_{q=1,N}\boldsymbol{\sigma}^{pq}(\omega), \tag{19}$$

where ω is the frequency, onto the macroscopic permittivity tensor $\boldsymbol{\varepsilon}(\omega)=\{\varepsilon_{\mu\nu}(\omega)\mu,\nu=x,y,z\}$

$$f:\boldsymbol{\sigma}(\omega)\rightarrow\boldsymbol{\varepsilon}(\omega)$$

such that

$$\boldsymbol{\varepsilon}^{pq}(\omega)=\frac{1}{N}\left[1-\frac{4\pi i}{\omega}\boldsymbol{\sigma}^{pq}(\omega)\right] \tag{20}$$

one then can evaluate optical properties,[11,12] or, for example, establish a well-defined macroscopical model for the evaluation of Kerr angles.[11,13]

It turned out[13] that in most cases investigated up-to-now it was sufficient to consider only layer-resolved permittivities $\boldsymbol{\epsilon}^{p}_{\mu\nu}(\omega)$

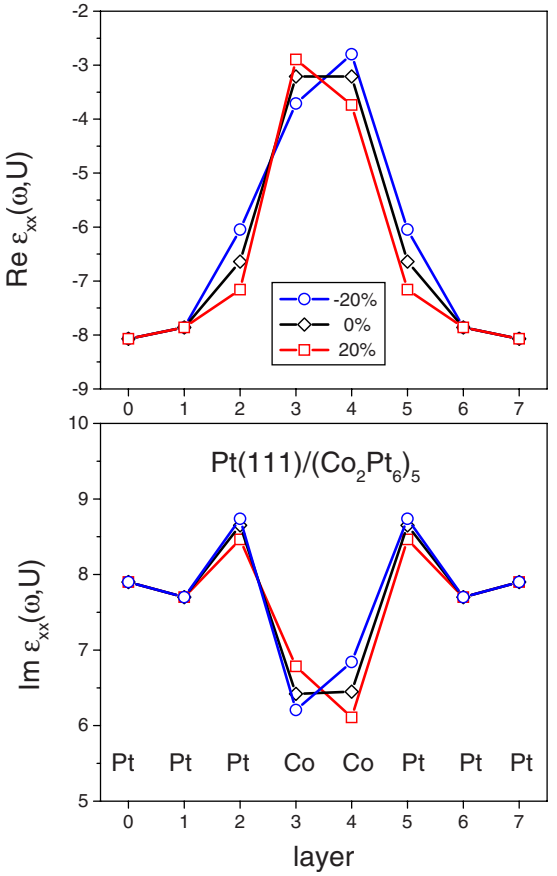

FIG. 5. (Color online) Real (top) and imaginary (bottom) part of the xx component of layer-resolved permittivity tensors in $Pt(111)/(Co_2Pt_6)_5$ relaxing the interlayer distance with respect to that in fcc Pt(111) only in the interface $PtCo_2Pt$ and leaving all other interlayer distances at the value corresponding to that in the Pt(111) substrate. The unrelaxed data are from Ref. 14, $\hbar\omega=3$ eV.

$$\boldsymbol{\epsilon}^{p}_{\mu\nu}(\omega)=\sum_{q=1,N}\boldsymbol{\epsilon}^{pq}_{\mu\nu}(\omega),\quad \boldsymbol{\epsilon}_{\mu\nu}(\omega)=\sum_{q=1,N}\boldsymbol{\epsilon}^{p}_{\mu\nu}(\omega) \tag{21}$$

in order to describe accurately magneto-optical phenomena. Clearly, the permittivity tensor $\boldsymbol{\epsilon}(\omega)$ is a physical property for which relaxation effects cannot even be guessed since one has to investigate the real and the imaginary parts of the diagonal and the off-diagonal components of all relevant layer-resolved permittivity tensors.

In Figs. 5–7 the layer-resolved permittivities in the vicinity of the Co/Pt interface in $Pt(111)/(Co_2Pt_6)_5$ (Ref. 14) are shown when changing the interlayer distance by $\pm 20\%$. As can be seen there are slight changes in the real and the imaginary part of $\boldsymbol{\epsilon}^{p}_{xx}(\omega)$ and $\boldsymbol{\epsilon}^{p}_{zz}(\omega)$, mostly located in the two Co layers, those in $\boldsymbol{\epsilon}^{p}_{xx}(\omega)$ being more pronounced than in $\boldsymbol{\epsilon}^{p}_{zz}(\omega)$. It is interesting to note that the contributions of the two Co layers to the total permittivity tensor are different whether contraction or relaxation is considered. This particular feature, which also can be seen in the xy components, is most likely caused by different kinds of magnetic interactions between the two Co layers with increasing (decreasing) interlayer distance.

