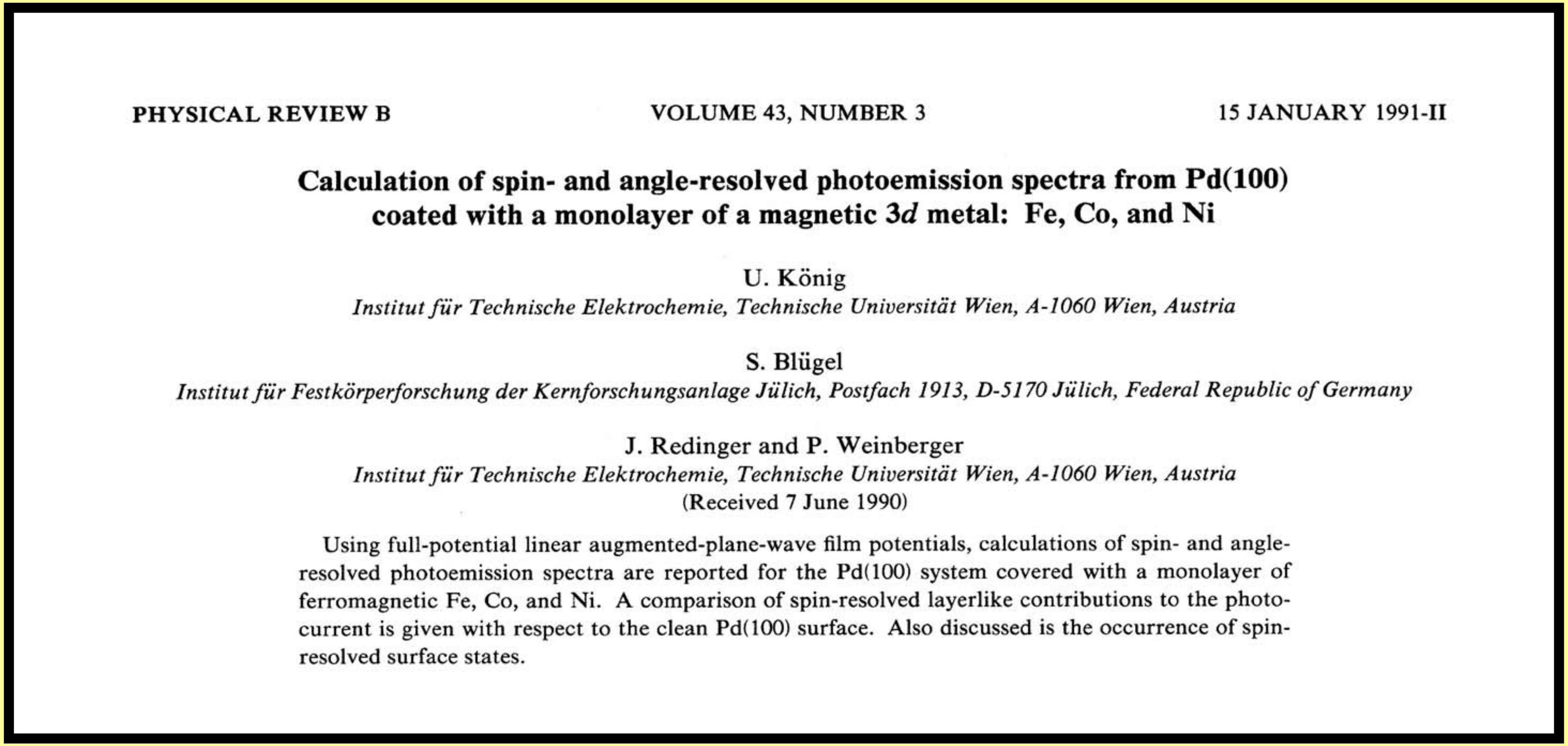
CMS

From photoemission to surface spin waves via (years of) magnetic anisotropies:

a more than 15 years lasting collaboration between experiment & theory

At the beginning there was photoemission



PHYSICAL REVIEW B VOLUME 43, NUMBER 3 15 JANUARY 1991-II

Calculation of spin- and angle-resolved photoemission spectra from Pd(100) coated with a monolayer of a magnetic 3*d* metal: Fe, Co, and Ni

U. König
Institut für Technische Elektrochemie, Technische Universität Wien, A-1060 Wien, Austria

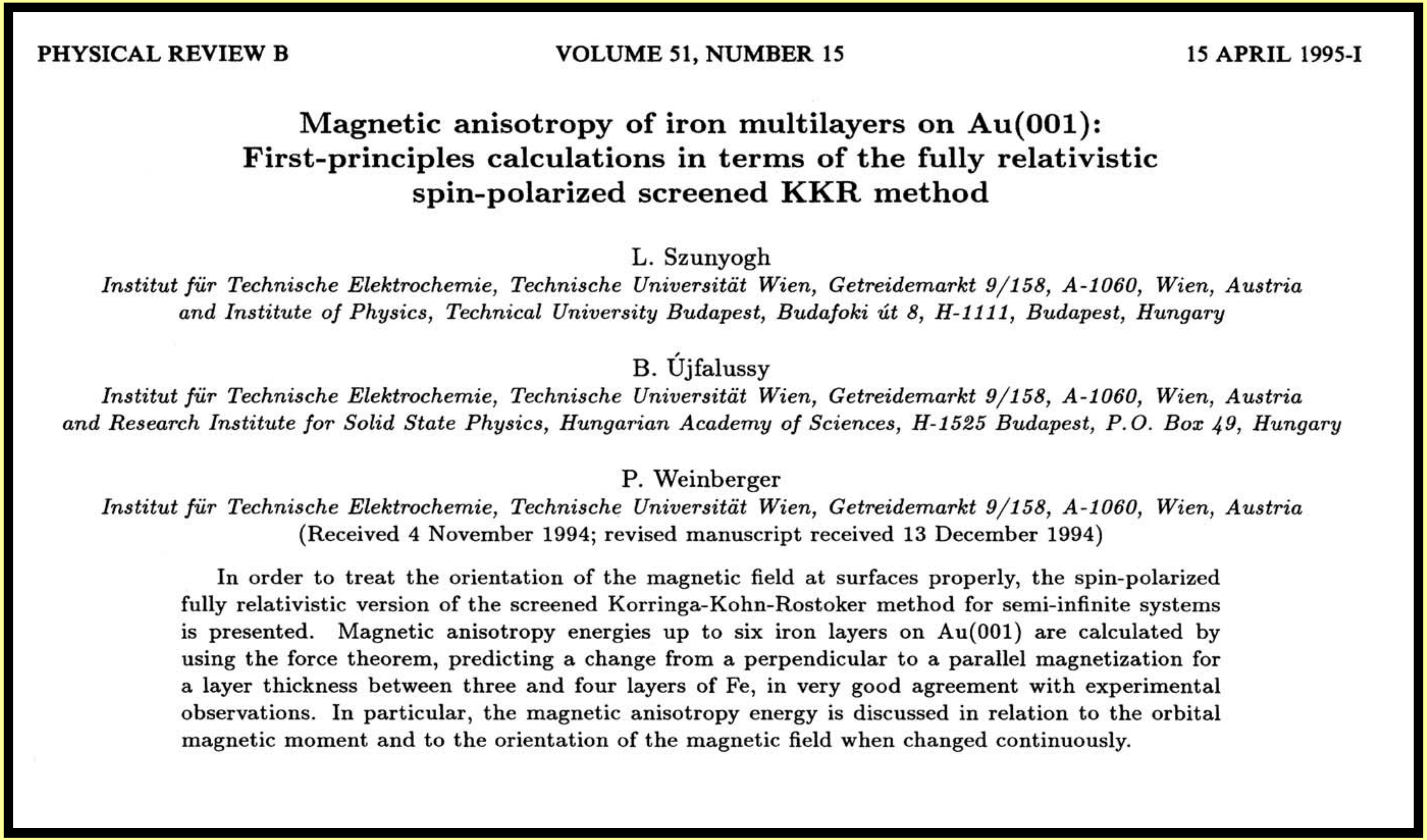
S. Blügel
Institut für Festkörperforschung der Kernforschungsanlage Jülich, Postfach 1913, D-5170 Jülich, Federal Republic of Germany

J. Redinger and P. Weinberger
Institut für Technische Elektrochemie, Technische Universität Wien, A-1060 Wien, Austria

(Received 7 June 1990)

Using full-potential linear augmented-plane-wave film potentials, calculations of spin- and angle-resolved photoemission spectra are reported for the Pd(100) system covered with a monolayer of ferromagnetic Fe, Co, and Ni. A comparison of spin-resolved layerlike contributions to the photocurrent is given with respect to the clean Pd(100) surface. Also discussed is the occurrence of spin-resolved surface states.

Magnetic anisotropies or the need of thinking relativistically



PHYSICAL REVIEW B VOLUME 51, NUMBER 15 15 APRIL 1995-I

Magnetic anisotropy of iron multilayers on Au(001): First-principles calculations in terms of the fully relativistic spin-polarized screened KKR method

L. Szunyogh
Institut für Technische Elektrochemie, Technische Universität Wien, Getreidemarkt 9/158, A-1060, Wien, Austria and Institute of Physics, Technical University Budapest, Budafoki út 8, H-1111, Budapest, Hungary

B. Újfalussy
Institut für Technische Elektrochemie, Technische Universität Wien, Getreidemarkt 9/158, A-1060, Wien, Austria and Research Institute for Solid State Physics, Hungarian Academy of Sciences, H-1525 Budapest, P.O. Box 49, Hungary

P. Weinberger
Institut für Technische Elektrochemie, Technische Universität Wien, Getreidemarkt 9/158, A-1060, Wien, Austria

(Received 4 November 1994; revised manuscript received 13 December 1994)

In order to treat the orientation of the magnetic field at surfaces properly, the spin-polarized fully relativistic version of the screened Korringa-Kohn-Rostoker method for semi-infinite systems is presented. Magnetic anisotropy energies up to six iron layers on Au(001) are calculated by using the force theorem, predicting a change from a perpendicular to a parallel magnetization for a layer thickness between three and four layers of Fe, in very good agreement with experimental observations. In particular, the magnetic anisotropy energy is discussed in relation to the orbital magnetic moment and to the orientation of the magnetic field when changed continuously.

Fe/Au(100)

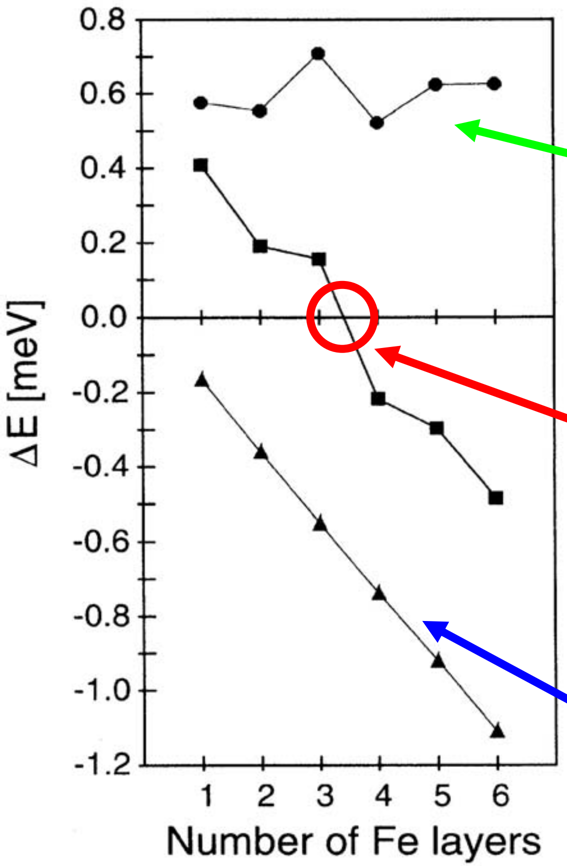


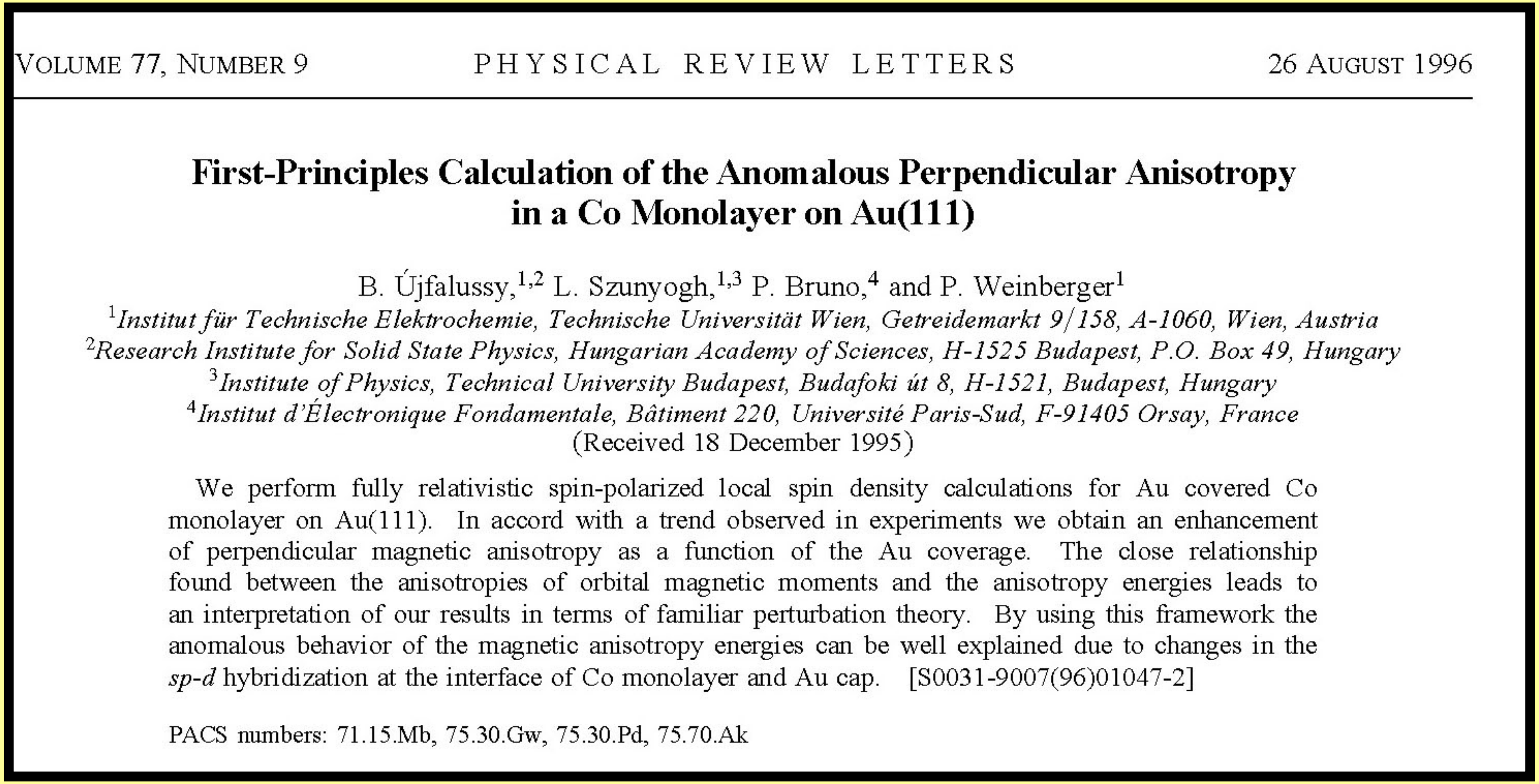
FIG. 3. Calculated magnetic anisotropy energies for Fe multilayers on Au(001). ΔE_b: circles, ΔE_{dd}: triangles, $\Delta E = \Delta E_b + \Delta E_{dd}$: squares. Solid lines serve as a guide for the eye.

