Strain field measurement at inversion domain boundaries of indium-doped zinc oxide

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Zinc oxide (ZnO) is probably the most widely used oxide in advanced materials and industrial chemicals; it plays an outstanding role in many aspects of science and engineering owing to its unique optical, semiconducting, piezoelectric and catalytic properties [1]. To tailor the properties, ZnO is commonly doped with other oxides. Small additions of trivalent ions of e.g. indium and iron to ZnO result in the formation of domain structures where the polar *c* axis is inverted at the domain boundaries [2]. The inversion domain boundaries (IDBs) can not be studied by X-ray diffraction; however, they are ideal objects for characterization by TEM methods. In this contribution we investigate the two-dimensional strain field from single HR-TEM images. To obtain highly precise atom positions, images were acquired with the latest generation of electron microscopes equipped with aberration correctors at the Ernst Ruska-Center, FZ Jülich.

The material was produced by sintering powders of ZnO and In_2O_3 in 30 to 1 molar ratio. An image taken at the 'bright-atom' contrast condition (C_s = -12.7 µm, Δf = 5.9 nm) close to the edge of a thinned crystal is shown in Fig. 1. Inversion domains 1 to 4 and an IDB parallel to the basal plane (b-IDB) and two IDBs parallel to pyramidal planes (p-IDBs) of type $\{2\bar{1}\,\bar{1}\,3\}$ are observed. The lattice image contains atom columns with spacings of 2.60 Å and 1.62 Å from lattice planes (0002) and $(2\bar{1}\,\bar{1}\,0)$ of ZnO, respectively, and it could be shown that the bright dots coincide with the position of metal columns only. For strain analysis, the atom column positions (x_1, x_2) were defined by the 'peak-finding' method (Dali program [3]). A region in domain 1 was chosen as reference lattice and the displacement field with components u_1 (horizontal) and u_2 (vertical) was determined from the differences of vectors (x_1, x_2) and the nodes of the reference lattice. The strain field was calculated from the displacements [3] and the 2D tensor components ε_{11}, ε_{22}, ε_{12} and ω_{21} are shown in Fig. 2 in false colour (grey scale) representation. It can be seen that the strain field inside the ZnO domains is close to zero. The component ε_{11} indicates a maximum dilatation of (4 ± 0.8) %·located at the two p-IDBs whereas the component ε_{22} is very small at the p-IDBs and shows a jump-like strain behavior at the b-IDB. The strain component ε_{12} displays the shear of the lattice concentrated again at the p-IDBs, with same absolute values but opposite shear directions. This is the result of mirror symmetry of the displacements represented by a vertical line through the meeting point of the two p-IDBs. Finally, the rotation component ω_{21} yields the tilt angle of the lattice at the p-IDBs with maximum of 1.7 ± 0.3º [4].

1. Ü. Özgür, Ya. I. Alivov, C. Liu, et al., J. Appl. Phys. 98 (2005) 041301.
2. C. Li, Y. Bando et al., J. Solid State Chem. 139 (1998) 347.
3. A. Rosenauer, S. Kaiser, T. Reisinger, J. Zweck, W. Gebhardt & D. Gerthsen, Optik 102 (1996) 63.
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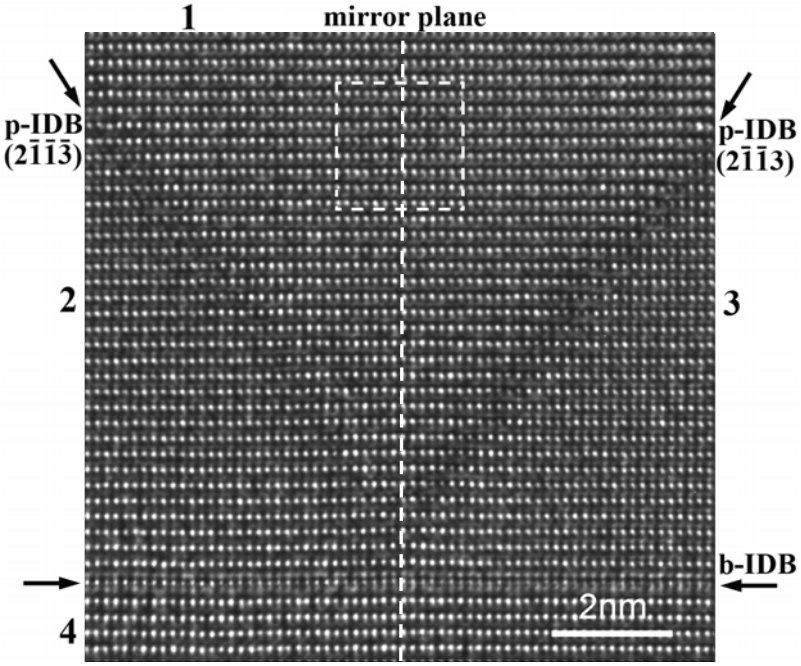

