CEMS interface study of Fe(100)/Pd film structures

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The magnetic hyperfine fields B_{hf} near the interface in epitaxial Fe(100)/Pd thin film structures were analyzed using in-situ ^{57}Fe conversion electron Mössbauer spectroscopy. B_{hf} is enhanced by about 12% in the 2nd Fe monolayer and approaches the Fe bulk value after a few oscillations within 8–10 Fe monolayers. This oscillating behavior can be described by a superposition of an exponential short-range and an RKKY-like long-range exchange interaction.

Modern theoretical methods of band structure calculations [1] and the monolayer (ML) resolution achieved experimentally using the ^{57}Fe conversion electron Mössbauer spectroscopy (CEMS) have strongly stimulated the investigation of magnetic surfaces and interfaces in thin film systems [2,3]. So far, essentially the interfaces between Fe and W, Ag [4], Cr [5], Gd, Y [6] were investigated revealing more or less pronounced deviations of the Fe magnetic hyperfine (hf) field at the interface from its bulk value. These deviations are of short range in the case of Fe(100, 110)/Cr (~4 MLs) [5], but can also extend up to ~20 MLs into the Fe film in the case of Fe(110)/Gd [6], indicating a corresponding range of the magnetic exchange interactions. In this work, we report on a CEMS study of the hf field dependence near the interface in Fe(100)/Pd thin film structures.

The in-situ experiments were performed in an ultrahigh vacuum (UHV) system combining a CEMS chamber and a preparation chamber equipped with RHEED, LEED and AES for the characterization of the thin films. The setup for the CEMS measurements consisted of a 30 mCi (^{57}Co)Rh source outside the UHV irradiating the thin film sample under 75° angle of incidence (with respect to the sample normal) through a Be window. The conversion electrons were registered by a channeltron electron detector. Thin Fe(100)/Pd films of the composition as shown in fig. 1b were grown by evaporation in UHV on MgO(100) single crystalline substrates. The substrate temperatures for the growth of the 40 nm thick Cr buffer layer, the ^{56}Fe/^{57}Fe layers, and the 1.5 nm thick Pd layer were 680 °C, 190 °C and 20 °C, respectively. Sharp p(1 × 1) LEED patterns were obtained from the Cr and Fe layers. The RHEED patterns of the Cr and Fe layers showed narrow stripes lying on a semicircle, as is typical for smooth surfaces. Well-defined RHEED oscillations indicated layer-by-layer growth of the Fe layers. The 1st Pd layer grew on

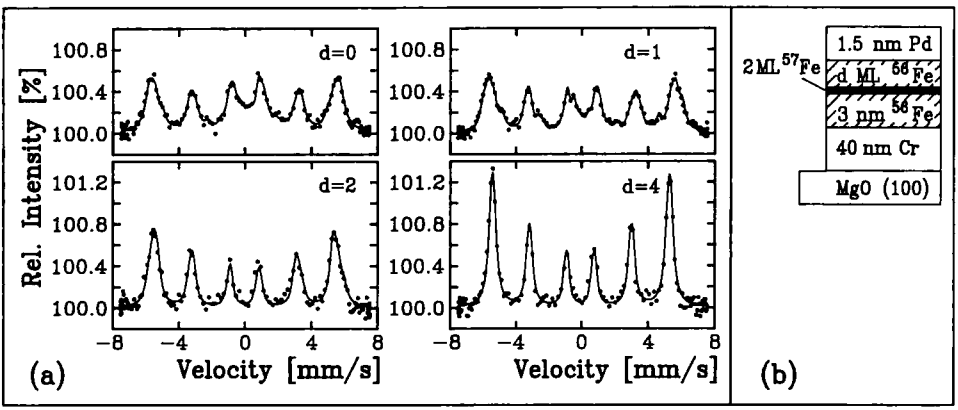

Fig. 1. (a) CEM spectra at $T = 300$ K of a 2 ML thick ^{57}Fe probe layer at different distances d[ML] from the Fe(100)/Pd interface. (b) Composition of the Fe/Pd thin film samples.

Fe pseudomorphically, while from the 2nd to 3rd Pd ML island growth started (Stranski–Krastanov growth).