„band energy“ contribution

critical thickness of reorientation transition

magnetic dipole-dipole contribution

The first surprises:



VOLUME 77, NUMBER 9 PHYSICAL REVIEW LETTERS 26 AUGUST 1996

First-Principles Calculation of the Anomalous Perpendicular Anisotropy in a Co Monolayer on Au(111)

B. Újfalussy,[1,2] L. Szunyogh,[1,3] P. Bruno,[4] and P. Weinberger[1]
[1]*Institut für Technische Elektrochemie, Technische Universität Wien, Getreidemarkt 9/158, A-1060, Wien, Austria*
[2]*Research Institute for Solid State Physics, Hungarian Academy of Sciences, H-1525 Budapest, P.O. Box 49, Hungary*
[3]*Institute of Physics, Technical University Budapest, Budafoki út 8, H-1521, Budapest, Hungary*
[4]*Institut d'Électronique Fondamentale, Bâtiment 220, Université Paris-Sud, F-91405 Orsay, France*

(Received 18 December 1995)

We perform fully relativistic spin-polarized local spin density calculations for Au covered Co monolayer on Au(111). In accord with a trend observed in experiments we obtain an enhancement of perpendicular magnetic anisotropy as a function of the Au coverage. The close relationship found between the anisotropies of orbital magnetic moments and the anisotropy energies leads to an interpretation of our results in terms of familiar perturbation theory. By using this framework the anomalous behavior of the magnetic anisotropy energies can be well explained due to changes in the *sp-d* hybridization at the interface of Co monolayer and Au cap. [S0031-9007(96)01047-2]

PACS numbers: 71.15.Mb, 75.30.Gw, 75.30.Pd, 75.70.Ak

Au/Co/Au(111)

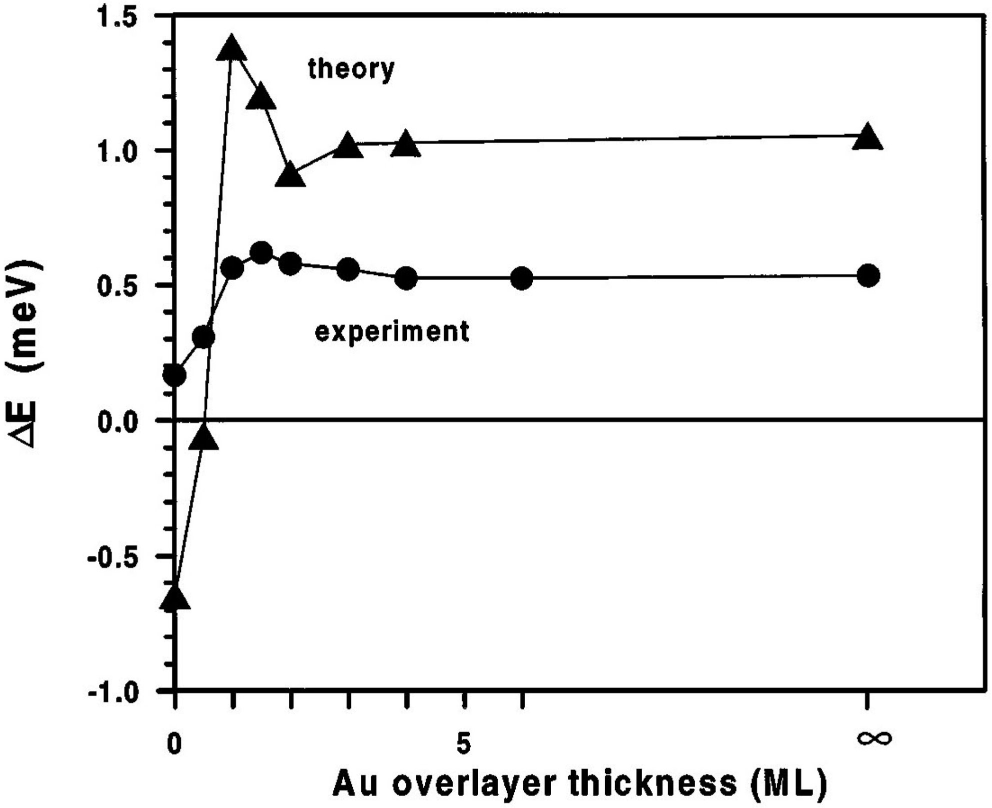
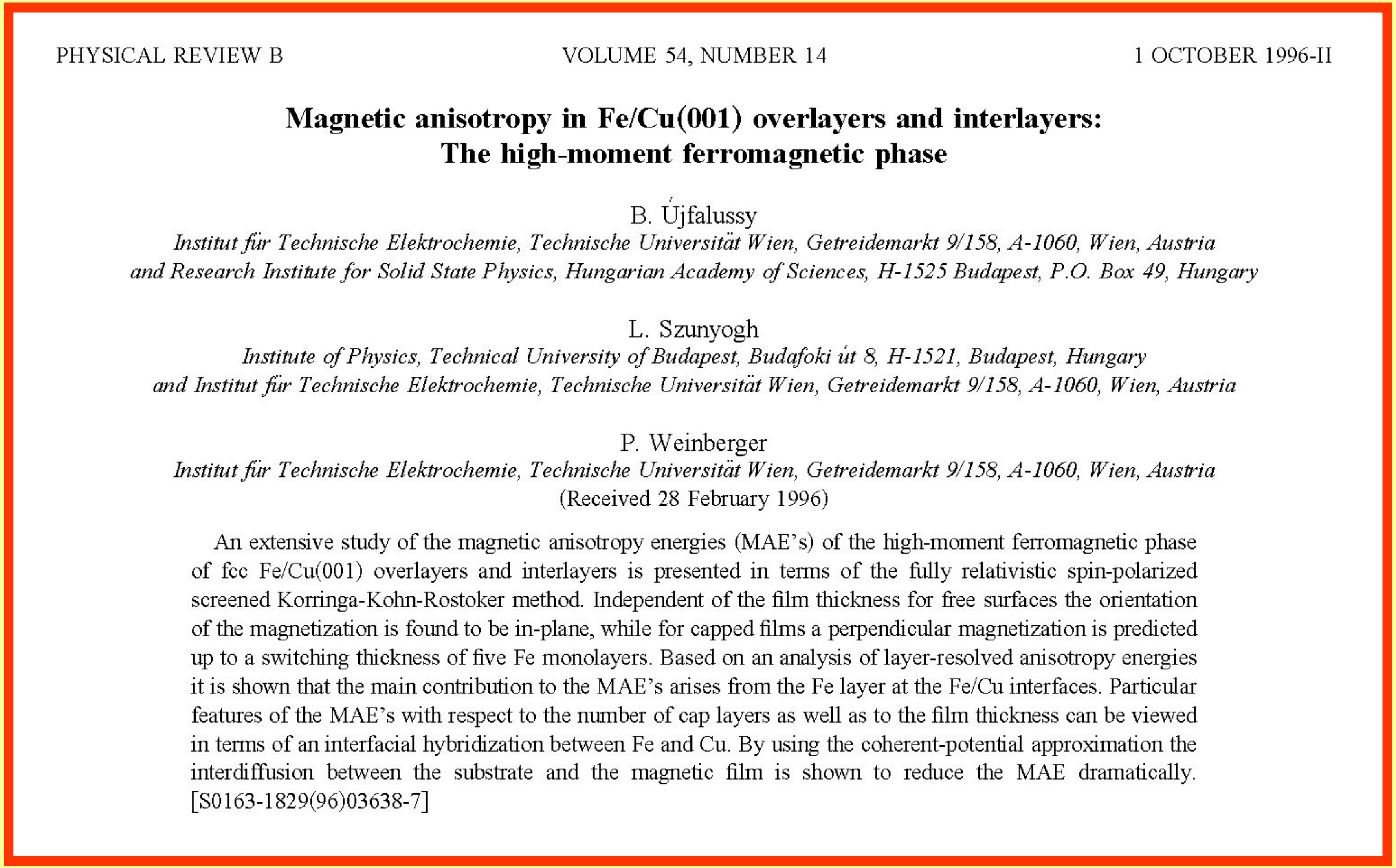


FIG. 1. Total magnetic anisotropy energies ΔE for a Co monolayer on Au(111) with different Au coverages. Triangles: calculated results; circles: experimental results from Ref. [4]. Solid lines serve as a guide to the eye.

Still unresolved: Fe/Cu(100) the first attempt



PHYSICAL REVIEW B VOLUME 54, NUMBER 14 1 OCTOBER 1996-II

Magnetic anisotropy in Fe/Cu(001) overlayers and interlayers: The high-moment ferromagnetic phase

B. Újfalussy
Institut für Technische Elektrochemie, Technische Universität Wien, Getreidemarkt 9/158, A-1060, Wien, Austria
and Research Institute for Solid State Physics, Hungarian Academy of Sciences, H-1525 Budapest, P.O. Box 49, Hungary

L. Szunyogh
Institute of Physics, Technical University of Budapest, Budafoki út 8, H-1521, Budapest, Hungary
and Institut für Technische Elektrochemie, Technische Universität Wien, Getreidemarkt 9/158, A-1060, Wien, Austria

P. Weinberger
Institut für Technische Elektrochemie, Technische Universität Wien, Getreidemarkt 9/158, A-1060, Wien, Austria

(Received 28 February 1996)

An extensive study of the magnetic anisotropy energies (MAE's) of the high-moment ferromagnetic phase of fcc Fe/Cu(001) overlayers and interlayers is presented in terms of the fully relativistic spin-polarized screened Korringa-Kohn-Rostoker method. Independent of the film thickness for free surfaces the orientation of the magnetization is found to be in-plane, while for capped films a perpendicular magnetization is predicted up to a switching thickness of five Fe monolayers. Based on an analysis of layer-resolved anisotropy energies it is shown that the main contribution to the MAE's arises from the Fe layer at the Fe/Cu interfaces. Particular features of the MAE's with respect to the number of cap layers as well as to the film thickness can be viewed in terms of an interfacial hybridization between Fe and Cu. By using the coherent-potential approximation the interdiffusion between the substrate and the magnetic film is shown to reduce the MAE dramatically. [S0163-1829(96)03638-7]

Ferromagnetic coupling ...

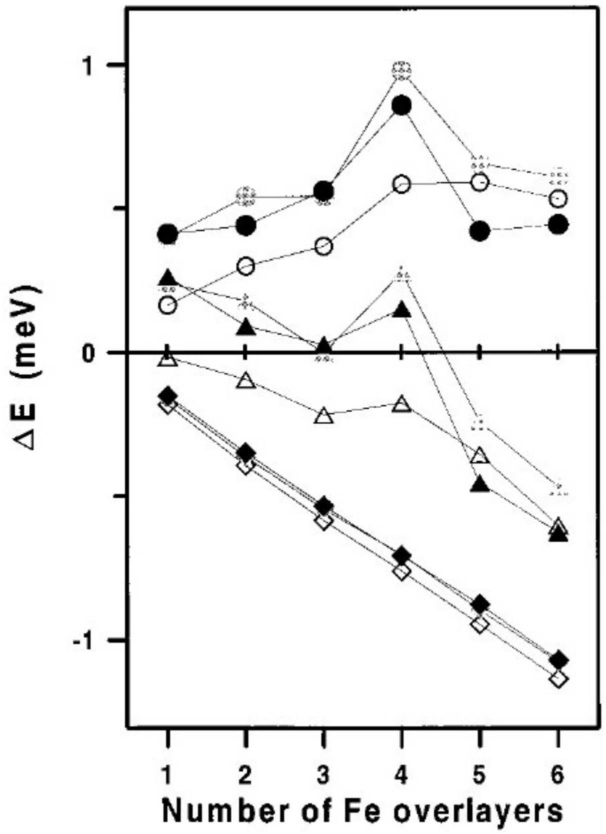
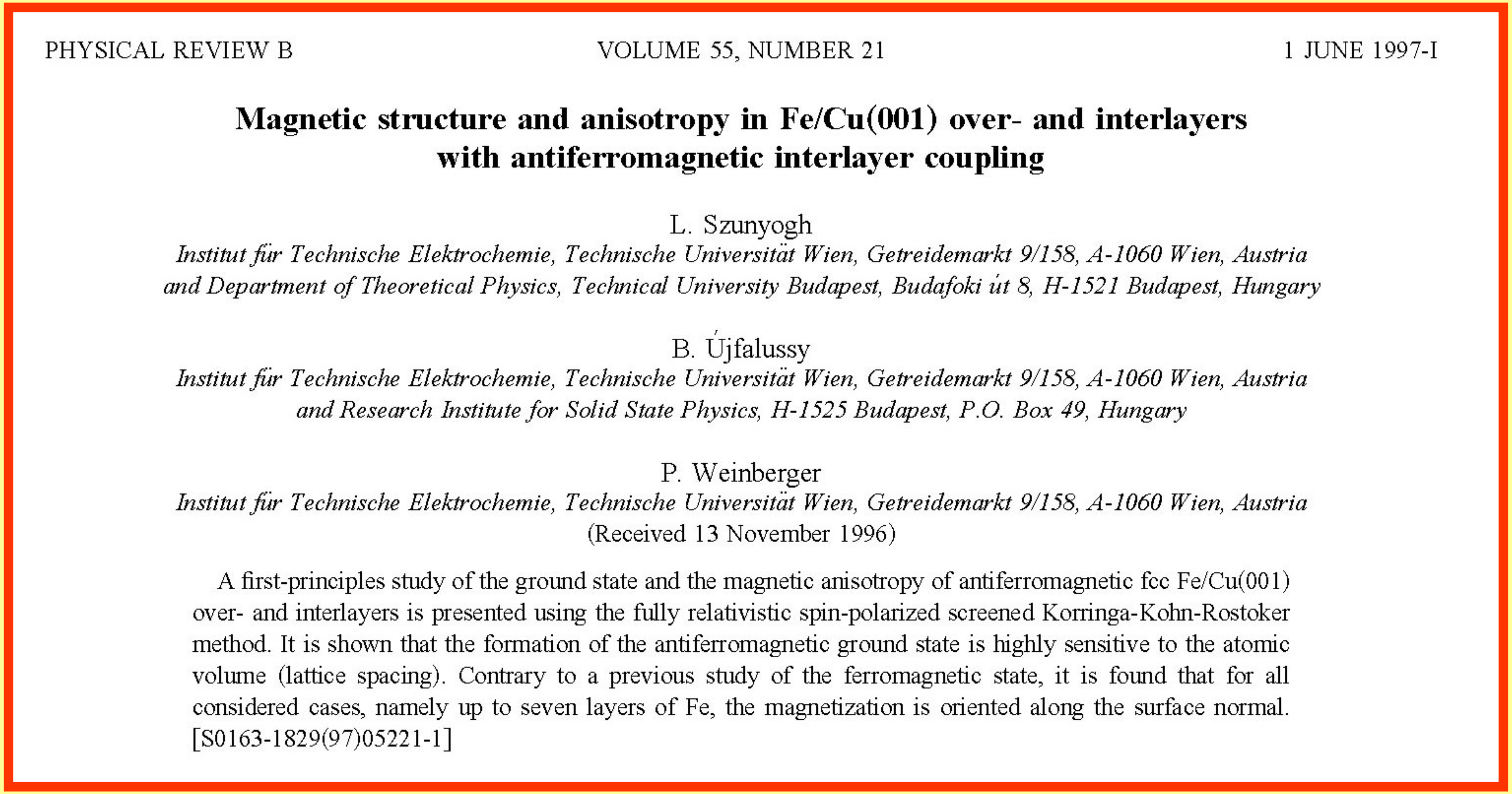


