Atomic Structure of EuO/Si Spin Contact for Spintronic Applications

Control and manipulation of the spin of conduction electrons in industrial semiconductors such as silicon are suggested as an operating principle for a new generation of spintronic devices [1]. Injection of spin polarization into Si from ferromagnetic metals is ineffective due to impedance mismatch suggesting the use of all-semiconductor heterostructures. The ferromagnetic semiconductor EuO is a prospective spin injector into silicon. The growth of a EuO/Si spin contact is a long-standing problem [2-4]. Recently, we achieved a direct epitaxial stabilization of EuO on Si [5, 6]. The structural coupling between EuO and Si is established with X-ray techniques [7]. The application of EuO as a spin injector into silicon is justified by SX-ARPES analysis of the band structure at the EuO/Si contact [8]. However, engineering of an efficient spin contact requires a detailed knowledge of the atomic structure of the EuO/Si interface.

The goal of the project was to map the layer-by-layer atomic structure in the vicinity of the buried EuO/Si interface, with special emphasis on potential transformations of 1×2 and 1×5 Eu submonolayers used as templates for the growth. With molecular beam epitaxy we synthesized a number of samples: different reconstructions of Eu on Si, products of their chemical reaction with oxygen, EuO/Si films with the thickness ranging from 1 monolayer (ML) of EuO to 400 Å. To produce an atomic model of the EuO/Si interface we applied the CTR method while the structure of relatively thick epitaxial layers (20-400 Å) was analysed with RSM.

The experiments were carried out at the beamline BM25 (experimental hatch 2 branch B) employing the surface diffraction setup. Maximal values of the momentum transfer were achieved with radiation energy of 17 keV. The intensity of CTR was measured in the geometry "2D+3S" of the diffractometer with a constant grazing angle of 0.5 deg. To improve the integration of the scattered intensity we modified the standard measurement scheme of beamline BM25: the 2D detector Maxipix was installed on the detector arm instead of the 1D detector. The slits were fully open for collection of the rod profile spectrum. The measurements of any given *hkl* rod were carried out in the standard mode: for each value of *l* the raw data were read from the 2D detector, peak regions found for each image, background estimated and subtracted, the intensity integrated in the direct space (in analogy with [9, 10]). More advanced approaches for collection and initial analysis of the data [11] with integration in the reciprocal space could not be applied due to technical restrictions of the BM25 beamline.

A number of rods -11l, 22l, 20l, 31l, 33l as well as their mirror counterparts – were recorded for each sample studied. It turned out that the rods 11l were the most informative as well as quite similar for 1 ML EuO and Eu reconstructions 1×2 and 1×5. We found the rods to be asymmetric (Figure 1) with a shoulder at the node 111 and a steep rise at the node 113. Such form of rods is a characteristic feature of the system substrate + surface atomic layer (Eu) with some displacement from the regular positions. According to our preliminary estimates this displacement is about -6% ÷ -10% for both 1×2 and 1×5 reconstructions. We also noticed that the structure factor for the 1×5 reconstruction is larger. Such effect is similar to the influence of the surface roughness. However, it can be also attributed to different coverage of the surface by Eu atoms for the two reconstructions.



Figure 1

Oxidation of the reconstructions does not induce significant changes of the rod profiles. It certifies that the atomic structure of the Eu-Si interface is conserved. According to our data oxygen does not react with the surface Si atoms. Instead, it probably forms bonds with the surface Eu atoms without significant changes to the Eu-Si distance. The changes in the RHEED images, observed *in situ* when the reconstructions are oxidized, are probably caused by lateral reorganization of the Eu layer. The CTR data for the oxidized Eu-Si layer are in sharp contrast to the common model for the Sr-Si system, where oxygen atoms are assumed to be incorporated between Sr and Si with formation of Sr-O-Si bonds [12-14]. The best way forward to analyse the influence of oxygen on the reconstructions would be wide in-plane reciprocal space mapping (h, k map at l=0.5). However, the restrictions of the beamline BM25 on the bending magnet prevented us from doing the experiment.



Figure 2

Samples of 1 ML of EuO on the reconstructions 1×2 and 1×5 demonstrate a more complex form of CTR (Figure 2). Remarkably, the profile does not depend noticeably on the type of the reconstruction. A qualitative analysis of such rod profiles is very difficult: a theoretical simulation of the experimental curves is necessary. We are planning such a study based on detailed atomic models for the interface, resulting in quantitative estimates.

The crystal quality of the epitaxial structures with thicknesses ranging from 20 Å to 400 Å was estimated according to RSM at the node 113. Figures 3a and 3b clearly show the node 113 from the Si substrate and the epitaxial layer of EuO, as well as a fragment of the 11*l* rod. The structure of the epitaxial layer can be extracted from the corresponding scattering intensity profile. The position and form of the EuO node suggest that the thick epitaxial layer of EuO is fully relaxed and exhibits a sufficiently high structural quality.





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