By shifting the 2 ML thick ^{57}Fe probe layer (fig. 1(b)) within the ^{56}Fe films, the hf interactions can be measured layer by layer as a function of the distance from the Fe/Pd interface. Some CEM spectra taken in this way are shown in fig. 1(a). While for a distance $d = 4-6$ ML of the ^{57}Fe probe from the interface a bulk-like 6-line pattern with slightly broadened lines was obtained, the spectra for $d < 4$ ML clearly reveal additional structures. One cannot expect the ^{57}Fe probe layer to be confined exactly to 2 MLs. Due to mainly mono-atomic steps, it will rather be spread to 1 + 2 + 1 = 4 MLs. Therefore, assuming discrete hf field values for each Fe-ML near the Fe/Pd interface, we analyzed our CEM spectra by a superposition of 4 magnetically split subspectra. The analysis was performed in two alternative ways: (i) Using the sharpening method by integral transformations of Afanas'ev and Tsymbal [7], hf field distributions $P(B_{hf})$ were evaluated from the CEM spectra. Then, these $P(B_{hf})$ curves were fitted altogether in one computer run by a common set of discrete hf field values corresponding to the different Fe-MLs. (ii) The CEM spectra were fitted individually in the usual way by a superposition of four 6-line patterns with Lorentzian line shape. The results of procedure (ii) are shown in fig. 2(a) for the hf fields and in fig. 2(b) for the isomer shift values. Both procedures gave good quantitative agreement with respect to the hf fields, while the isomer shift data could be evaluated only using procedure (ii).

In the 2nd Fe-ML at the Fe/Pd interface, the hf field reveals a strong enhancement of about 12% compared to the Fe bulk value, fading out in a damped oscillation within 8–10 Fe-MLs. This effect is clearly larger than similar enhancements observed for the Fe/Cr, Fe/Y and Fe/Gd interfaces [6]. Recent ab initio FLAPW bandstructure calculations of the layer dependence of the hf field in a 1 ML Pd/11 ML Fe/1 ML Pd

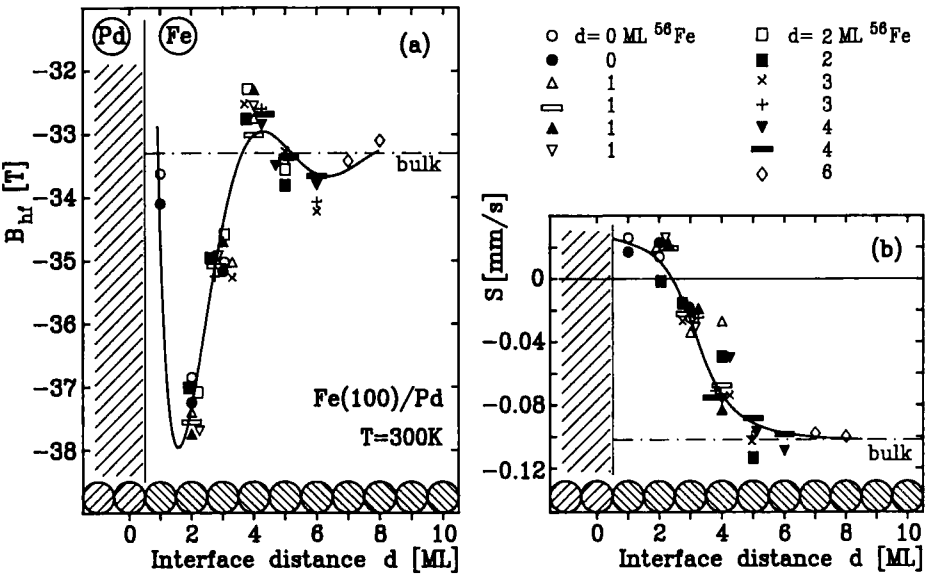

Fig. 2. Distance dependence with respect to the Fe(100)/Pd interface of: (a) The magnetic Fe hf field B_{hf}. For the fit (solid line) see text; (b) The isomer shift S. The solid line is only a guide to the eye. $T = 300$ K.

slab [8] could reproduce the same damped oscillation behavior and even showed a fairly good quantitative agreement with our experimental results.

As can be seen from fig. 2(a), one can fit the hf field data in another approach quite well by a superposition of a short-range exponential distance dependence and an RKKY like oscillating term:

$$B_{hf} = B_{bulk} + \alpha \cdot \exp(-d/\delta) + \beta \cdot \cos(2\pi d/\Lambda)/d^2. \quad (1)$$