FIG. 1. Calculated magnetic anisotropy energies of $Cu_mFe_n/Cu(001)$ multilayers for $m=0$ (open symbols), $m=1$ (shaded symbols), and $m=\infty$ (solid symbols). ΔE_b, circles; ΔE_{dd}, squares; $\Delta E = \Delta E_b + \Delta E_{\mathrm{dd}}$, triangles. Solid lines serve as a guide for the eye.

Fe/Cu(100) the second attempt



PHYSICAL REVIEW B VOLUME 55, NUMBER 21 1 JUNE 1997-I

Magnetic structure and anisotropy in Fe/Cu(001) over- and interlayers with antiferromagnetic interlayer coupling

L. Szunyogh
Institut für Technische Elektrochemie, Technische Universität Wien, Getreidemarkt 9/158, A-1060 Wien, Austria
and Department of Theoretical Physics, Technical University Budapest, Budafoki út 8, H-1521 Budapest, Hungary

B. Újfalussy
Institut für Technische Elektrochemie, Technische Universität Wien, Getreidemarkt 9/158, A-1060 Wien, Austria
and Research Institute for Solid State Physics, H-1525 Budapest, P.O. Box 49, Hungary

P. Weinberger
Institut für Technische Elektrochemie, Technische Universität Wien, Getreidemarkt 9/158, A-1060 Wien, Austria

(Received 13 November 1996)

A first-principles study of the ground state and the magnetic anisotropy of antiferromagnetic fcc Fe/Cu(001) over- and interlayers is presented using the fully relativistic spin-polarized screened Korringa-Kohn-Rostoker method. It is shown that the formation of the antiferromagnetic ground state is highly sensitive to the atomic volume (lattice spacing). Contrary to a previous study of the ferromagnetic state, it is found that for all considered cases, namely up to seven layers of Fe, the magnetization is oriented along the surface normal. [S0163-1829(97)05221-1]

or antiferromagnetic coupling?

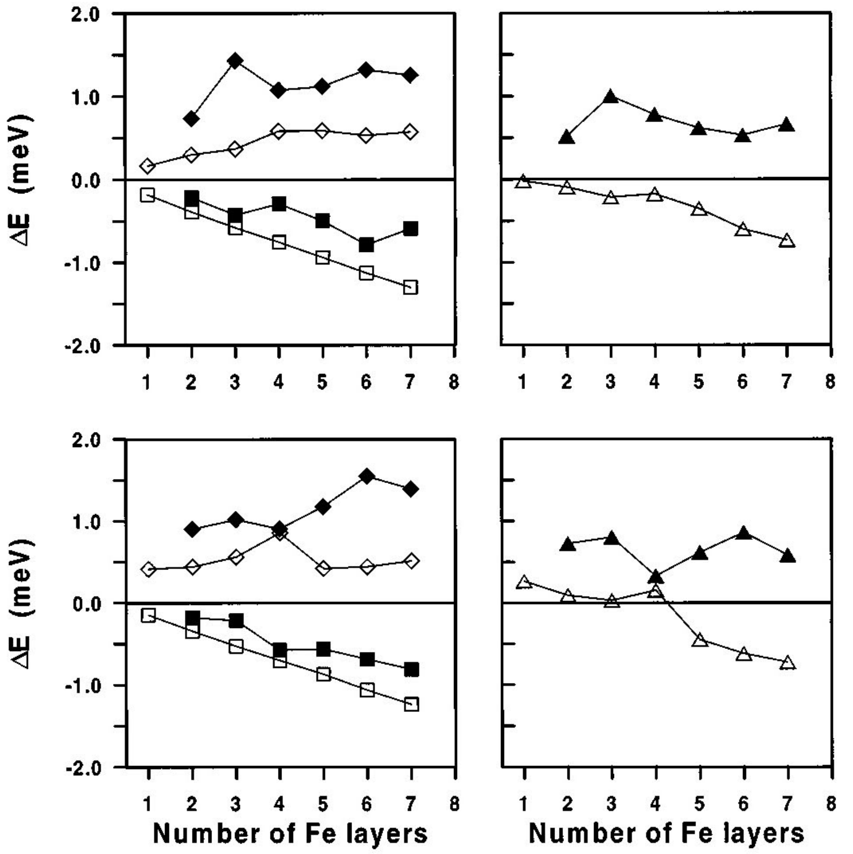
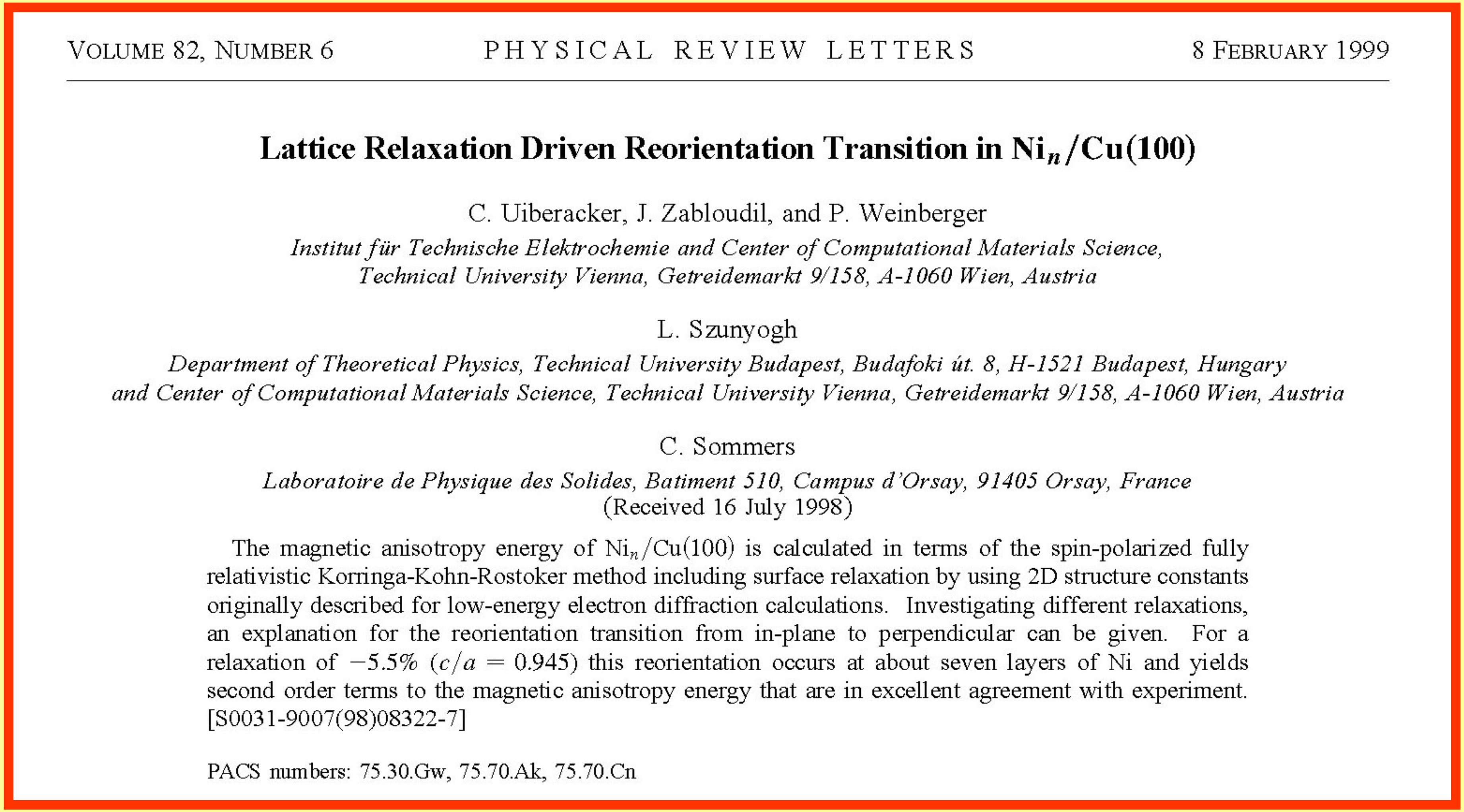


FIG. 3. Calculated magnetic anisotropy energies for the Fe_n/Cu(001) overlayer (upper panels) and for the Cu/Fe_n/Cu(001) interlayer (lower panels) systems. Diamonds: ΔE_b, squares: ΔE_{dd}, triangles: $\Delta E = \Delta E_b + \Delta E_{dd}$. Full symbols: antiferromagnetic ground states (but for $n=2$), open symbols: ferromagnetic state (Ref. 8). The solid lines serve as a guide for the eye.

... and another unsolved problem



VOLUME 82, NUMBER 6 PHYSICAL REVIEW LETTERS 8 FEBRUARY 1999

Lattice Relaxation Driven Reorientation Transition in $\mathrm{Ni}_n/\mathrm{Cu}(100)$

C. Uiberacker, J. Zabloudil, and P. Weinberger
Institut für Technische Elektrochemie and Center of Computational Materials Science,
Technical University Vienna, Getreidemarkt 9/158, A-1060 Wien, Austria

L. Szunyogh
Department of Theoretical Physics, Technical University Budapest, Budafoki út. 8, H-1521 Budapest, Hungary
and Center of Computational Materials Science, Technical University Vienna, Getreidemarkt 9/158, A-1060 Wien, Austria

C. Sommers
Laboratoire de Physique des Solides, Batiment 510, Campus d'Orsay, 91405 Orsay, France

(Received 16 July 1998)

The magnetic anisotropy energy of $\mathrm{Ni}_n/\mathrm{Cu}(100)$ is calculated in terms of the spin-polarized fully relativistic Korringa-Kohn-Rostoker method including surface relaxation by using 2D structure constants originally described for low-energy electron diffraction calculations. Investigating different relaxations, an explanation for the reorientation transition from in-plane to perpendicular can be given. For a relaxation of -5.5% ($c/a = 0.945$) this reorientation occurs at about seven layers of Ni and yields second order terms to the magnetic anisotropy energy that are in excellent agreement with experiment. [S0031-9007(98)08322-7]

PACS numbers: 75.30.Gw, 75.70.Ak, 75.70.Cn

Ni/Cu(100)

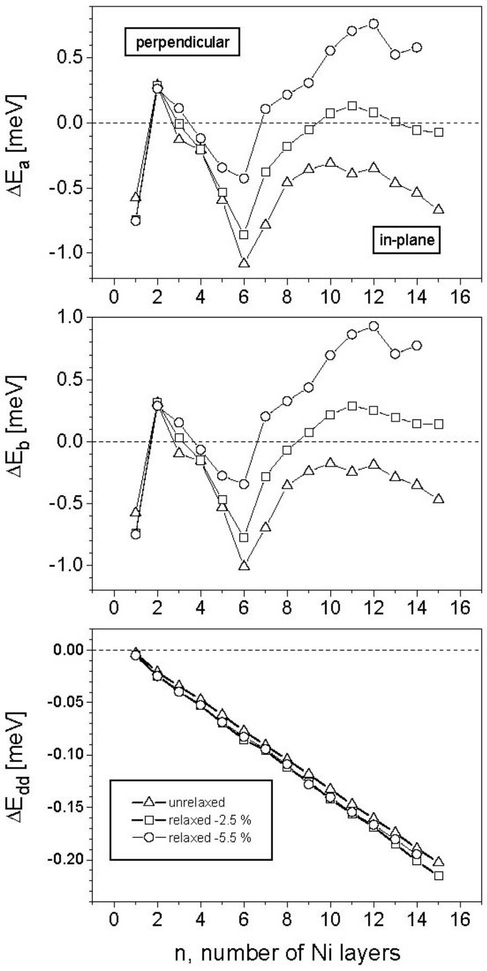


FIG. 1. Magnetic anisotropy energy ΔE_a (top), band energy difference ΔE_b (middle), and magnetic dipole-dipole energy difference ΔE_{dd} (bottom) versus the number of Ni layers on Cu(100). Triangles, squares, and circles refer in turn to a uniform relaxation by 0%, −2.5%, and −5.5%, i.e., to a c/a ratio of 1, 0.975, and 0.945.

