TEM investigation of electron beam evaporated epitaxial Fe_3Si films on GaAs (100) substrates

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The interest in iron silicide on the metal-rich side of the phase diagram is based on prospective applications in the field of electronics, thermoelectrics, optoelectronics and magnetism. Fe_3Si is a representative of the Heusler family that is known as a candidate for a high spin-polarization. For the epitaxial growth of the Fe_3Si films on substrates mainly the extensive molecular beam epitaxial (MBE) technique or (more unusually) magnetron sputtering has been used (see e.g. [1]).

We deposited epitaxial Fe_3Si films on GaAs(100) substrates by electron beam evaporation in an ultrahigh vacuum chamber. Beside the lower costs this technique allows the production of magnetic tunnel junctions in the most used technological approach. These tunnel junctions are important for applications as well as for measurements of the magnetic properties of the films.

To determine the orientation relation between GaAs substrate and Fe_3Si film by transmission electron microscopy cross section specimens were prepared by the conventional face-to-face technique with grinding and Ar^+ ion milling. For the investigations we used a TEM/STEM Tecnai F30 ST. Figure 1 shows an overview of the cross section and the corresponding measured nanobeam diffraction patterns. The patterns show the basic correlation of the substrate (GaAs) and the Fe_3Si lattices. Both patterns can be indexed assuming the zone axis [0 -1 -1] as the viewing direction in the cross section. As expected, the [100] direction lies in the diffraction plane, perpendicular to the zone axis and characterizing the surface normal of the substrate as well as of the film, indicating an epitaxial orientation relation.

The second goal was the characterization of the interface between substrate and Fe_3Si layer in more detail. This was done using the high resolution TEM supported by image simulations with JEMS [2]. Different super cells of the interface region have been created with different distances free of atoms between the GaAs substrate and the Fe_3Si layer as well as different shifts between the atomic columns in the interface plane. Basing on this matrix possible HRTEM pictures have been calculated with a variation of defocus and specimen thickness. The best fit of the measured images of the undisturbed interface region could be obtained with the assumption of a super cell with continuation of the GaAs crystal lattice into the iron silicide by replacing of the As positions with Si atoms (see Figure 2).

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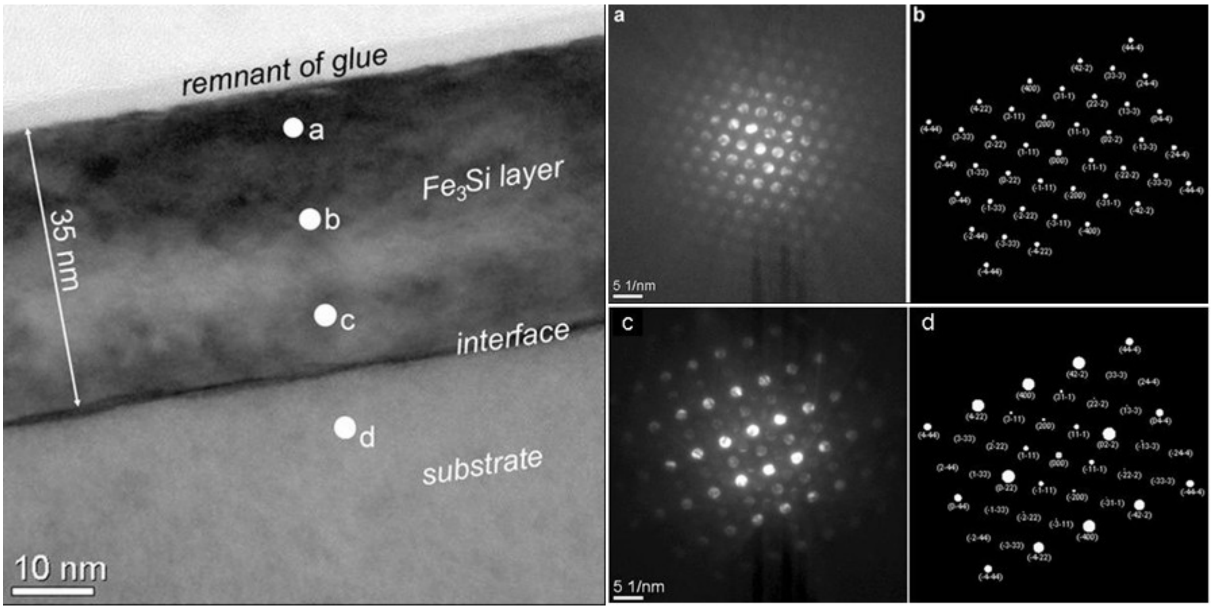

