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Structural and magnetic properties of fcc Pt/Fe(111) multilayers

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The structural, electronic, and magnetic properties of the 2Pt/5Fe/2Pt(111) system were investigated using the total energy full-potential linearized augmented-plane-wave method. The interplanar relaxation, determined by the atomic force approach, was found to be large between the nearest Pt–Fe and Fe–Fe distances, thus altering the electronic and magnetic properties of the system. We find an enhancement of the spin and orbital Fe magnetic moment ($2.44 \mu_B$) at the interface, and a large induced magnetic moment ($0.27 \mu_B$) at the interfacial Pt site, which is relatively short ranged. The effects of the interface on the contact hyperfine fields is evaluated: The (negative) core-polarization contribution is found to scale with the moment, but the valence contribution changes from negative in the interior to *positive* at the interface. The trend of the calculated layer-by-layer hyperfine fields agrees well with experiment. © 1996 American Institute of Physics. [S0021-8979(96)51408-X]

I. INTRODUCTION

Recent experiments have revealed that (Co,Fe)/(Pd,Pt) multilayers where the ferromagnetic layers are only a few monolayers thick show perpendicular magnetic anisotropy; combined with the large magneto-optical Kerr rotation, these multilayers appear to be promising candidates for high-density magneto-optical storage media.^{1,2} It is well known that Pd and Pt are considered to be “nearly magnetic” with anomalously large susceptibility. A small percentage (0.1 at. %) of Fe in bulk Pd induces magnetic moments on the surrounding Pd atoms giving rise to giant magnetic moments of $10 \mu_B$ per Fe atom. Similarly, Pd or Pt atoms at an Fe/Pd or Fe/Pt interface are strongly polarized by the Fe atoms.^{3,4} Magnetization measurements on Fe/Pt multilayers have shown an enhanced magnetization by about 15% over the bulk Fe value for Fe thicknesses larger than 12 Å.¹⁵ Recent magnetization and Mössbauer measurements⁶ on Fe/Pt multilayers have shown a strong enhancement of about 15% of the hyperfine field in the second Fe monolayer below the interface, which fades out in a damped oscillation within 6–10 Fe monolayers. A similar trend of the layer-by-layer hyperfine field was observed for the Fe/Pd multilayers.⁷

In order to understand the changes in electronic structure induced at the Fe/Pt interface, and their effects on modifying the atomic magnetic moments and hyperfine fields as compared to the corresponding bulk values, we have carried out a series of self-consistent spin-polarized local-spin-density total energy calculations with the use of the full-potential linearized augmented-plane-wave (FLAPW) method.⁸ Because of the high density of states at the Fermi level in Pt and the sensitivity of the number of the Fe majority spin holes on the local environment,³ structural changes should reflect themselves in the magnetic response of the Fe and Pd atoms near the interface and in the interlayer magnetic coupling. Thus a well determined atomic structure is always a prerequisite for obtaining reliable predictions of the electronic and magnetic properties—especially for those systems with strong overlayer–substrate hybridization.

II. COMPUTATIONAL METHOD AND RESULTS

In this article, the structural properties of the 2Pt/5Fe/2Pt(111) sandwich were determined using the atomic force approach,⁹ which yields a well-optimized atomic structure. The Pt/Fe(111) system is simulated by a slab consisting of five layer of Fe and two layers of Pt on each side. We have carried out two sets of electronic structure calculations with the in-plane lattice constant frozen to either that of bulk fcc Pt ($a_{\text{Pt}}=5.243$ a.u.) or to the value of $a=5.063$ a.u., which is about the average of the bulk Fe and Pt interatomic distances. The interplanar distances of *all* layers in the slab are adjusted efficiently according to the calculated forces.⁹ In the FLAPW approach, no shape approximations are made to the charge densities, potentials, and wave functions. The Kohn–Sham equations are solved self-consistently with an energy cutoff of 13 Ry for the variational plane-wave basis set. Within the muffin-tin spheres ($r_{\text{Fe}}=2.15$ a.u. and $r_{\text{Pt}}=2.45$ a.u.), lattice harmonics with angular momentum l up to 8 are employed to expand the charge density, potential, and wave functions. Summations over 18 k points in the $\frac{1}{12}$ irreducible 2D Brillouin zone are employed for k -space integrations. When the mean-root-square difference between the input and output charge and spin densities in the semirelativistic iterations is converged to better than $1.0 \times 10^{-4} e/(\text{a.u.})^3$, the spin–orbit coupling is invoked as a perturbation in a second variational way.¹⁰

