

Surface electronic properties of Fe(001) probed via hyperfine interactions

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The Fe(001) surface is relevant for many magnetic systems [1]. Its electronic structure was studied in the past using angle-resolved photoelectron spectroscopy (ARUPS) [1, and references therein] and scanning tunnelling microscopy and spectroscopy (STM/STS) [2]. ARUPS and STM measurements demonstrated surface electronic states, which are very sensitive to surface topography and contamination. As far as the magnetic properties are concerned, detailed data, including estimation of magnetic moments, have only been published for Fe(001) covered with MgO, while direct measurements of surface magnetic moments for a clean surface are not available. Details of surface magnetism come only from theoretical studies [3], which are consistent in predictions that the ground state magnetic moment of the surface atoms is strongly enhanced to about $2.9 \mu_B$ (as compared to $2.2 \mu_B$ in the bulk). While local measurements of magnetic moments with depth resolution are challenging, hyperfine magnetic fields were measured near the Fe(110) surface using Mössbauer spectroscopy [4] or its synchrotron counterpart, the nuclear resonant scattering of synchrotron radiation [5]. The measured hyperfine magnetic field (B_{hf}) for the Fe(110) surface at room temperature is slightly reduced compared to the bulk (31 T and 33 T, respectively), which is in fair agreement with *ab initio* calculations [6]. It should be noted that the slight reduction of B_{hf} corresponds to the 20% enhancement of the theoretical magnetic moment, from $2.2 \mu_B$ to $2.65 \mu_B$.

Here we present the experimental analysis of the hyperfine interactions at the Fe(001) surface. It is more open than Fe(110), and the contrast between the calculated surface behaviour of the hyperfine magnetic field and the magnetic moment is much stronger. We studied the surface of an epitaxial Fe(001) film on MgO(001). The 500 nm thick film was deposited using the non-Mössbauer ^{56}Fe isotope and treated as an iron single crystal to produce a clean and well-ordered surface, as confirmed with LEED, AES and STM

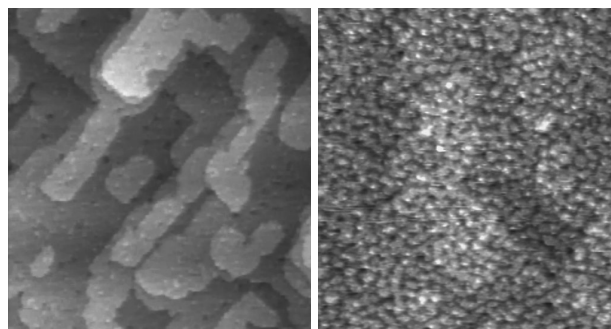


Figure 1 $100 \times 100 \text{ nm}^2$ STM topographic images of Fe(001) surface before (left) and after (right) deposition of 2 ML of iron at room temperature.

(Fig. 1a). On such a surface, a 2 ML ^{57}Fe probe layer was deposited at room temperature, to minimize $^{57}\text{Fe}/^{56}\text{Fe}$ intermixing. The low deposition temperature resulted in a change of the surface topography. The STM image (Fig. 1b) revealed that the 2 ML ^{57}Fe material was distributed over three different atomic levels of small (3 nm in average) terraces. The conversion electron Mössbauer spectroscopy (CEMS) result is shown in Fig. 2a. The spectrum was measured *in situ* under UHV conditions over several days. In an ideal case of a flat surface, the 2 ML ^{57}Fe probe would produce a two-component spectrum, with a surface and sub-surface hyperfine magnetic field of $B_{\text{hf}1} = 25.2$ T and $B_{\text{hf}2} = 39.5$ T, respectively (according to 0 K theory [3]). Instead, we observed a complex spectrum fitted with six components split in two groups. The green group (light, $B_{\text{hf}} = 33.2$ T, and dark, $B_{\text{hf}} = 36.1$ T) have a hyperfine magnetic field equal to or exceeding the bulk value and a negligible quadrupole interaction. We assign these components to sub-surface ^{57}Fe atoms that have at least the first coordination shell, as in the bulk. The second group includes three magnetically-split components with a strongly reduced B_{hf} (25.7 T, 23.3 T, 18.5 T, denoted as T, S and C, respectively), and a non-magnetic doublet. These components are attributed to low-coordinated surface atoms at different sites. The STM image clearly showed the small terraces, for which a significant number of atoms were located on steps and corners. The corresponding spectral component could be identified by a high quadrupole interaction for the components S (from the step atoms) and C (from the corner atoms). The component T showed only very small quadrupole interaction and therefore we assigned it to the atoms on terraces, with a symmetric distribution of the nearest neighbours. Further support for the above interpretation comes from additional CEMS experiments. Figure 2b shows the spectrum after covering the 2 ML ^{57}Fe probe layer with 2 ML of ^{56}Fe . The additional iron layer, nominally assuring a bulk-like coordination within the first and second coordination shell of the ^{57}Fe probe layer, almost fully restores the bulk-like CEMS spectrum. When the ^{57}Fe probe layer was reduced to 1 ML, the CEMS spectrum could be fitted within the same model (Fig. 2c) and only contributions of different spectral components were adjusted accordingly.

In summary, we performed surface analysis of the hyperfine fields at the Fe(001) surface, showing that the magnetic hyperfine field is reduced down to 25 T. This is in excellent agreement with theory, which parallelly predicts a strong enhancement of the surface magnetic moments [3].

References

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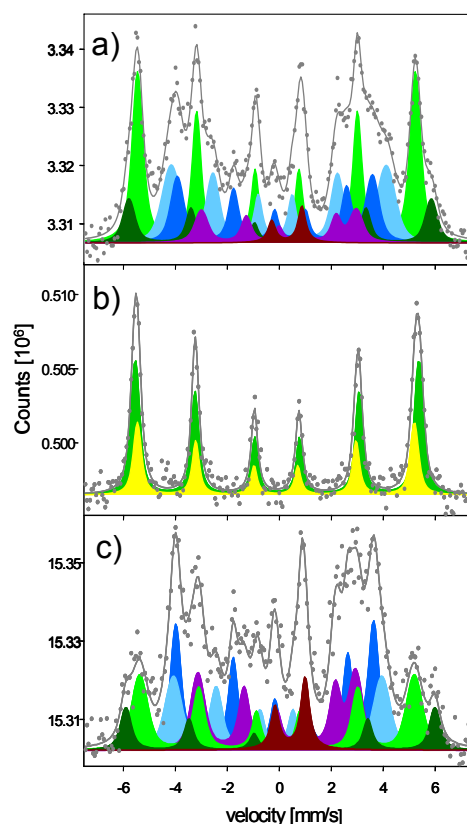


Figure 2 CEMS spectra for: (a) 2 ML ^{57}Fe probe layer on the $^{56}\text{Fe}(001)$ surface, (b) sample from (a) covered with a 2 ML ^{56}Fe layer, (c) 1 ML ^{57}Fe probe layer on the $^{56}\text{Fe}(001)$.