Figure 1. Left side: Overview of a cross section with the positions on which the diffraction patterns were recorded. Right side: Nanobeam diffraction patterns with indexing: a) Substrate (region d on the right), b) Indexing for GaAs, zone axis [0-1-1], c) Overlay of the Patterns from regions a, b, c on the right, d) Indexing for Fe_3Si, zone axis [0-1-1],.

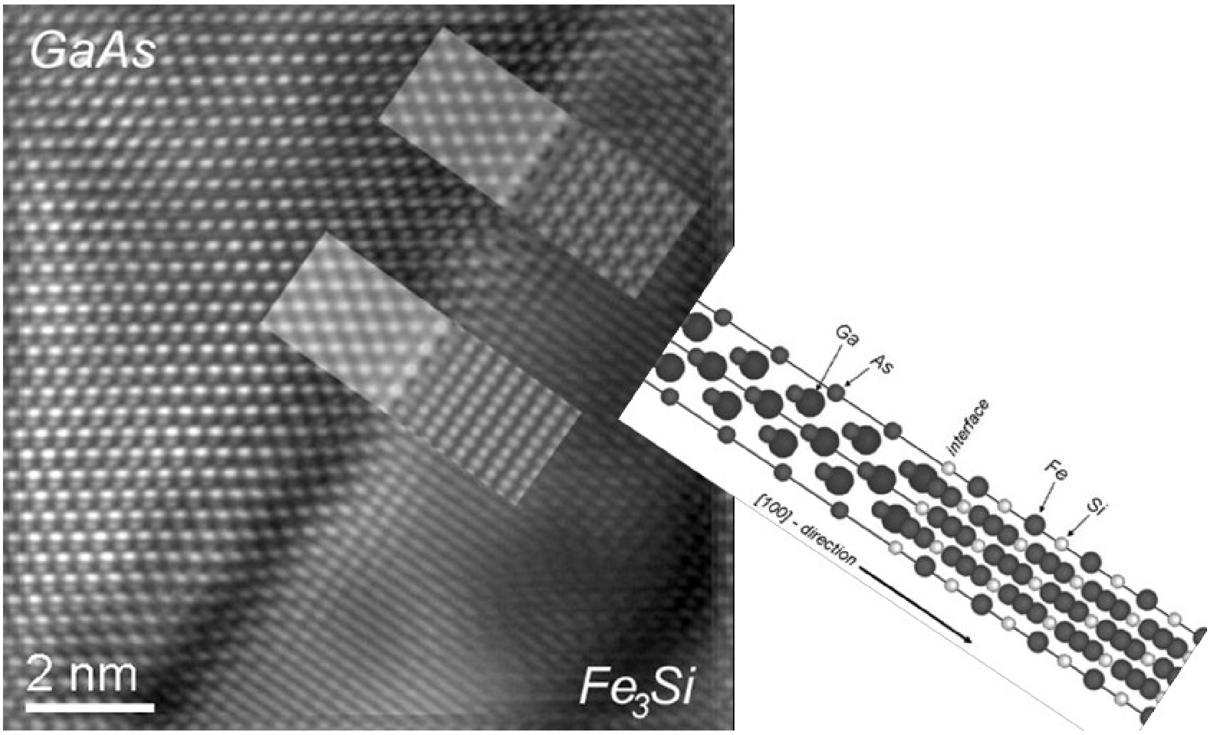

Figure 2. HRTEM image of the interface between GaAs and Fe_3Si with inserted super cells calculated by JEMS with defocus – 2 nm, thickness 20.8 nm (top) and -2 nm, 16.0 nm (middle), respectively. Right side: Sketch of the super cell used for the calculations.