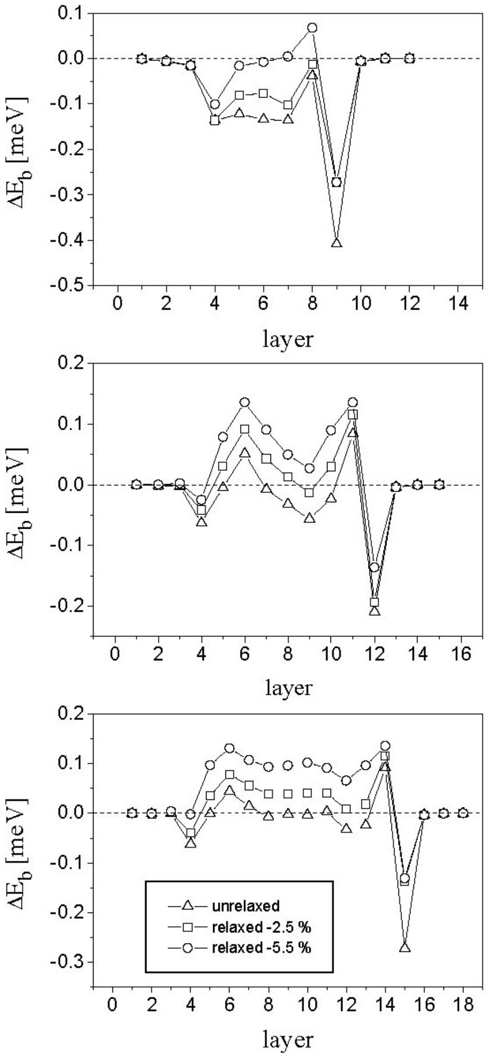
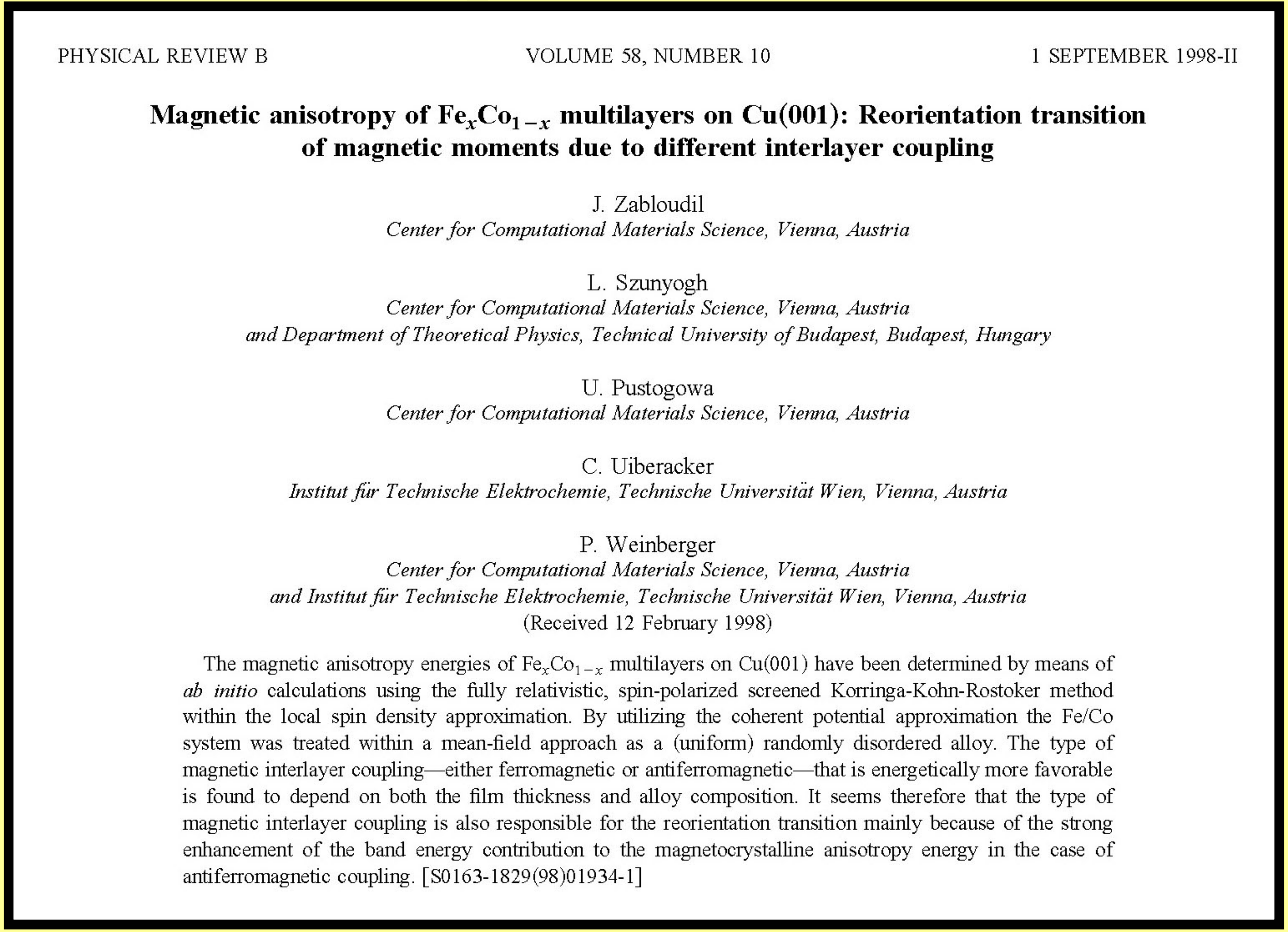


FIG. 2. Layer resolved band energy differences ΔE_b^n for six (top), nine (middle), and twelve (bottom) Ni layers on Cu(100). Triangles, squares, and circles refer in turn to a uniform relaxation by 0%, −2.5%, and −5.5%, i.e., to a c/a ratio of 1, 0.975, and 0.945.

this was yet another Kirschner problem



PHYSICAL REVIEW B VOLUME 58, NUMBER 10 1 SEPTEMBER 1998-II

Magnetic anisotropy of Fe_xCo_{1-x} multilayers on Cu(001): Reorientation transition of magnetic moments due to different interlayer coupling

J. Zabloudil
Center for Computational Materials Science, Vienna, Austria

L. Szunyogh
Center for Computational Materials Science, Vienna, Austria
and Department of Theoretical Physics, Technical University of Budapest, Budapest, Hungary

U. Pustogowa
Center for Computational Materials Science, Vienna, Austria

C. Uiberacker
Institut für Technische Elektrochemie, Technische Universität Wien, Vienna, Austria

P. Weinberger
Center for Computational Materials Science, Vienna, Austria
and Institut für Technische Elektrochemie, Technische Universität Wien, Vienna, Austria

(Received 12 February 1998)

The magnetic anisotropy energies of Fe_xCo_{1-x} multilayers on Cu(001) have been determined by means of *ab initio* calculations using the fully relativistic, spin-polarized screened Korringa-Kohn-Rostoker method within the local spin density approximation. By utilizing the coherent potential approximation the Fe/Co system was treated within a mean-field approach as a (uniform) randomly disordered alloy. The type of magnetic interlayer coupling—either ferromagnetic or antiferromagnetic—that is energetically more favorable is found to depend on both the film thickness and alloy composition. It seems therefore that the type of magnetic interlayer coupling is also responsible for the reorientation transition mainly because of the strong enhancement of the band energy contribution to the magnetocrystalline anisotropy energy in the case of antiferromagnetic coupling. [S0163-1829(98)01934-1]

a „phasediagram“ of reorientations:

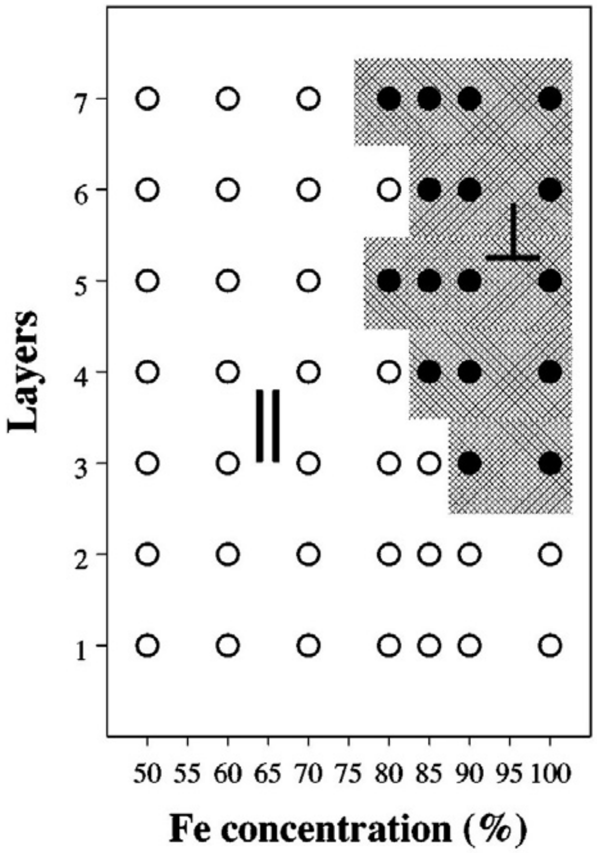
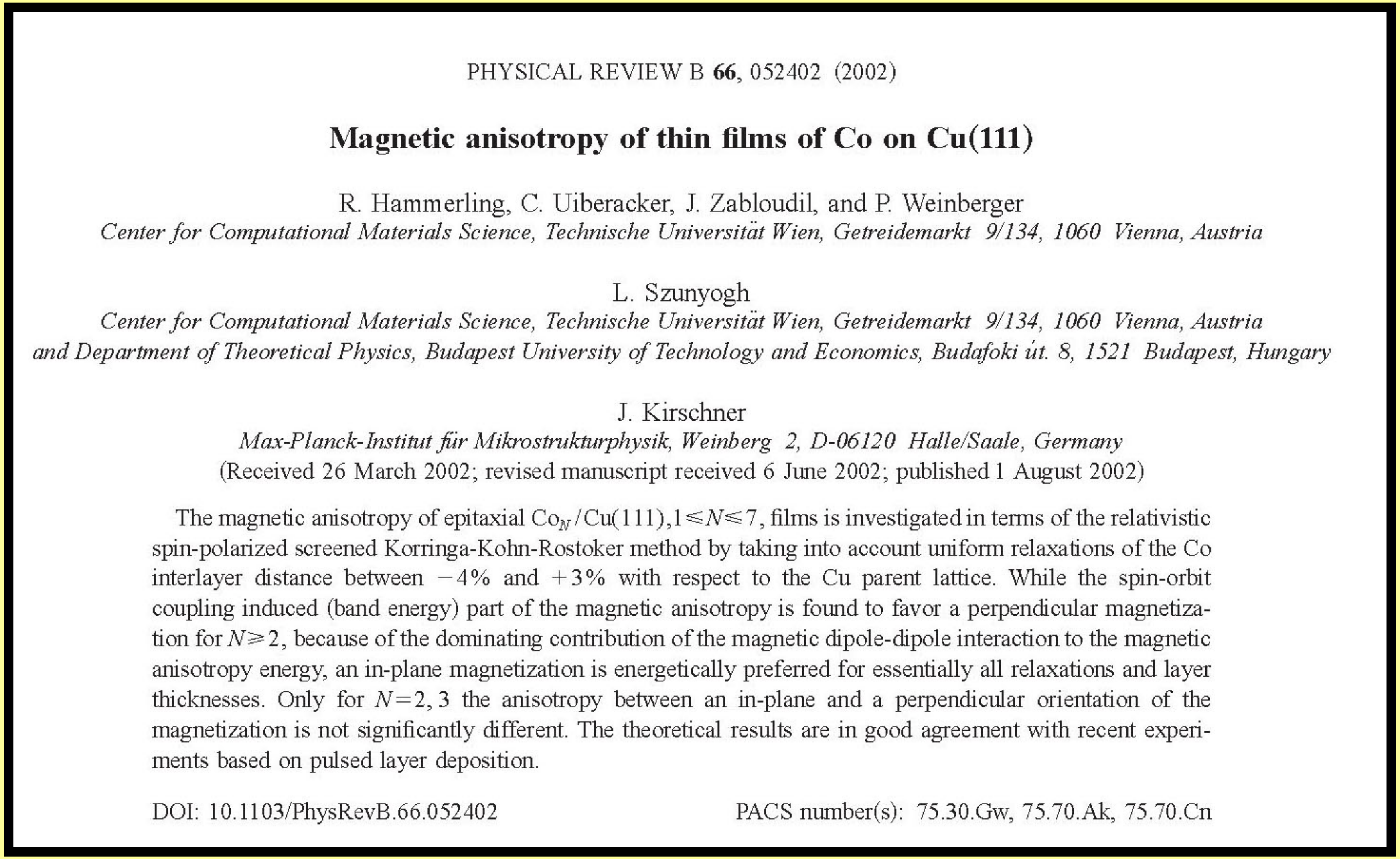


FIG. 4. ‘‘Phase diagram’’ of the reorientation transition in terms regions of perpendicular and in-plane magnetization. Solid circles in the shaded region correspond to a positive MAE and therefore to a perpendicular magnetization. Open circles indicate a negative MAE and an in-plane orientation of the magnetic moments.