The distance d is given in Fe-MLs with $d = 0.143$ nm for Fe(100). The RKKY term is adopted from refs. [9,10] and depends on d^{-2} (instead of d^{-3}) due to the two-dimensionality. For the free fit parameters we obtained, $B_{bulk} = -33.3$ T, $\alpha = -4.2$ T, $\delta = 1.65$ ML, $\beta = 12.2$ T · ML^2, and $\Lambda = 4.43$ ML. The exponential short-range term may be explained by the hybridization of the Fe-3d and the Pd-4d wave functions at the interface. The range parameter $\delta = 1.65$ ML = 0.24 nm is of the same size as was observed for the spin wave parameter b near the interface of Fe with other 4d metals like Fe(100)/Ag ($\delta = 1.5$ ML = 0.22 nm) [4] and Fe(110)/Y ($\delta = 1.3$ ML = 0.26 nm) [6]. These spin wave parameters, reflecting the local exchange interaction, also reveal an exponential distance dependence [16] near all Fe/M interfaces investigated so far [4,6].

The wavelength $\Lambda = 4.43$ ML = 0.633 nm of the oscillating term is large compared to typical RKKY wavelengths as observed, e.g. for Cu ($\lambda \approx 0.25$ nm).

This is strongly suggestive of the large periods found for the oscillating antiferro-/ferromagnetic interlayer coupling effect in, e.g. Fe/Cr/Fe systems [11]. Meanwhile, this effect is explained by an RKKY-type exchange interaction coupling the two Fe layers across the Cr interlayer [9,10]. By adopting this model to our experiments, we have to consider the so-called aliasing effect [12] which takes into account that the RKKY spin polarization of the conducting electrons is experimentally probed at discrete equidistant positions, i.e. MLs, only. Using the relationship [12] $\lambda = \Lambda/(n\Lambda - 1)$, with $n = 0, 1, 2, \ldots$, one obtains the real RKKY period $\lambda = 1.29$ ML $= 0.185$ nm ($n = 1$). From this, a Fermi vector in k-space of $k_F = \pi/\lambda = 1.70$ Å^{-1} is derived. When searching for such a k-vector on the Fermi surface of ferromagnetic Fe, one has to keep in mind the following conditions [9,10] which must be fulfilled in order to obtain appreciable oscillation amplitudes: (i) due to the (100) film orientation $\boldsymbol{k}_F$ must be parallel to the $\Gamma - H$ direction on the Fermi surface, (ii) the vector $2\,\boldsymbol{k}_F$ must link 2 points on the Fermi surface with antiparallel group velocities and small curvature ("stationary" points), and (iii) $\boldsymbol{k}_F$ must be perpendicular to the Fermi surface. Using these criteria and the Fermi surface of ferromagnetic Fe [13,14], one would expect the strongest oscillation for $2\,\boldsymbol{k}_F$ connecting the large Γ-centered spin-up electron surface along the $\Gamma - H$ direction. This would result in an oscillation wavelength $\lambda \approx 2$ ML which, however, is not observed in fig. 2(b). But usually, such short oscillations are wiped out by interface roughness. Our experimental result $k_F = 1.70$ Å^{-1}, however, fits quite well to the Fermi vector $k_F \approx 1.65$ Å^{-1} [14] belonging to the Γ-centered spin-down electron surface. There is also another Fermi vector $k_F \approx 1.92$ Å^{-1} (H-centered spin-up hole surface) which should give an additional oscillation, but with smaller amplitude due to the stronger curvature.

Summarizing, in view of the fact that eq. (1) represents an asymptotic approximation for $d \geq 5$ MLs [15] and that the Fe Fermi surface is rather complex, which may lead to a superposition of several spin polarization oscillations with different wavelengths and amplitudes, our simple formula eq. (1) describes the experimental results surprisingly well.

In principle, one would expect an oscillating behavior for the isomer shift in dependence of the interface distance as well, due to Friedel oscillations. However, within the scattering of the data points, such an effect could not be observed (fig. 2(b)). Rather, the isomer shift smoothly follows the trend, as expected from Fe–Pd alloys.

In conclusion, we suggest that the behavior of the magnetic hf field within the Fe film near the Fe(100)/Pd interface can be explained by an exponentially decreasing exchange interaction of relatively short range, mainly due to 3d–4d hybridization [16]. This interaction is superposed by an oscillating RKKY-type long-range exchange interaction mediated by conduction electrons.

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[15] J. Mathon, D.M. Edwards, R.B. Muniz and M.S. Phan, J. Magn. Magn. Mater. 104–107(1992)1721.
[16] Note added in proof: Meanwhile, we found a nearly linear relationship between the range parameter δ and the 3d-, 4d-, 5d-bandwidth of the contacting metal film. This supports our conclusion that the hybridization increasing from 3d to 5d elements should be responsible for the range of the exponential interaction term.