Thin Films and Coatings

MS.5.P145
Substrate strain measurements by convergent beam electron diffraction in epitaxially grown $Ba(Fe_{1-x}Co_x)_2As_2$ thin films

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Keywords: CBED, strain, thin film, superconductivity

Superconductivity and antiferromagnetism in ironpnictides are affected by chemical doping, stress or strain [1]. Thin film growth on a substrate with slightly different lattice parameters is one way to produce an in-plane strain [2]. Epitaxial $Ba(Fe_{1-x}Co_x)_2As_2$ (Ba122) thin films with x = 0.06 have been produced by pulsed laser deposition (PLD) on a $MgAl_2O_4$ spinel substrate with a 30 nm thick iron buffer layer, also produced by PLD. Because of a small lattice mismatch between unstrained bulk substrate ($d_{100}/4$ = 0.2021 nm), bulk iron (d_{110} = 0.2027 nm) and bulk Ba122 ($d_{100}/2$ = 0.198 nm) strain is introduced to the 60 nm thick Ba122 layer. In addition, on top of the first Ba122 layer a second very thin iron layer (7 nm) and a 55 nm thick Ba122 layer were deposited by PLD (Fig. 1). TEM lamellae were cut by the focused ion beam technique. X-ray diffraction as well as electron diffraction experiments confirmed that the layers were epitaxially grown on the substrate.

It is a major task to clarify, whether the strain state in the Ba122 layer is dictated by the substrate or rather by the iron buffer layer in between. To provide an answer, the convergent beam electron diffraction (CBED) technique [3] in the transmission electron microscope (TEM) with an acceleration voltage of 200 kV was applied.

With the beam close to the spinel [1 12 0] direction Kossel patterns from the substrate were recorded at different distances to the spinel/iron interface. Approaching the spinel/iron interface, major changes are observed (Fig. 2): The higher order Laue zone (HOLZ) lines corresponding to lattice planes with a normal containing a [001] component start to split. HOLZ line splitting can be explained by the bending of the thin TEM lamella due to strain relaxation [4]. However, almost no splitting is observed for HOLZ lines if the corresponding lattice plane normal is close to the [010] direction. Therefore, only the latter HOLZ lines are used for analysis by comparing their change in position with Kossel patterns dynamically simulated with the software TEMStrain developed by A. Morawiec [5]. Two different assumptions are made in the simulation: The first "thin film" assumption considers the specimen as a completely relaxed (very thin) TEM lamella yielding a stress only along the [100] spinel direction. The second assumption considers the TEM lamella as an unrelaxed bulk specimen. Due to specimen symmetry in this case it is assumed that the stresses in the [100] and [010] direction are the same. For both assumptions there are no additional stress components. The change of the distance ratio L1/L2 (Fig. 2) in the measured patterns (as a function of the distance from the spinel/iron interface) and in the simulated patterns (as a function of the in-plane lattice parameter of spinel) is plotted in Fig. 3. To interpret the result, it is necessary to point to the lattice parameter where the simulated ratio L1/L2 is the same as the measured one (dotted lines in Fig. 3). Qualitatively both assumptions show an increase of the in-plane lattice parameters in spinel. Regarding the lattice parameters of the unstrained bulk materials it may be concluded that the 30 nm thick iron layer is not thin enough to adopt lattice parameters somewhere between the spinel substrate and Ba122. As a consequence, the strain in Ba122 is mainly determined by the iron buffer layer and not by the substrate.

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Support of this work by the German Research Foundation (DFG) within the framework of the Research Training Group 1621 is gratefully acknowledged.

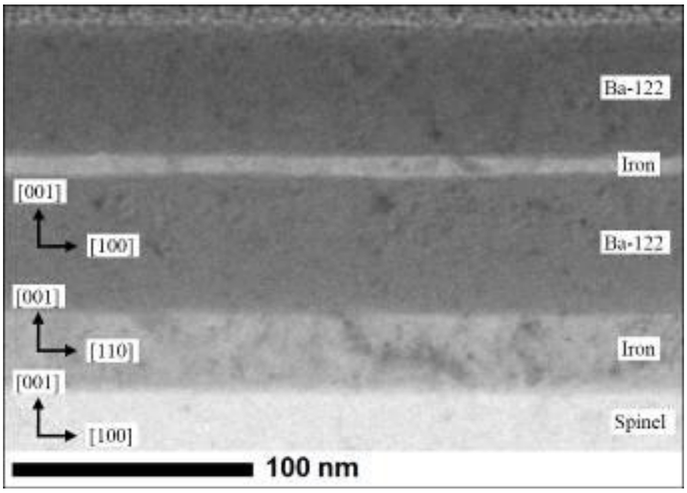

Figure 1. TEM bright field micrograph of the thin film. Beam is parallel to the [010] direction of spinel.