The first joint publication



PHYSICAL REVIEW B **66**, 052402 (2002)

Magnetic anisotropy of thin films of Co on Cu(111)

R. Hammerling, C. Uiberacker, J. Zabloudil, and P. Weinberger
Center for Computational Materials Science, Technische Universität Wien, Getreidemarkt 9/134, 1060 Vienna, Austria

L. Szunyogh
Center for Computational Materials Science, Technische Universität Wien, Getreidemarkt 9/134, 1060 Vienna, Austria
and Department of Theoretical Physics, Budapest University of Technology and Economics, Budafoki út. 8, 1521 Budapest, Hungary

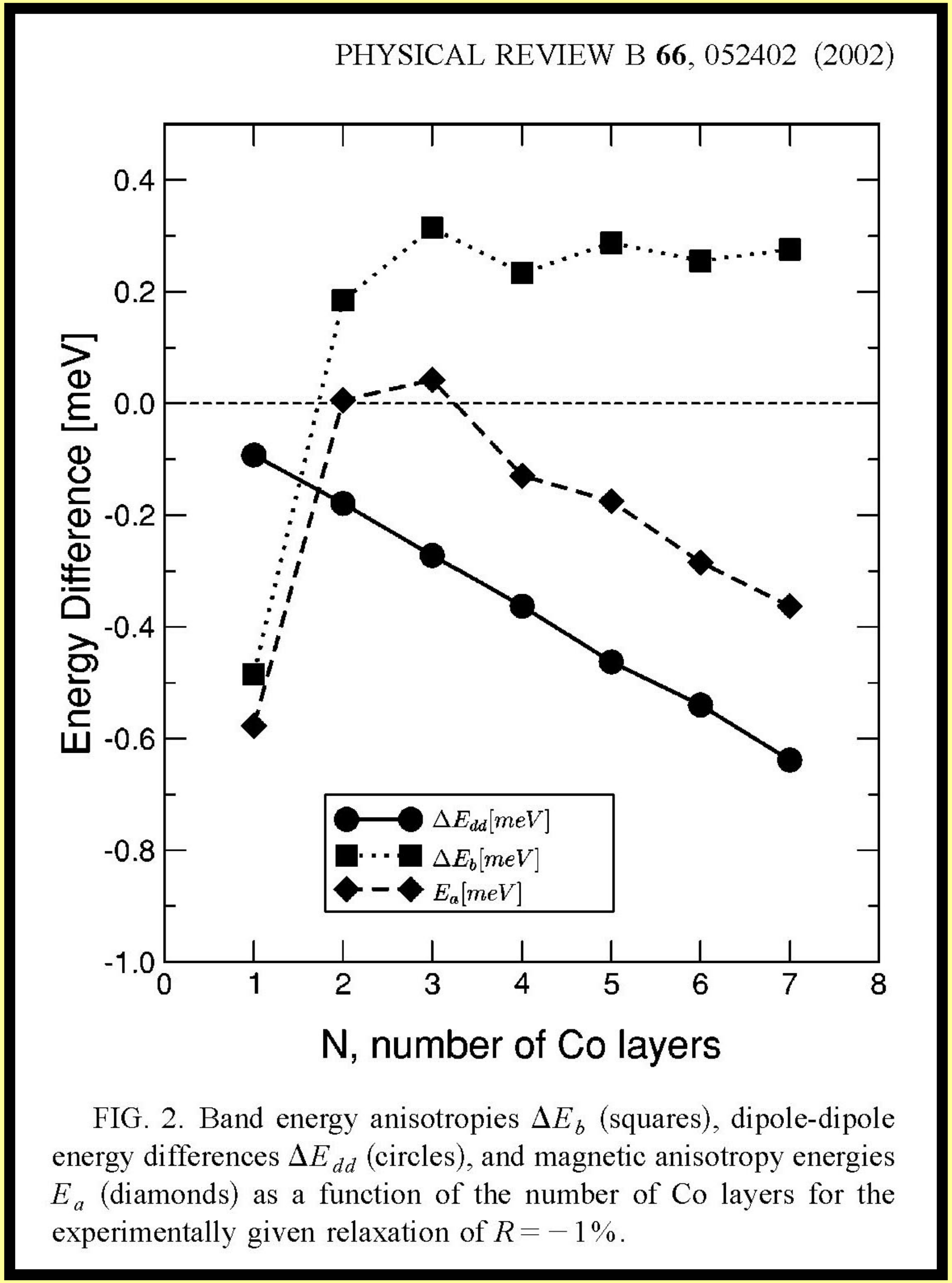
J. Kirschner
Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle/Saale, Germany

(Received 26 March 2002; revised manuscript received 6 June 2002; published 1 August 2002)

The magnetic anisotropy of epitaxial $\mathrm{Co}_N/\mathrm{Cu}(111), 1 \leqslant N \leqslant 7$, films is investigated in terms of the relativistic spin-polarized screened Korringa-Kohn-Rostoker method by taking into account uniform relaxations of the Co interlayer distance between -4% and $+3\%$ with respect to the Cu parent lattice. While the spin-orbit coupling induced (band energy) part of the magnetic anisotropy is found to favor a perpendicular magnetization for $N \geqslant 2$, because of the dominating contribution of the magnetic dipole-dipole interaction to the magnetic anisotropy energy, an in-plane magnetization is energetically preferred for essentially all relaxations and layer thicknesses. Only for $N=2, 3$ the anisotropy between an in-plane and a perpendicular orientation of the magnetization is not significantly different. The theoretical results are in good agreement with recent experiments based on pulsed layer deposition.

DOI: 10.1103/PhysRevB.66.052402 PACS number(s): 75.30.Gw, 75.70.Ak, 75.70.Cn

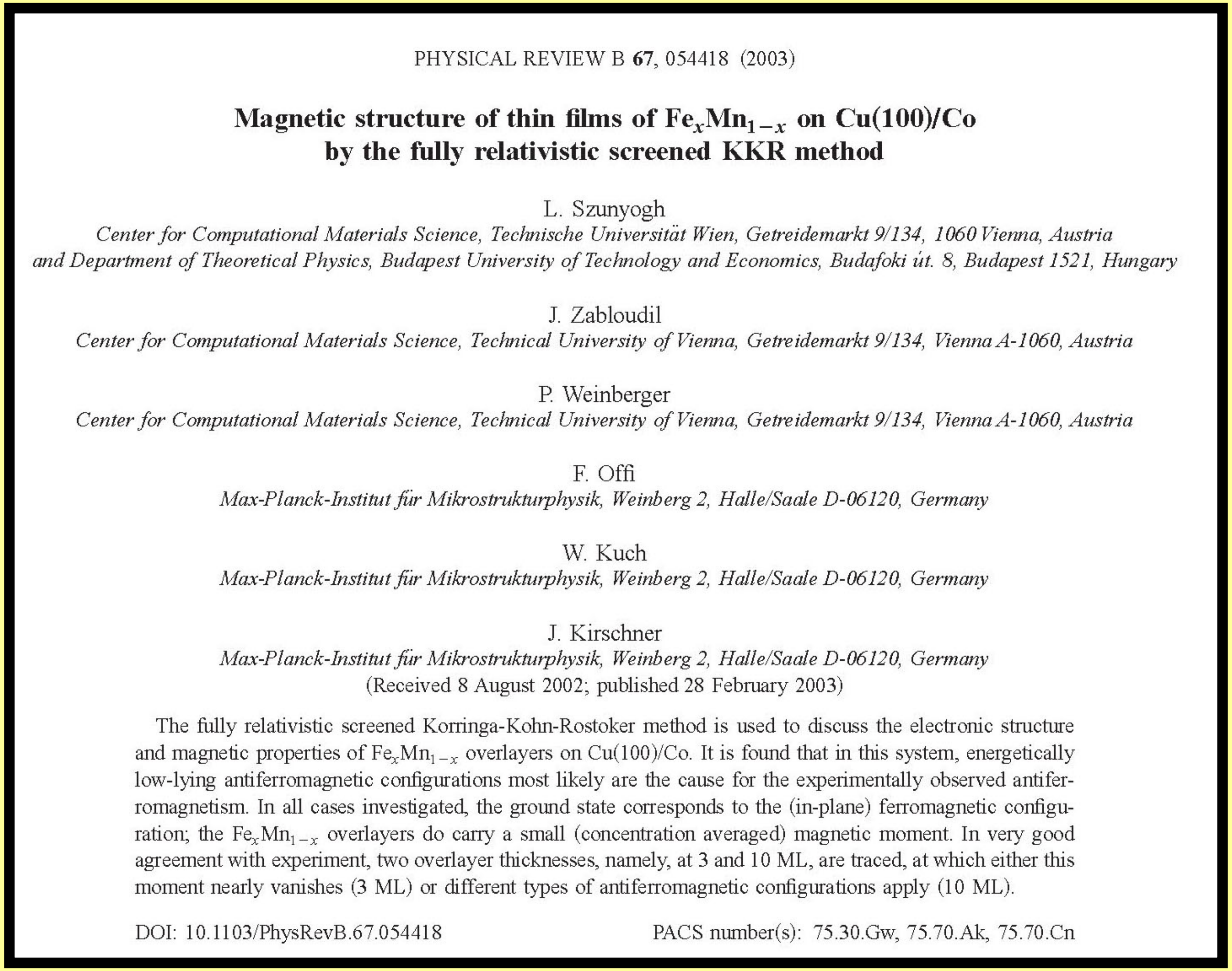
Co/Cu(111)



PHYSICAL REVIEW B **66**, 052402 (2002)

FIG. 2. Band energy anisotropies ΔE_b (squares), dipole-dipole energy differences ΔE_{dd} (circles), and magnetic anisotropy energies E_a (diamonds) as a function of the number of Co layers for the experimentally given relaxation of $R = -1\%$.

and another one:



PHYSICAL REVIEW B **67**, 054418 (2003)

Magnetic structure of thin films of Fe_xMn_{1-x} on Cu(100)/Co by the fully relativistic screened KKR method

L. Szunyogh
Center for Computational Materials Science, Technische Universität Wien, Getreidemarkt 9/134, 1060 Vienna, Austria and Department of Theoretical Physics, Budapest University of Technology and Economics, Budafoki út. 8, Budapest 1521, Hungary

J. Zabloudil
Center for Computational Materials Science, Technical University of Vienna, Getreidemarkt 9/134, Vienna A-1060, Austria

P. Weinberger
Center for Computational Materials Science, Technical University of Vienna, Getreidemarkt 9/134, Vienna A-1060, Austria

F. Offi
Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, Halle/Saale D-06120, Germany

W. Kuch
Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, Halle/Saale D-06120, Germany

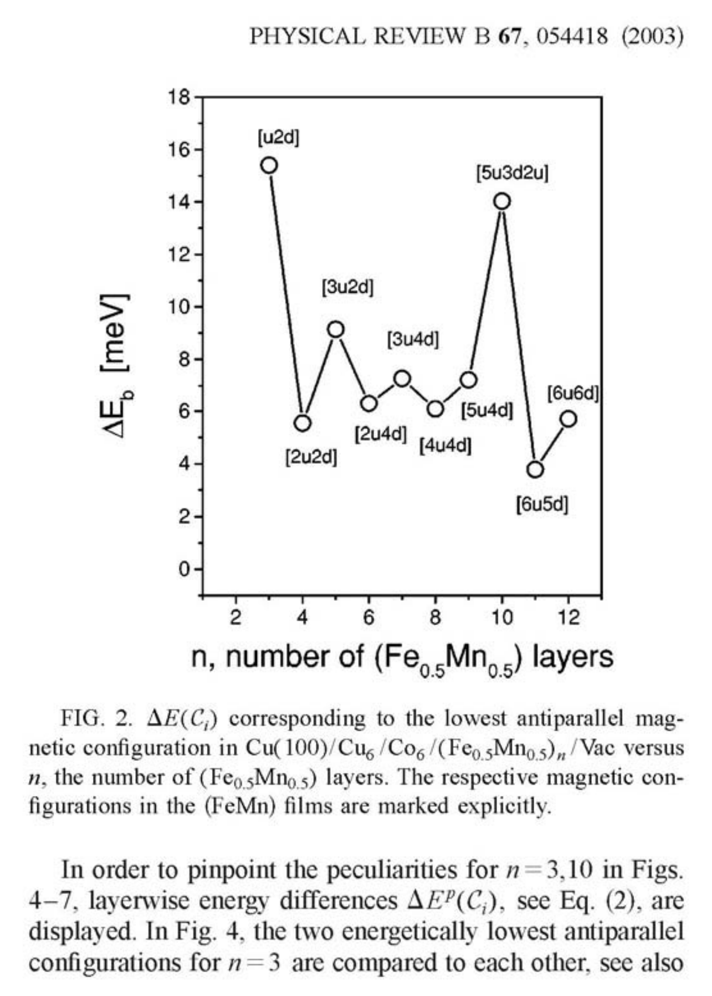
J. Kirschner
Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, Halle/Saale D-06120, Germany

(Received 8 August 2002; published 28 February 2003)

The fully relativistic screened Korringa-Kohn-Rostoker method is used to discuss the electronic structure and magnetic properties of Fe_xMn_{1-x} overlayers on Cu(100)/Co. It is found that in this system, energetically low-lying antiferromagnetic configurations most likely are the cause for the experimentally observed antiferromagnetism. In all cases investigated, the ground state corresponds to the (in-plane) ferromagnetic configuration; the Fe_xMn_{1-x} overlayers do carry a small (concentration averaged) magnetic moment. In very good agreement with experiment, two overlayer thicknesses, namely, at 3 and 10 ML, are traced, at which either this moment nearly vanishes (3 ML) or different types of antiferromagnetic configurations apply (10 ML).

DOI: 10.1103/PhysRevB.67.054418 PACS number(s): 75.30.Gw, 75.70.Ak, 75.70.Cn

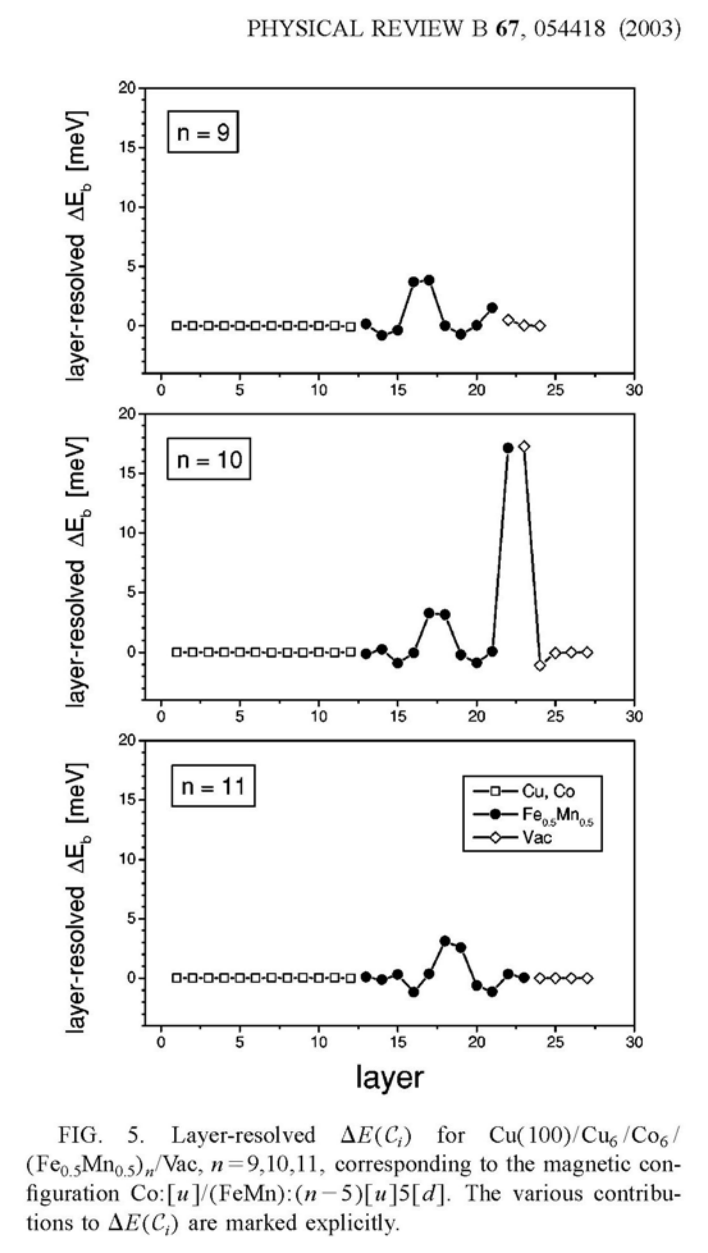
(FeMn)/Co/Cu(100)



PHYSICAL REVIEW B **67**, 054418 (2003)

FIG. 2. $\Delta E(\mathcal{C}_i)$ corresponding to the lowest antiparallel magnetic configuration in Cu(100)/Cu_6/Co_6/$(Fe_{0.5}Mn_{0.5})_n$/Vac versus n, the number of $(Fe_{0.5}Mn_{0.5})$ layers. The respective magnetic configurations in the (FeMn) films are marked explicitly.