Calculated results for the layer-by-layer vertical atomic positions, spin and orbital magnetic moments, and Fermi contact hyperfine fields broken down into valence ($H_{\text{CF},v}$) and core contributions $H_{\text{CF},c}$ are listed in Table I, for the two values of the in-plane lattice constant. The structure with the bulk fcc Pt in-plane lattice constant is found to be the most stable (lowest total energy). Large multilayer relaxations are found for the Pt–Fe and Fe–Fe interplanar distances which play an important role on the electronic and magnetic properties of the system. The interlayer Fe–Fe distance, 3.26 a.u. in the interior region and 3.23 a.u. in the interfacial region, is much smaller than the corresponding Pt–Pt interlayer dis-

TABLE I. Calculated layer-by-layer vertical atomic positions, z (in a.u.), spin and orbital magnetic moments, M and L_z (in μ_B), Fermi contact hyperfine fields H_{CF} broken down into valence ($H_{CF,v}$) and core ($H_{CF,c}$) contributions (in kG), and the ratios $H_{CF,c}/M$ in (kG/ μ_B) for Fe/Pt(111), for two values ($a=5.243$ a.u. and $a=5.063$ a.u.) of the in-plane lattice constant.

Atom	Fe(C)	Fe(I-1)	Fe(I)	Pt(I)	Pt(S)
$a=5.243$ a.u.					
z	0.00	3.26	6.49	10.03	14.27
M	2.07	2.11	2.44	0.27	0.05
L_z	0.04	0.07	0.12	0.08	0.01
H_{CF}	-315	-328	-275	...	...
$H_{CF,v}$	-30	-39	+60	...	...
$H_{CF,c}$	-285	-289	-335	...	...
$H_{CF,c}/M$	-137.7	-137.6	-137.6	...	...
$a=5.063$ a.u.					
z	0.00	3.30	6.57	10.19	14.52
M	1.95	2.00	2.32	0.25	0.07
L_z	0.04	0.05	0.10	0.06	0.02
H_{CF}	-308	-319	-282	...	...
$H_{CF,v}$	-39	-43	+36	...	...
$H_{CF,c}$	-269	-276	-318	...	...
$H_{CF,c}/M$	-137.9	-138.0	-137.4	...	...

tance of 4.28 a.u. in bulk fcc Pt. This is expected, of course, since the size of Fe atoms is much smaller than that of Pt atoms. Nevertheless, the Fe–Fe interatomic distance of 4.45 a.u. is still smaller by about 5% than that of 4.69 a.u. in bcc Fe. This shrinkage of the Fe–Fe distance can be attributed (i) to interfacial effects and (ii) to the failure of the local density approximation (LDA) imposed on the density functional

FIG. 1. Calculated charge and spin densities for Pt/Fe(111). Contours start from $\pm 1 \times 10^{-3} e/a.u.^3$ and increase successively by a factor of $\sqrt{2}$. Solid (dotted) lines in (b) denote the positive (negative) spin density, respectively.

FIG. 2. Calculated layer-by-layer density of states for Pt/Fe(111). Solid and dashed lines stand for majority and minority spin parts, respectively. Energies are measured with respect to the Fermi energy.

theory which is known for underestimating the lattice constants of 3d transition metals by about 3%.¹¹ Note that while there is, as expected, an expansion of the interlayer distances for the smaller (5.063 a.u.) in-plane lattice constant, the Fe–Fe interatomic distance remains almost intact (within 1%). For both sets of calculations, the Pt–Fe and Pt–Pt interatomic distances are 4.65 and 5.22 a.u., respectively. These results clearly indicate that metal atoms tend to preserve their volumes upon slight changes of local environment. Surprisingly, while the Pt–Fe distance shrinks by 6.5% compared to the average of the bond lengths in bulk Fe and Pt, no relaxation ($<1\%$) is found between the Pt–Pt layers, despite the presence of the surface and the interface on either side of the Pt layers.