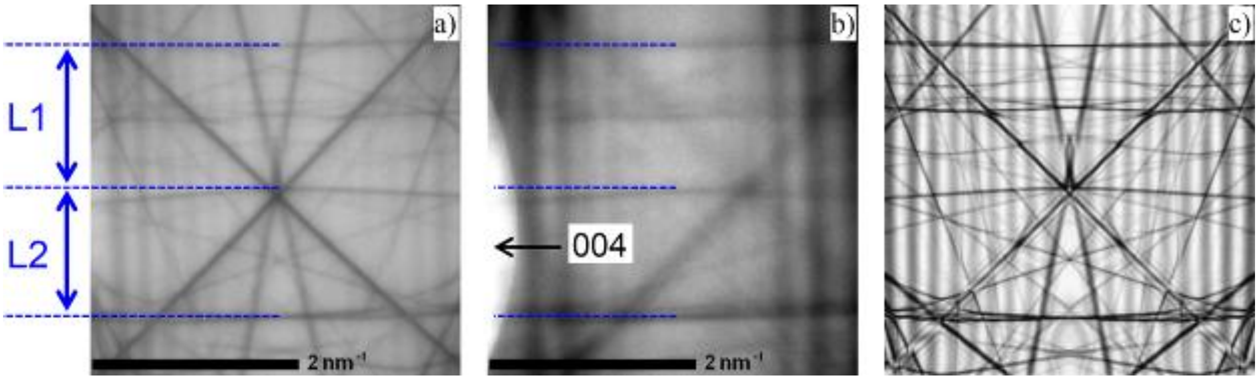

Figure 2. a) Kossel pattern taken 800 nm from the spinel/iron interface, b) Kossel pattern taken 50 nm from the spinel/iron interface and c) dynamically simulated pattern assuming unstrained spinel.

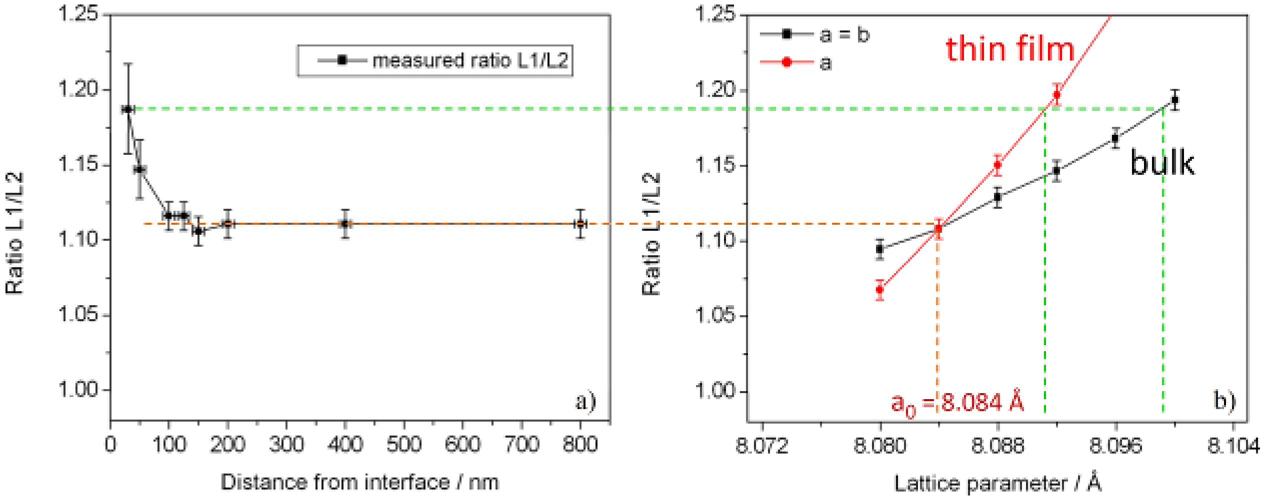

Figure 3. a) L1/L2 ratio of recorded Kossel patterns in spinel as a function of distance from the spinel/iron interface and b) L1/L2 ratio of simulated Kossel patterns as a function of the in-plane lattice parameter of spinel (variation of a = b in the "bulk" and variation of a in the "thin film" assumption).