In order to pinpoint the peculiarities for $n=3,10$ in Figs. 4–7, layerwise energy differences $\Delta E^p(\mathcal{C}_i)$, see Eq. (2), are displayed. In Fig. 4, the two energetically lowest antiparallel configurations for $n=3$ are compared to each other, see also



PHYSICAL REVIEW B **67**, 054418 (2003)

FIG. 5. Layer-resolved $\Delta E(\mathcal{C}_i)$ for Cu(100)/Cu_6/Co_6/$(Fe_{0.5}Mn_{0.5})_n$/Vac, $n=9,10,11$, corresponding to the magnetic configuration Co:$[u]$/(FeMn):$(n-5)[u]5[d]$. The various contributions to $\Delta E(\mathcal{C}_i)$ are marked explicitly.

Complicated stuff: interdiffusion, antiferro-ordering and all the rest

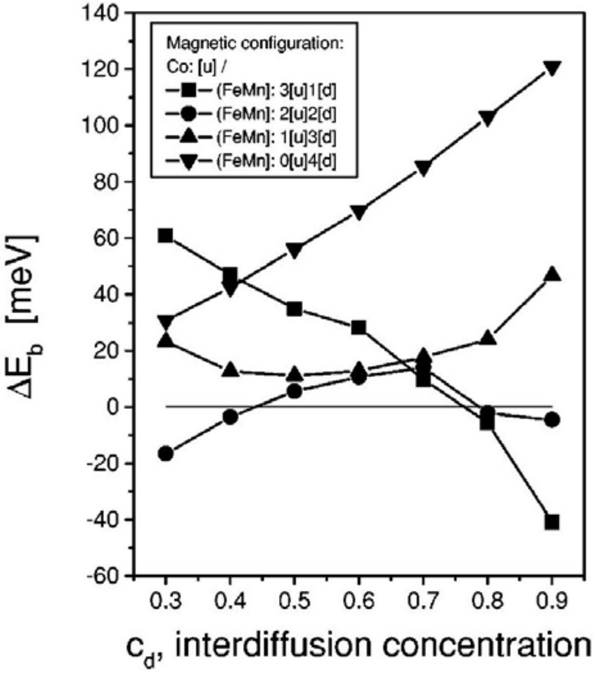


FIG. 9. $\Delta E(C_i)$ in $\mathrm{Cu(100)/Cu_6/Co_6/(Fe_{x_d}Mn_{1-x_d})(Fe_{1-x_d}Mn_{x_d})(Fe_{1-x_d}Mn_{x_d})(Fe_{x_d}Mn_{1-x_d})/Vac}$ versus the interdiffusion concentration x_d. The various antiparallel magnetic configurations investigated are marked explicitly.

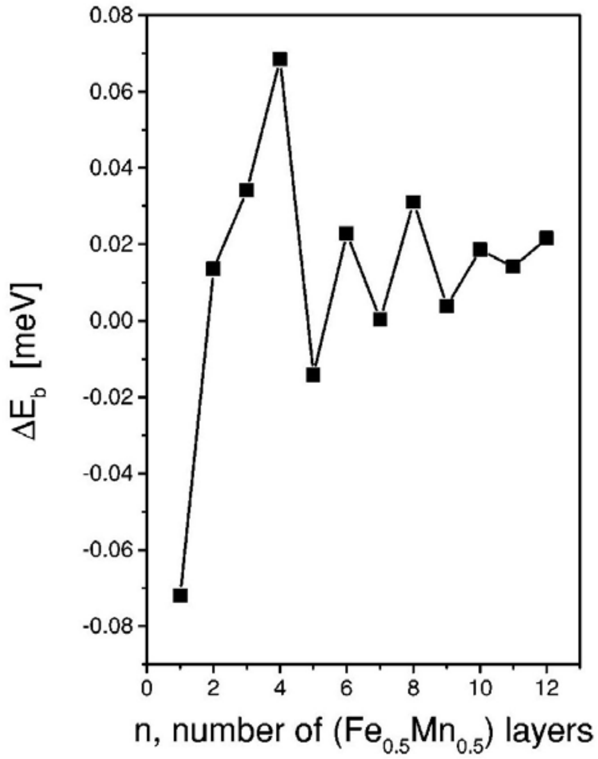
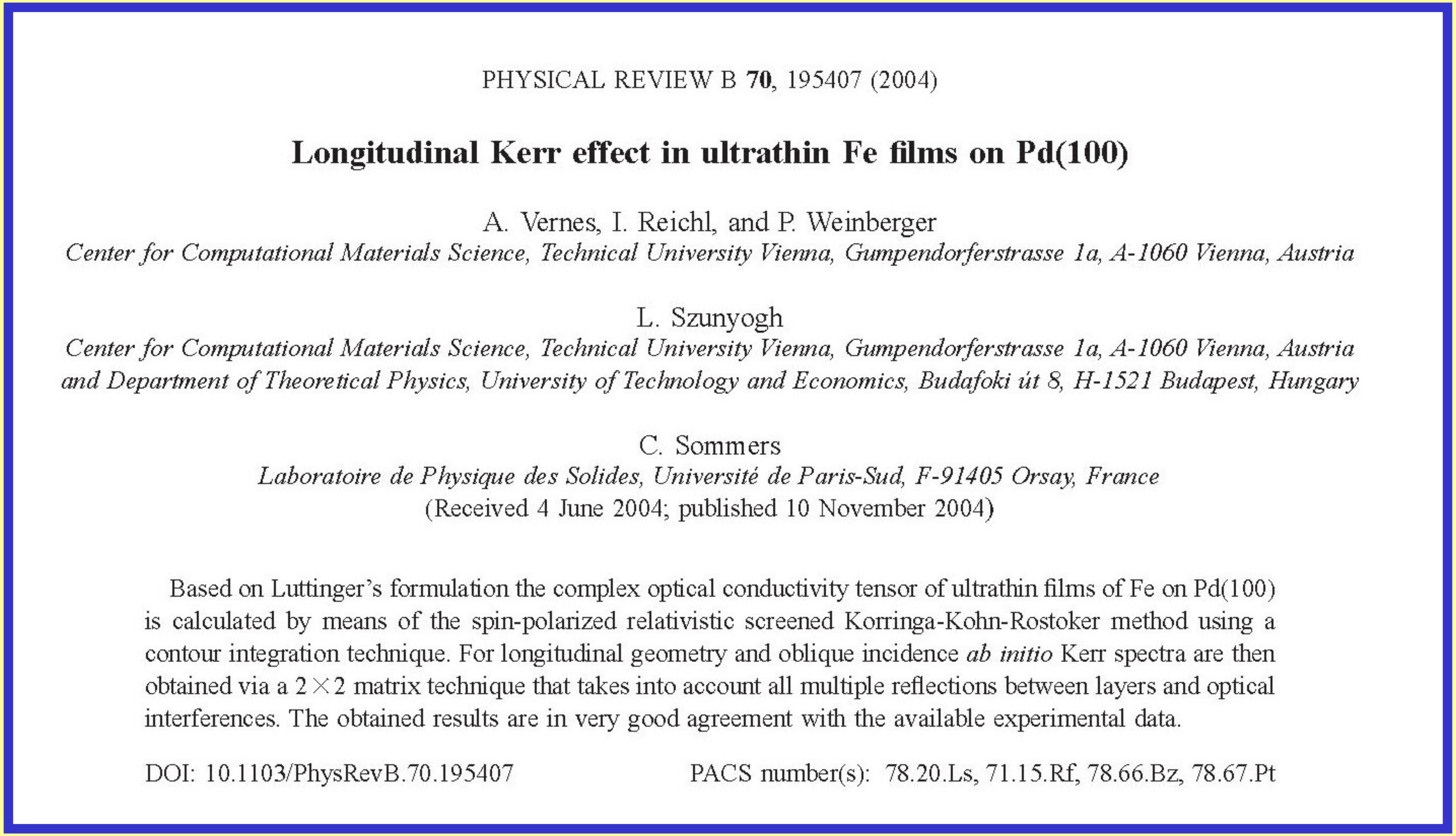


FIG. 14. Band energy part of the magnetic anisotropy energy in $\mathrm{Cu(100)/Cu_6/Co_6/(Fe_{0.5}Mn_{0.5})_{\mathit{n}}/Vac}$ versus n, the number of $\mathrm{(Fe_{0.5}Mn_{0.5})}$ layers.

Magneto-optics



PHYSICAL REVIEW B **70**, 195407 (2004)

Longitudinal Kerr effect in ultrathin Fe films on Pd(100)

A. Vernes, I. Reichl, and P. Weinberger
Center for Computational Materials Science, Technical University Vienna, Gumpendorferstrasse 1a, A-1060 Vienna, Austria

L. Szunyogh
Center for Computational Materials Science, Technical University Vienna, Gumpendorferstrasse 1a, A-1060 Vienna, Austria and Department of Theoretical Physics, University of Technology and Economics, Budafoki út 8, H-1521 Budapest, Hungary

C. Sommers
Laboratoire de Physique des Solides, Université de Paris-Sud, F-91405 Orsay, France

(Received 4 June 2004; published 10 November 2004)

Based on Luttinger's formulation the complex optical conductivity tensor of ultrathin films of Fe on Pd(100) is calculated by means of the spin-polarized relativistic screened Korringa-Kohn-Rostoker method using a contour integration technique. For longitudinal geometry and oblique incidence *ab initio* Kerr spectra are then obtained via a 2×2 matrix technique that takes into account all multiple reflections between layers and optical interferences. The obtained results are in very good agreement with the available experimental data.

DOI: 10.1103/PhysRevB.70.195407 PACS number(s): 78.20.Ls, 71.15.Rf, 78.66.Bz, 78.67.Pt

Fe/Pd(100)

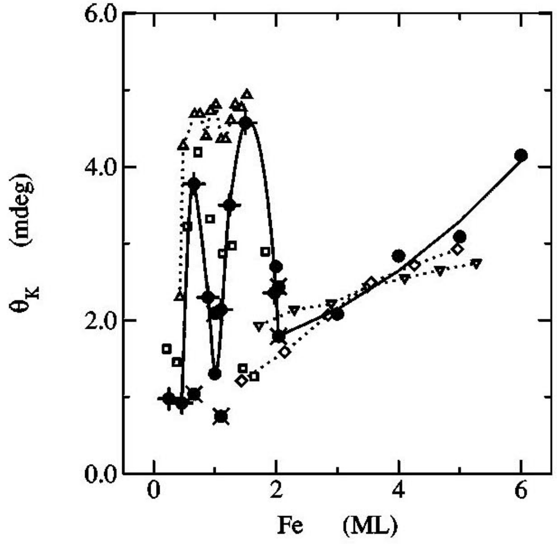
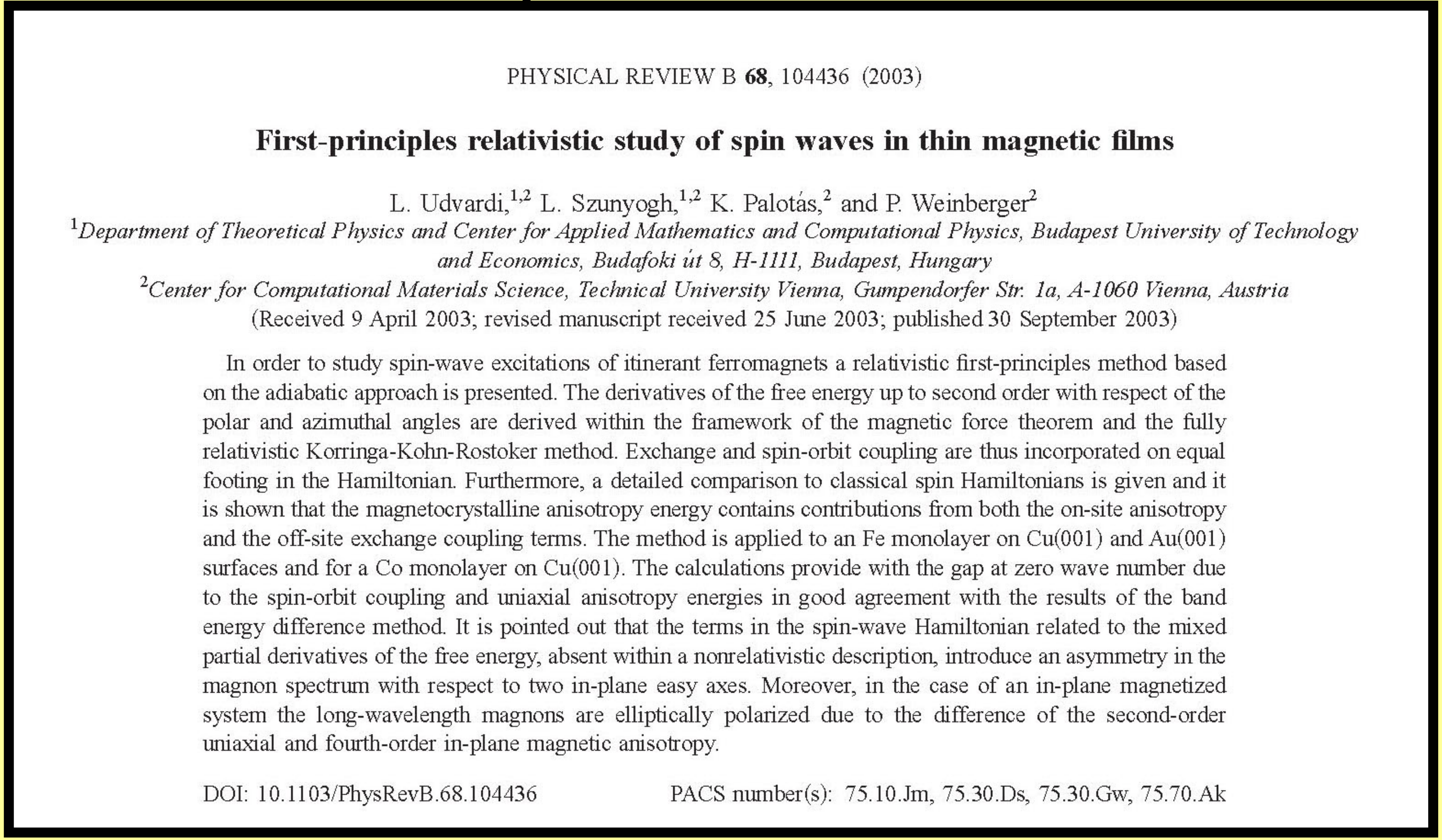


FIG. 1. Longitudinal Kerr rotation angle for oblique incidence ($\theta=70°$) and p-polarized light ($\hbar\omega=1.847\,654$ eV) in the case of fcc Fe/Pd(100). The calculated Kerr rotation angles θ_K in mdeg (10^{-3} deg) corresponding to concentration profiles I (II) are shown as pluses (crosses) and those corresponding to the ordered layered systems $\mathrm{Fe}_N/\mathrm{Pd}(100)$, with $N \in \mathbb{N}$, as solid circles. The properly scaled experimental Kerr signals (arbitrary units) from Ref. 3 refer to open symbols: squares, up and down triangles denote data from samples obtained by pulse laser deposition performed at temperatures $T=50-70$ K, while diamonds represent data recorded from thermal deposited probes at room temperature. Dashed lines connect different experimental Kerr signal sets; the solid line follows the regression of the calculated Kerr rotation angles for concentration profiles I and for the ordered layered systems.