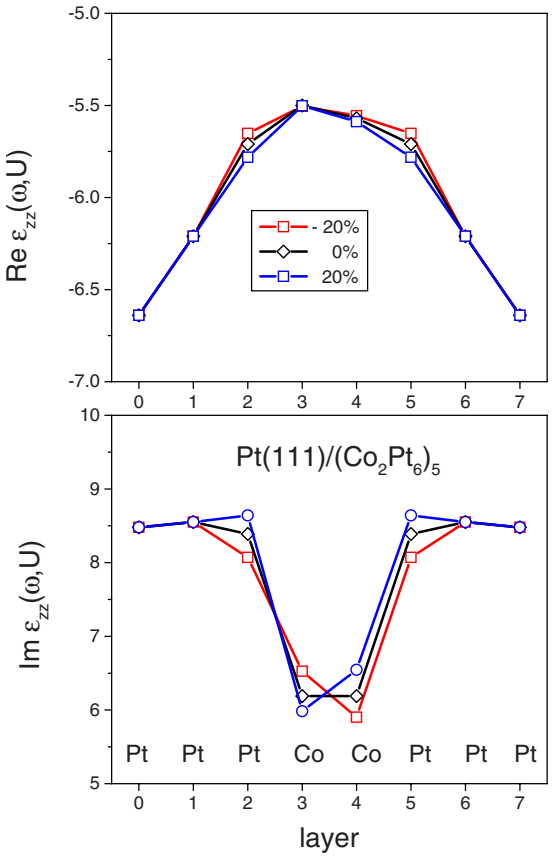

FIG. 6. (Color online) Real (top) and imaginary (bottom) part of the *zz* component of layer-resolved permittivity tensors in $Pt(111)/(Co_2Pt_6)_5$ relaxing the interlayer distance with respect to that in fcc Pt(111) only in the interface $PtCo_2Pt$ and leaving all other interlayer distances at the value corresponding to that in the Pt(111) substrate. The unrelaxed data are from Ref. 14, $\hbar\omega$=3 eV.

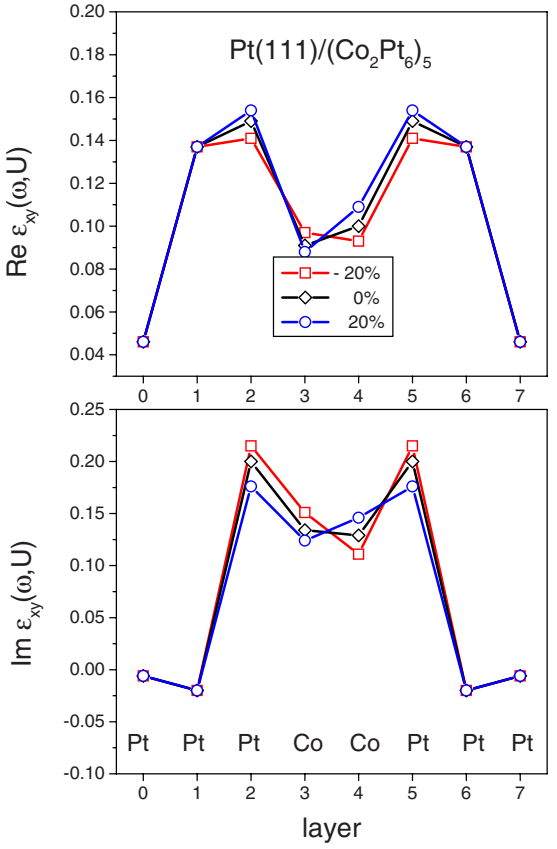

FIG. 7. (Color online) Real (top) and imaginary (bottom) part of the *xy* component of layer-resolved permittivity tensors in $Pt(111)/(Co_2Pt_6)_5$ relaxing the interlayer distance with respect to that in fcc Pt(111) only in the interface $PtCo_2Pt$ and leaving all other interlayer distances at the value corresponding to that in the Pt(111) substrate. The unrelaxed data are from Ref. 14, $\hbar\omega$=3 eV.

Considering that relaxations on the order of 20% are rather large, their effect on the permittivity has to be regarded as small. It should be noted that in using the so-called two-matrix approach surface reflectivities subject to relaxations could now be evaluated including all reflections and interferences. From the elements of the surface reflectivity matrix finally Kerr rotation and ellipticity angles would follow.[11,13] However, since experimentally almost exclusively only Kerr intensities are recorded and not (absolute) Kerr angles, it can be expected that for these intensities relaxation effects might not be important at all: in most experiments surface roughness is perhaps the much bigger problem.