The charge density of the Pt/Fe(111) is presented in Fig. 1(a). The charge density in the interfacial region between Fe and Pt is greater than that between Pt and Pt atoms, indicating a strong Fe–Pt bonding. The strong interfacial interaction between the magnetic Fe overlayer and the Pt substrate can be seen more clearly in Fig. 2, where the layer-by-layer density of states (DOS) of the majority and minority spin are plotted. The profile of the DOS of the interface Fe(I) atom differs substantially from that of the central Fe(C) atom and even from that of the subinterface Fe(I-1) atom. Strong hybridization can be seen especially in the energy range of -6 to -4 eV and around the Fermi level for the majority spin, and around $+1$ eV and below -4 eV for the minority spin. As a result, the 5d bands of the interface Pt(I) and even of the surface Pt(S) are spin polarized. Note also that the d bands of the interfacial Fe(I) and Pt(I) layers are broadened, corresponding to the strong overlayer–substrate hybridization.

The spin density of the Pt/Fe(111) is shown in Fig. 1(b). The solid (dashed) lines label the positive (negative) contours. We find that (i) the Fe layers adopt ferromagnetic coupling in the distorted fcc structure; (ii) the induced magneti

zation of the Pt(*I*) site is parallel to that of Fe; and (iii) the magnetic disturbance in the Pt layers is short ranged [the volume associated with the positive spin density around Pt(*S*) becomes very small]. As can be seen more quantitatively in Table I, the spin magnetic moments of the Fe(*C*) and Fe(*I-1*) are 2.07 and 2.11 μ_B , respectively. These values are well below the calculated magnetic moment of 2.25 μ_B for bcc bulk Fe using the experimental lattice constant ($a=5.425$ a.u.), but close to that of 2.06 μ_B obtained using the LDA optimized lattice constant ($a=5.225$ a.u.). By invoking the spin-orbit coupling, small orbital magnetic moments, 0.03 and 0.05 μ_B , are found for the Fe(*C*) and Fe(*I-1*), respectively. From the DOS curves in Fig. 2, we see that there is a smaller number of majority spin *d* holes for the Fe(*I*) atom compared to that for the other Fe atoms. As a result, there is an enhancement of the Fe(*I*) magnetic moment (2.44 μ_B), which indicates the important role of the Pt-Fe interfacial hybridization on the Fe magnetization. The orbital magnetic moment of the Fe(*I*) is also found to be large, 0.1 μ_B . It is desirable to have experimental measurements using the magnetic circular dichroism technique to verify our theoretical predictions. The magnetic perturbation in the Pt layers is a shorter range effect since the induced spin (orbital) moment decreases quickly from 0.27 (0.08) μ_B in the Pt(*I*) layer to 0.05 (0.01) μ_B in the surface Pt(*S*) layer. It is important to note that the magnetic moments listed in Table I for the two values of the lateral lattice constants differ markedly, even though the interatomic distances remain almost unchanged. Clearly, this shows that the magnetism in Pt/Fe(111) is very sensitive to the details of the geometry, and thus a well-optimized atomic structure appears to be very important.¹²

The magnetic hyperfine interaction, which describes the interaction of the electronic spin moment with the nuclear magnetic moment, provides an important tool for the study of interface magnetism. Table I presents the calculated layer-by-layer Fermi contact hyperfine fields broken down into valence and core contributions. As established for many magnetic systems,³ the core contribution (negative in sign) is proportional to the local Fe magnetic moment. The ratio of the core-hyperfine-field and the magnetic moment (137.5 kG/ μ_B) is independent of the value of the in-plane lattice constant, and is very close to that obtained for other systems, 130–140 kG/ μ_B .³ While our results for the Fe(*I*) layer do show an enhancement of the interfacial magnetic moment, the total calculated H_{CF} is smaller in magnitude (–275 kG) due to the large positive (+60 kG) valence contribution,

which, however, is localized to the interface; the subinterface valence contributions are again negative. Thus, as in previous calculations,³ we find that while the core contribution is dominant, the valence contribution is very sensitive to the local environment. The trend of the calculated layer-by-layer H_{CF} agrees well with recent Mössbauer experiments;⁶ i.e., the total H_{CF} is relatively smaller at the Fe(*I*), increases by 8.5% at the Fe(*I-1*), and then decreases again by 4% at the Fe(*C*). However, due to the small Fe-Fe interlayer distances found in our calculations, the results for the total hyperfine fields and magnetic moments are about 8%–10% smaller than the measured values.¹²

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