This was one of the very few cases when theory was ahead of experiment

Response to his newest interest: surface spin waves

CMS



PHYSICAL REVIEW B **68**, 104436 (2003)

First-principles relativistic study of spin waves in thin magnetic films

L. Udvardi,[1,2] L. Szunyogh,[1,2] K. Palotás,[2] and P. Weinberger[2]
[1]*Department of Theoretical Physics and Center for Applied Mathematics and Computational Physics, Budapest University of Technology and Economics, Budafoki út 8, H-1111, Budapest, Hungary*
[2]*Center for Computational Materials Science, Technical University Vienna, Gumpendorfer Str. 1a, A-1060 Vienna, Austria*

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In order to study spin-wave excitations of itinerant ferromagnets a relativistic first-principles method based on the adiabatic approach is presented. The derivatives of the free energy up to second order with respect of the polar and azimuthal angles are derived within the framework of the magnetic force theorem and the fully relativistic Korringa-Kohn-Rostoker method. Exchange and spin-orbit coupling are thus incorporated on equal footing in the Hamiltonian. Furthermore, a detailed comparison to classical spin Hamiltonians is given and it is shown that the magnetocrystalline anisotropy energy contains contributions from both the on-site anisotropy and the off-site exchange coupling terms. The method is applied to an Fe monolayer on Cu(001) and Au(001) surfaces and for a Co monolayer on Cu(001). The calculations provide with the gap at zero wave number due to the spin-orbit coupling and uniaxial anisotropy energies in good agreement with the results of the band energy difference method. It is pointed out that the terms in the spin-wave Hamiltonian related to the mixed partial derivatives of the free energy, absent within a nonrelativistic description, introduce an asymmetry in the magnon spectrum with respect to two in-plane easy axes. Moreover, in the case of an in-plane magnetized system the long-wavelength magnons are elliptically polarized due to the difference of the second-order uniaxial and fourth-order in-plane magnetic anisotropy.

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Co/Cu(100) & Fe/Cu(100)

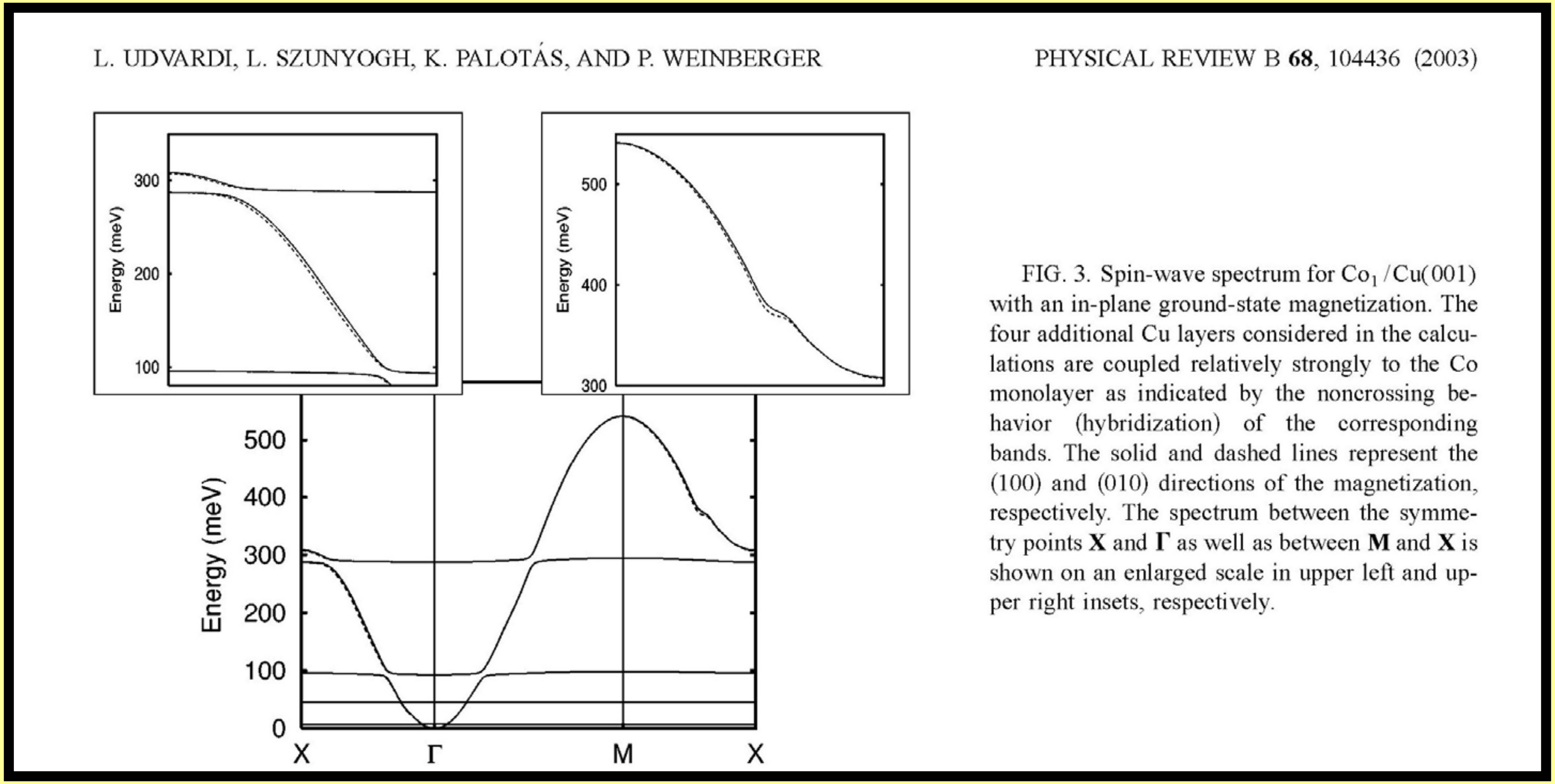

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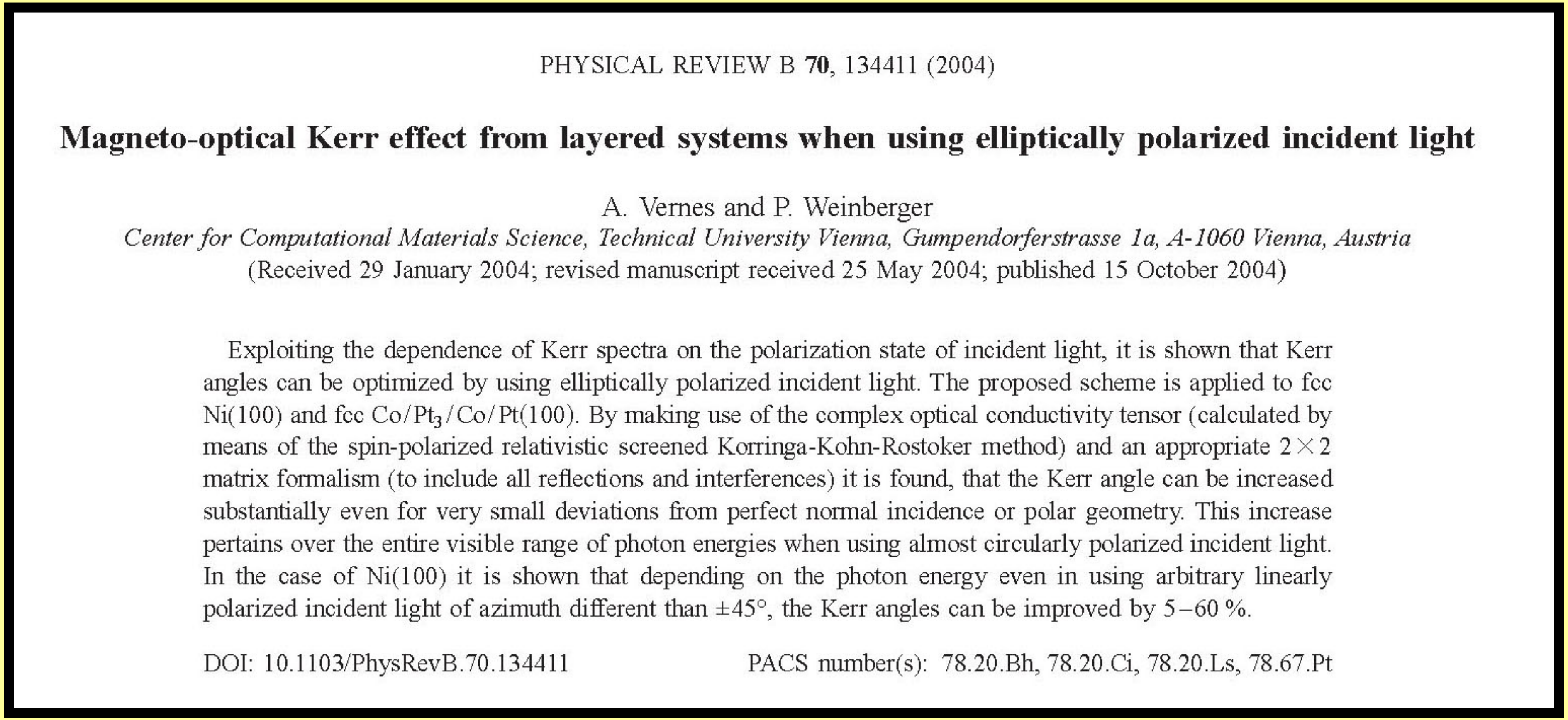
FIG. 3. Spin-wave spectrum for Co_1/Cu(001) with an in-plane ground-state magnetization. The four additional Cu layers considered in the calculations are coupled relatively strongly to the Co monolayer as indicated by the noncrossing behavior (hybridization) of the corresponding bands. The solid and dashed lines represent the (100) and (010) directions of the magnetization, respectively. The spectrum between the symmetry points **X** and **Γ** as well as between **M** and **X** is shown on an enlarged scale in upper left and upper right insets, respectively.

However, there were also topics with no experimental (Kirschner) response such as

magnetoelectronis (spintronics) and ....

a possible **optimization of Kerr angles** …



PHYSICAL REVIEW B **70**, 134411 (2004)

Magneto-optical Kerr effect from layered systems when using elliptically polarized incident light

A. Vernes and P. Weinberger
Center for Computational Materials Science, Technical University Vienna, Gumpendorferstrasse 1a, A-1060 Vienna, Austria

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Exploiting the dependence of Kerr spectra on the polarization state of incident light, it is shown that Kerr angles can be optimized by using elliptically polarized incident light. The proposed scheme is applied to fcc Ni(100) and fcc Co/Pt_3/Co/Pt(100). By making use of the complex optical conductivity tensor (calculated by means of the spin-polarized relativistic screened Korringa-Kohn-Rostoker method) and an appropriate 2×2 matrix formalism (to include all reflections and interferences) it is found, that the Kerr angle can be increased substantially even for very small deviations from perfect normal incidence or polar geometry. This increase pertains over the entire visible range of photon energies when using almost circularly polarized incident light. In the case of Ni(100) it is shown that depending on the photon energy even in using arbitrary linearly polarized incident light of azimuth different than $\pm 45°$, the Kerr angles can be improved by $5-60\,\%$.