Figure 1. HR-TEM image of inversion domains in ZnO with additions of In_2O_3 at bright atom contrast condition in [1$\bar{1}$00] direction. Reference lattice is marked by dashed square.

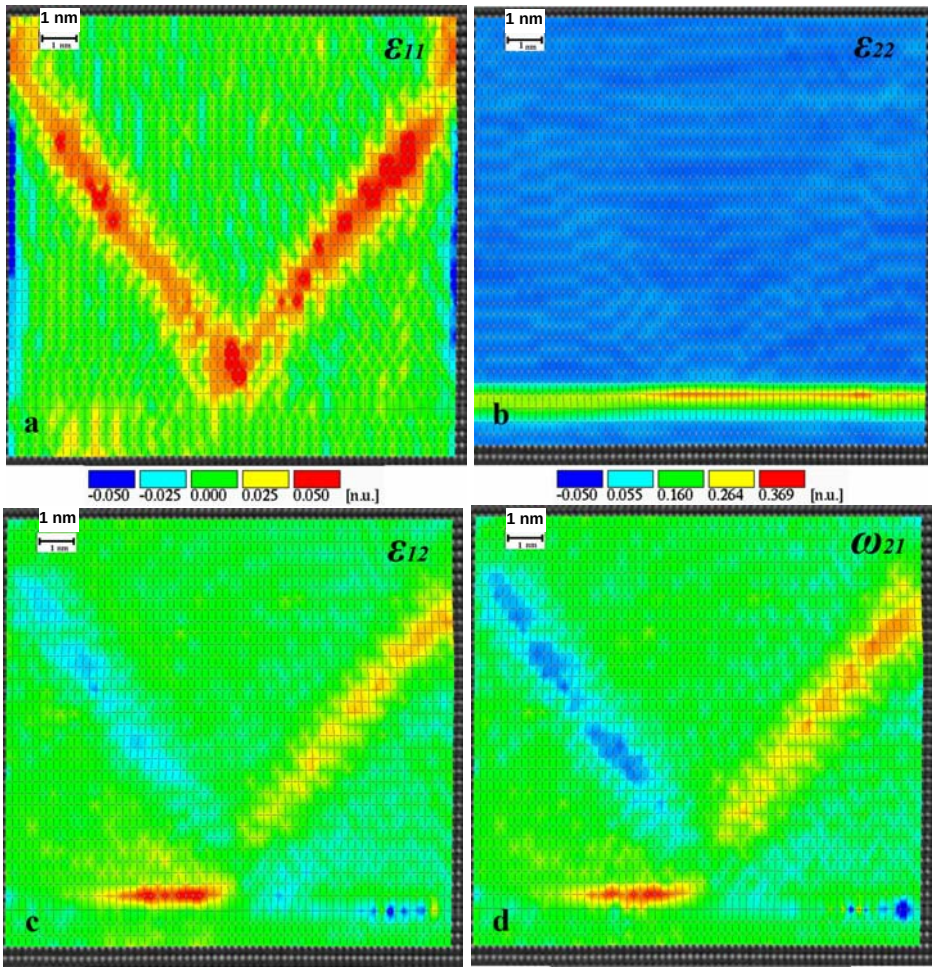

Figure 2. Components ε_{ij} of the strain tensor and the rotation component ω_{21} showing the distortion concentrated at the two p-IDBs.

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