



**Experiment title:**  
Structure Analysis of the Fe/MgO/Fe(001) TMR junction

**Experiment number:**  
32-03-613  
(CRG)

**Beamline:**  
BM32

**Date of experiment:**  
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21

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Report:

We have investigated the geometric and compositional structure of the Fe/MgO interface in the Fe/MgO/Fe(001) system using surface x-ray diffraction. This particular trilayer system is widely known as a prototype for tunneling magneto resistance applications[1][2]. The experiment was intended to investigate the influence of oxygen exposure during growth of the top Fe layer on the MgO since this has considerable effect on the expected tunneling magneto-resistance (TMR) ratio[3].

In the experiment, MgO films with a thickness of 2 and 4 monolayers were prepared by thermal evaporation on a clean Fe(100) single crystal surface, from a MgO rod. The Fe layer was then deposited either in UHV or at  $10^{-7}$  mbar  $O_2$  ambient pressure. In the latter case, the oxygen was turned off after the first 0,4 ML was grown and subsequent Fe was deposited in UHV.

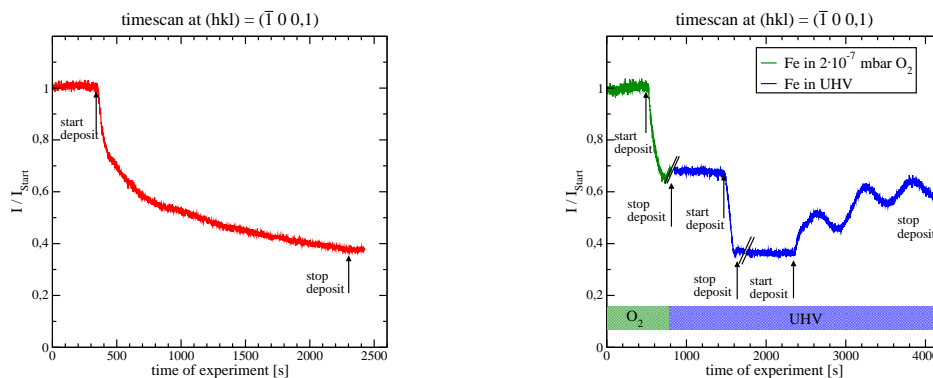


Figure 1: timescan at  $(hkl) = (\bar{1}00, 1)$  for Fe deposition under UHV conditions (left) and with oxygen backfilling (right)

During Fe deposition the antiphase (100) CTR-intensity was recorded as a function of the deposition time. Figure 1 shows the different results for UHV deposition and for initial FeO deposition. Epitaxial layer by layer growth can only be observed using oxygen atmosphere in the early stages.

For a detailed analysis of the interface formation, SXRD measurements were carried out on samples with Fe coverages in the range between 0,3 *ML* and 8 *ML*. The structure factor amplitude of several integer CTRs was measured for each sample. One representative result is shown in Figure 2 together with a high quality fit (line) of the measured CTR data (points). In this particular example a total of 2,5 *ML* Fe was deposited on MgO, with oxygen exposure for the first 0,4 *ML*. The detailed structure model used in this fit is shown in Figure 3.

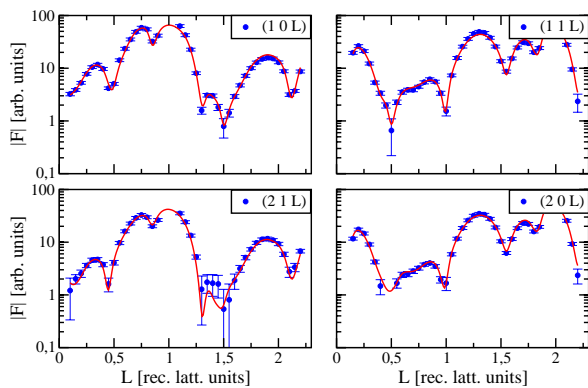


Figure 2: CTR data for 2,1 *ML* Fe/0,4 *ML* FeO/2,3 *ML* MgO

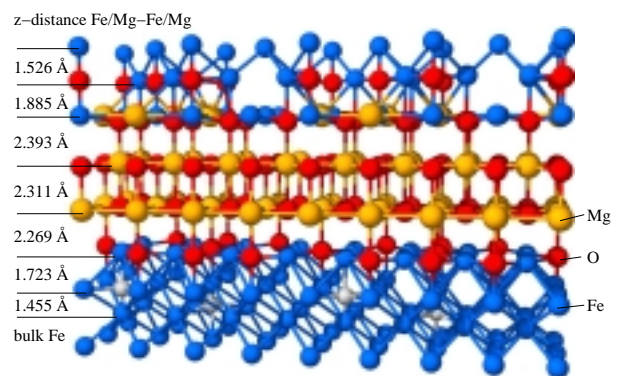


Figure 3: Structure model of the Fe/MgO/Fe interface

The bottom interface includes the  $FeO_{0,6}$  layer known from earlier experiments[4] with the first *MgO* layer 2,27 Å above, and an expanded (10%) interlayer spacing between the two *MgO* layers. At the top Fe/*MgO* interface a  $Fe_{0,7}Mg_{0,3}O_{0,8}$  layer is found 2.39 Å above the *MgO*. The mixture of Fe and Mg in this layer can be attributed to *MgO* islands since 2,3 *ML* *MgO* were deposited.

In contrast, for growth performed under UHV conditions, only a small fraction of Fe grows in registry. Albeit a  $FeO_{0,3}$  interface is formed, this does not extend over the whole surface and no epitaxial growth is possible. Our results may have important consequences on the theoretical interpretation of the actually observed tunneling magnetoresistance in such Fe/*MgO*/Fe junctions[5].

## References

- [1] W. H. Butler et al., Phys. Rev. B **63** (2000) 054416
- [2] J. Mathon et al., Phys. Rev. B **63** (2000) 220403
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- [5] S. Yuasa et al., Nature Materials **3** (2004) 868