DOI: 10.1103/PhysRevB.70.134411 PACS number(s): 78.20.Bh, 78.20.Ci, 78.20.Ls, 78.67.Pt

by changing the polarization of the incoming light

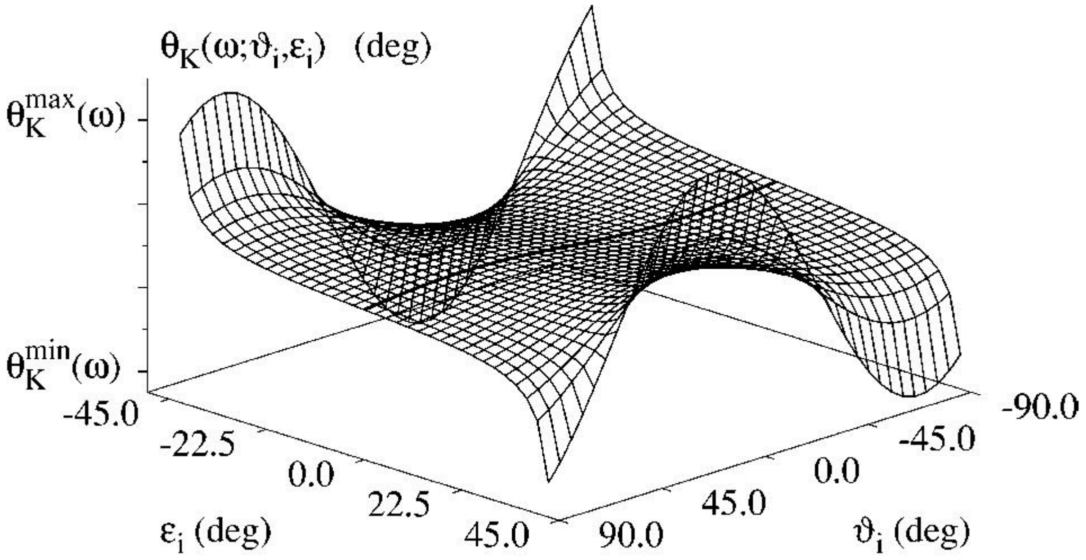
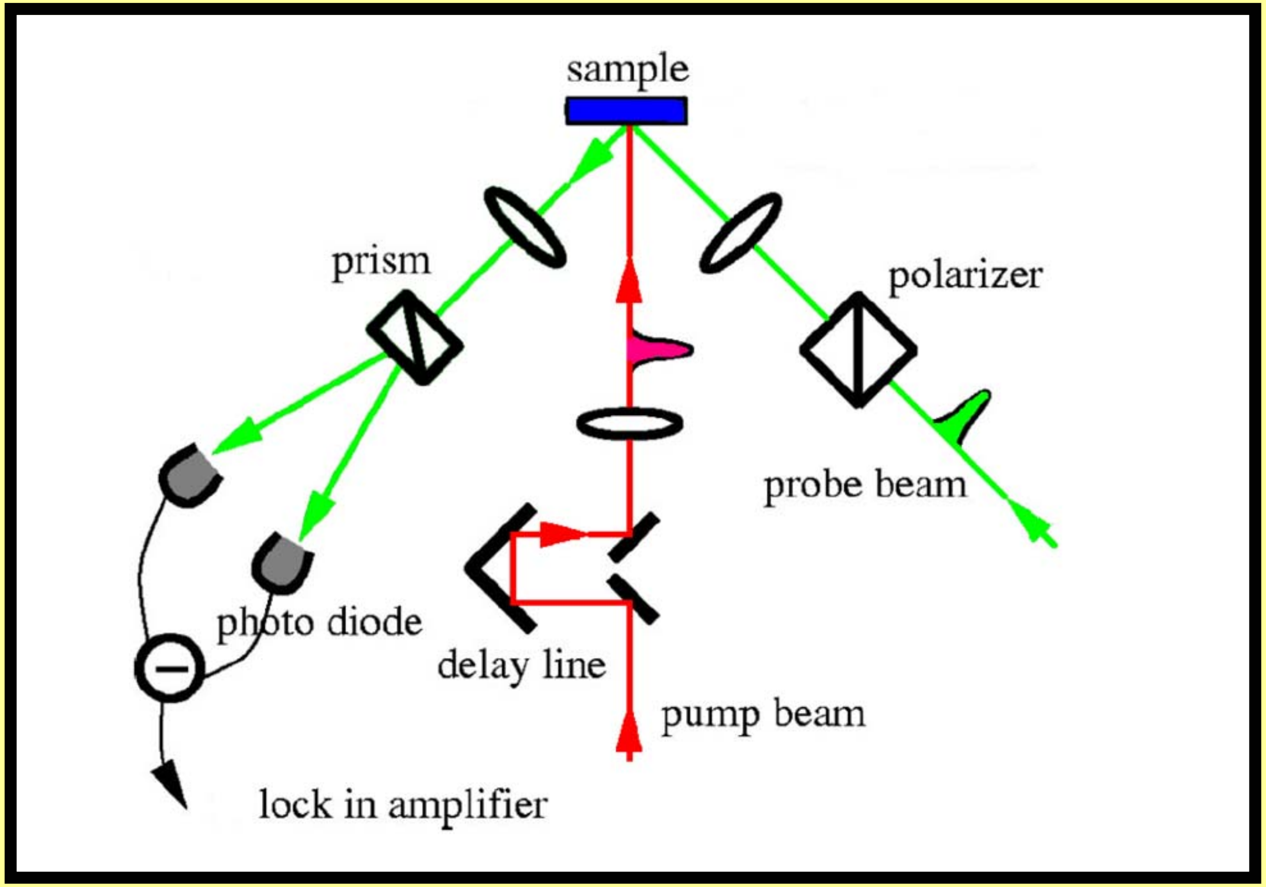


FIG. 2. Polar Kerr angle for almost normal incidence (θ=2°) and arbitrary photon energies ω within the visible spectrum in the case of fcc Ni(100) as a function of the polarization state of the incident light characterized by the azimuth ϑ_i and the ellipticity angle ϵ_i. The solid bold line represents the Kerr angle calculated for arbitrary linearly polarized light (ϵ_i=0). For ω=5 eV, for example, θ_K^{max} is at 0.3° and θ_K^{min} at −0.45°.

or: ultrafast time-resolved MOKE



Experimental set-up …

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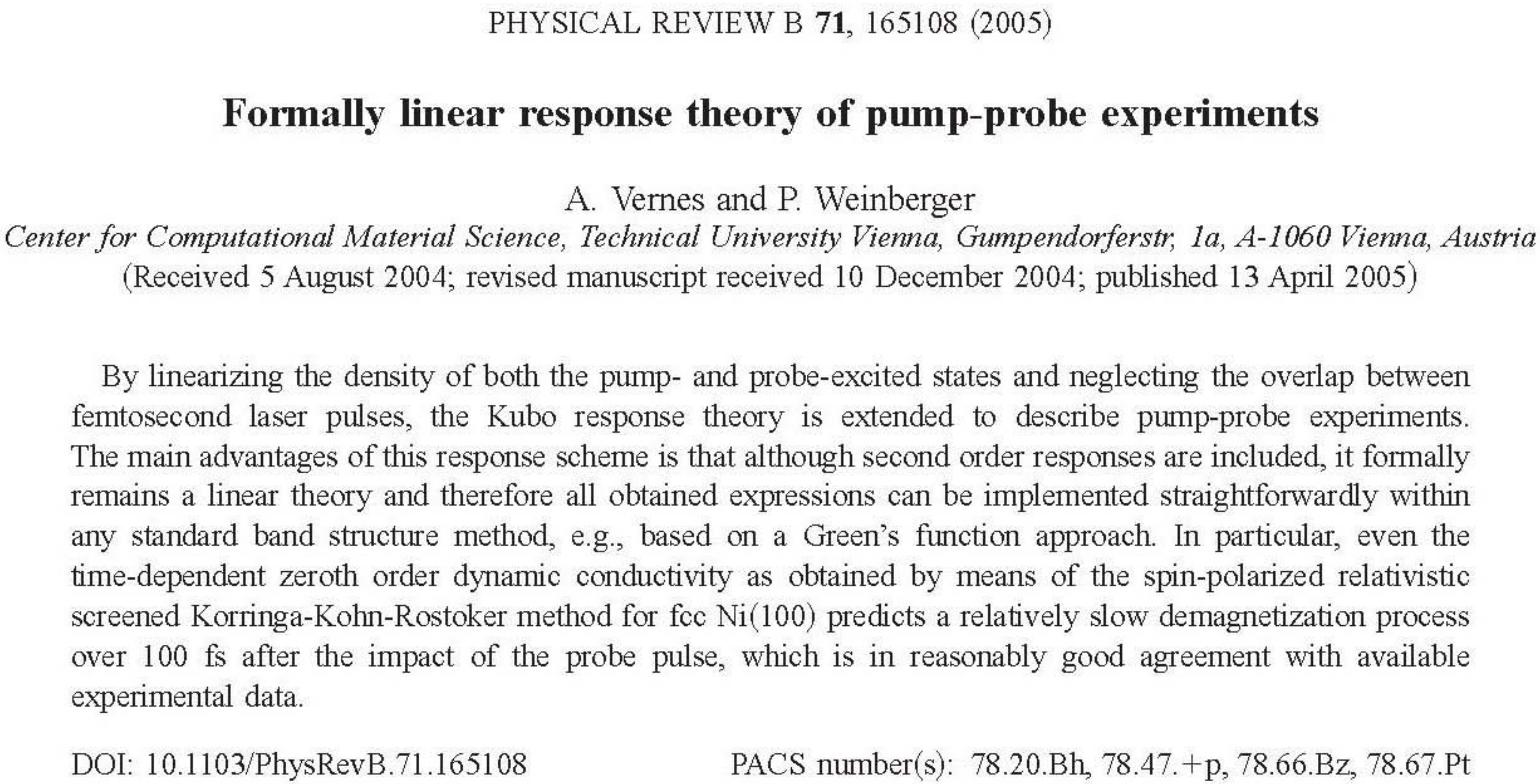
... with a new the theoretical approach



PHYSICAL REVIEW B **71**, 165108 (2005)

Formally linear response theory of pump-probe experiments

A. Vernes and P. Weinberger
Center for Computational Material Science, Technical University Vienna, Gumpendorferstr, 1a, A-1060 Vienna, Austria

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By linearizing the density of both the pump- and probe-excited states and neglecting the overlap between femtosecond laser pulses, the Kubo response theory is extended to describe pump-probe experiments. The main advantages of this response scheme is that although second order responses are included, it formally remains a linear theory and therefore all obtained expressions can be implemented straightforwardly within any standard band structure method, e.g., based on a Green's function approach. In particular, even the time-dependent zeroth order dynamic conductivity as obtained by means of the spin-polarized relativistic screened Korringa-Kohn-Rostoker method for fcc Ni(100) predicts a relatively slow demagnetization process over 100 fs after the impact of the probe pulse, which is in reasonably good agreement with available experimental data.

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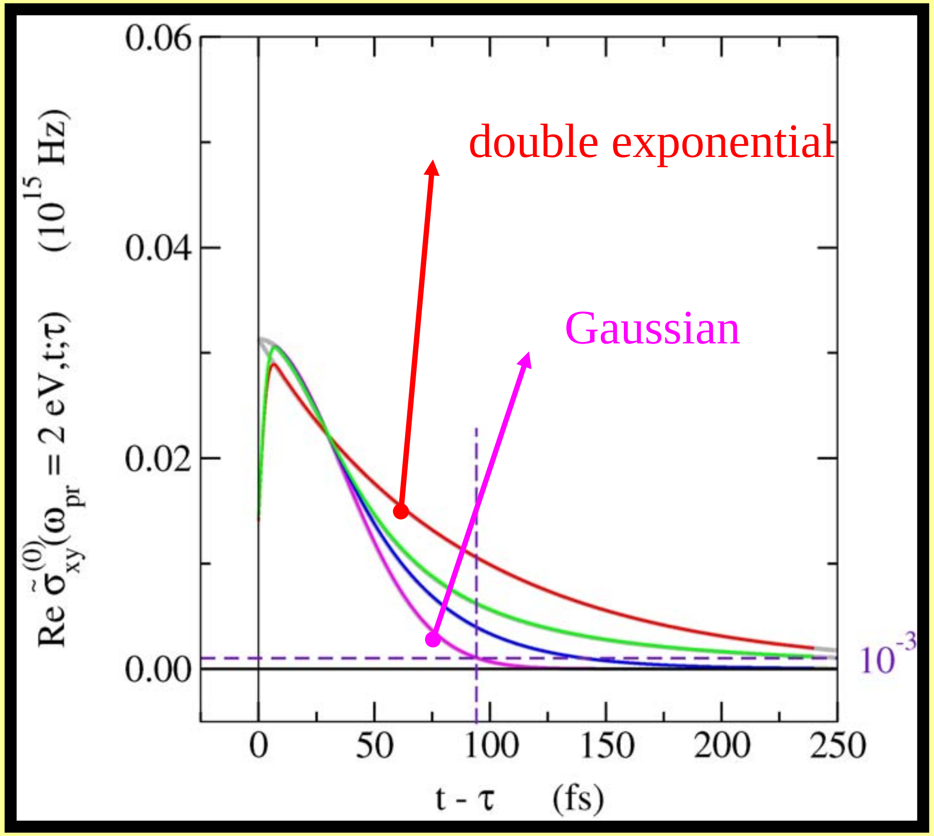
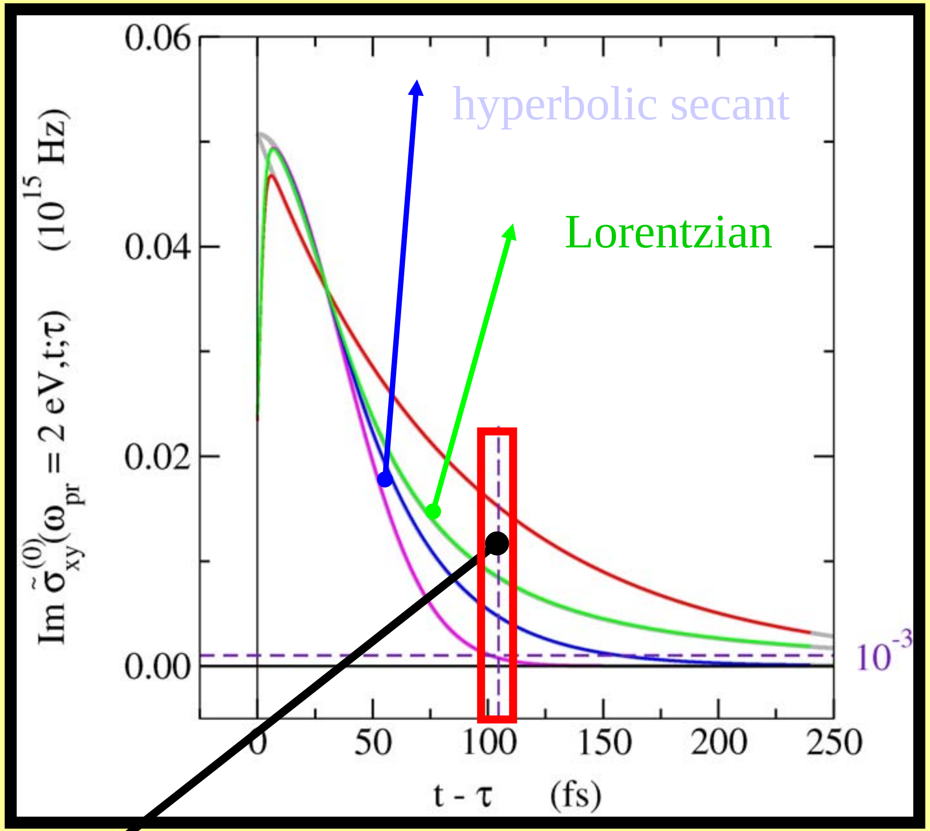
„Demagnetization time“ in Ni(100)





demagnetization time

a in particular interesting topic in which discussions and evaluations of perhaps „wrongly“ used terms such as „demagnetization“ would have been a great pleasure to have

So then: all the best and hopefully you get very soon to Cusco

and

.... Machu Picchu