VI. "ALMOST" TECHNOLOGICAL SAMPLES

While the above examples refer to experimentally well-characterized systems, for the vast majority of samples that might turn out to be of technological interest this is not the case. In particular, in the case of nanopillars and nanowires, the systems are mostly prepared by means of lithographic or other rather crude techniques that provide virtually no information about the actual interlayer spacing. Usually, all that is known, are thickness parameters in nanometers. Exactly for such systems the present approach offers unique possibilities since without great effort the influence of relaxation effects can easily be demonstrated. As a very typical example the case of a nanopillar-shaped spin-valve-type system is chosen with the following thickness parameters in (nanometer):

$$Cu_{30}Pt_3(Co_{0.25}Pt_{0.52})_4(Co_{0.25})Ni_{0.6}Co_{0.1}Cu_4(Co_{0.1}Ni_{0.6})_2Co_{0.25}Pt_3Cu_{20}$$

for which ultrafast current-induced switching was claimed[15] and which was cast theoretically[16] into a two-dimensional translational invariant system with fcc-Cu(111) interlayer spacing

$$Cu(111)/Cu_{12}Pt_{10}/\underbrace{Pt_4(CoPt_2)_4Co(Ni_2Co)_2Cu_4}_{\text{magnetic slab 1}}/Cu_{11}\underbrace{Cu_4(CoNi_2)_2Co}_{\text{magnetic slab 2}}/Pt_4/Pt_{10}Cu_{11}/Cu(111). \quad (22)$$

Of course in such a system immediately the question arises whether the rather thick Pt slabs pick up an interlayer spacing other than that of the leads, namely, a more fcc Pt(111)-like interlayer spacing, and, even more important, whether an increased interlayer spacing in the Pt layers influences the switching properties in this spin valve. This is, in particular, important since in contradiction to perhaps *ad hoc* believes it was shown[16] that by switching on a current first the first slab (magnetic slab 1), see Eq. (22), is forced into an in-plane orientation of the magnetization and only then the second magnetic slab (magnetic slab 2) follows en suite. The critical current necessary for the switching is therefore mostly determined by the reorientation energy of the first magnetic slab. In Fig. 8 the interlayer spacing in "magnetic slab 1" or in "magnetic slab 2" is increased up to a value that corresponds to the interlayer spacing in Pt(111). The inset of this figure shows the variation in the band energy for the second magnetic slab on an enlarged scale. As can be seen from this figure the changes with respect to relaxation are tiny on the scale of the difference between these two reorientation energies. The reason for the surprisingly small changes with respect to the interlayer spacing is Eq. (13): because the Cu spacer is rather thick the two magnetic slabs hardly interact. Therefore Eq. (13) is nearly fulfilled.

Quite obviously the theoretical arguing in Ref. 16 concerning the switching mechanism is robust as far as relaxation effects are concerned: the energetic path taken in current-induced switching leads via the reorientation of the first magnetic slab to a configuration in which the orientation of the magnetization is in plane in both slabs. As Fig. 8 shows this mechanism is independent of relaxation effects: the difference in reorientation energy is much too big to be influenced by relaxation effects.

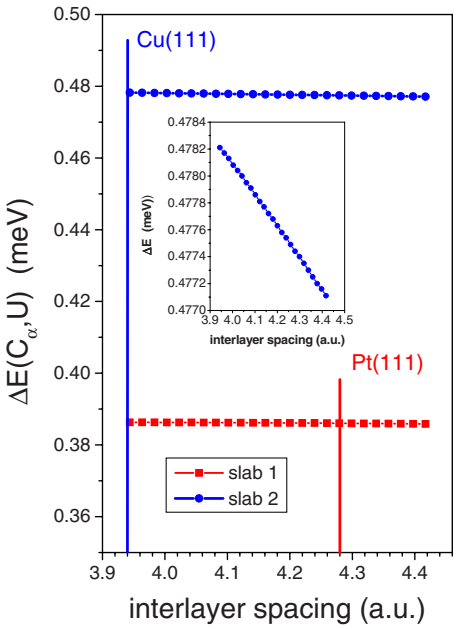

FIG. 8. (Color online) Band energy (with respect to a uniform perpendicular orientation of the magnetization) when the orientation of the magnetization in the first or in the second magnetic slab is in-plane. Squares refer to the case when in slab 1, see Eq. (22), the interlayer distance changes from that in fcc Cu(111) to fcc Pt(111) with all other interlayer distances corresponding to fcc Cu(111). Circles denote the case when the second slab is relaxed, confining all other interlayer distances to the one in fcc Cu(111). The interlayer spacing in Cu(111) and Pt(111) is marked explicitly. The inset shows the situation for the second magnetic slab on an enlarged scale. The unrelaxed data are from Ref. 16.

VII. CONCLUSION

It was shown that whenever physical properties can be expressed in theoretical descriptions as sums over layer-resolved quantities, then by means of Eq. (8) and by using a Taylor expansion, see Eq. (7), effects of layer relaxations can readily be estimated. Once the (unrelaxed) layer-resolved quantities are evaluated, which of course is the main computational effort, effects of changing the interlayer spacing can almost immediately be provided. Clearly, in the case of free surfaces such as a few layers of Co on a suitable substrate proper DFT calculations based on full potential approaches are preferable in order to discuss structural relaxation effects. For most systems in spintronics, however, this kind of "traditional approach" is completely out of reach, perhaps even not desirable, because not the structure of a particular system is of primary interest, but most likely its transport properties.

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