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Structural defects in ZnO thin films grown by atomic layer deposition at low temperatures

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In epitaxial thin films, stacking faults (SF's) on a crystal play an important role due their interaction with dislocations. Dislocations often divide into partial dislocations with the formation of a stacking fault connecting them [1]. On the synthesized thin films SFs parallel to the samples' interface can be seen not only on the substrate but also in the film where they appear to be more common. These parallel defects can be easily spotted when acquiring dark-field images. As the thin films and images differ in thickness and size, using the number of individual defects observed on a single image can be misleading. In a way of normalizing results SF's are counted in several DF images, considering the area of the film that is enclosed, to latter extrapolated these values for comparison. In this work, ZnO layers have been grown at low temperatures, 100, 150, and 200°C by atomic layer deposition (ALD). By using dark field imaging, basal and prismatic defects have been characterized and quantified. The films grown at the lower temperature shows the presence of grains along the film while in the case of the next two samples there is an increase of basal and prismatic defects. These dislocation density values approximately 2×10^{11} cm^{-2} are on the range of those reported in the literature for wurtzite structures such as GaN and ZnO [2-3]. Due to the presence of prismatic and basal stacking faults mainly in the samples 150°C and 200°C a deep analysis has been performed. Prismatic defects in the samples have been found good correlation with inversion domains (IDs) using high angle annular dark field scanning transmission electron microscopy (HAADF-STEM) in an aberration corrected microscope JEOL ARM200F operated at 200 kV. A preliminary analysis of the IDs was carried out using dark-field imaging under multi-beam conditions. This method is based on the Friedel's law, which states that the intensity of two diffraction contrast images obtained using ±**g** reflections is keep constant [4]. However, it is not fulfilled for noncentrosymmetric crystals (lack of inversion symmetry), leading up to an opposite contrast that comes from a change of polarity in the sample. In this way, the background contrast is reversed from one domain to another [5]. The hexagonal wurtzite structure has the noncentrosymmetric along the [0001] direction and the reflections g = 0002 and g =000-2 produce the inversion contrast in the regions of the IDs. SF's in hexagonal wurtzite structures can be represented by the 2H polytype [6]. Figure 1a shows individual basal stacking fault (SF) projected along [11-20] without presence of IDB's. This type of SF is denoted by the dissociation of a 1/3< 11-20 > dislocation into two Shockley partials (I2 type) [7]. As proof of the I2 SF, the Burgers circuit drawn around the faults does not exhibit any close failure as indicated in Figure 1a. A different case is presented in Figure 1b where an IDB's is separated by a basal SF, resulting in a Shockley partial dislocation [5], in which a reaction between Burgers vectors of the prismatic and basal stacking faults is taking place: 1/6< 20-23 > = 1/3< 10-10 > +1/2< 0001 >. Figure 1c shows the strain map of the interaction between the IDB and the SF using geometrical phase analysis method (GPA) [8]. Strain map of e_{yy} direction has been obtained rotating the image 90 degrees to avoid the flayback error, which is coming from the scan direction in STEM [9]. High strain concentration (±45%) is obtained at the Shockley partial dislocation, enlarged as an inset in Figure 1c. After the interaction between the basal stacking fault and the inversion domain, the inversion domains continue without modification towards the layer surface. Sample 150°C presents the highest number of basal stacking faults, which are in several regions interrupted by prismatic defects. Similar to the analysis performed in the sample 200 °C, Figure 2 shows an aberration-corrected STEM image of the interaction between a stacking fault and the prismatic inversion domain in sample 150 °C. Strain map obtained along the SFs indicates a strain of 6% with a periodic modulation of 2c, which is in agreement with the I2 model of the SFs previously reported for hexagonal wurtzite structures [6]. We acknowledge to the U.S. Department of Defense W911NF-18-1-0439. 1-200-23

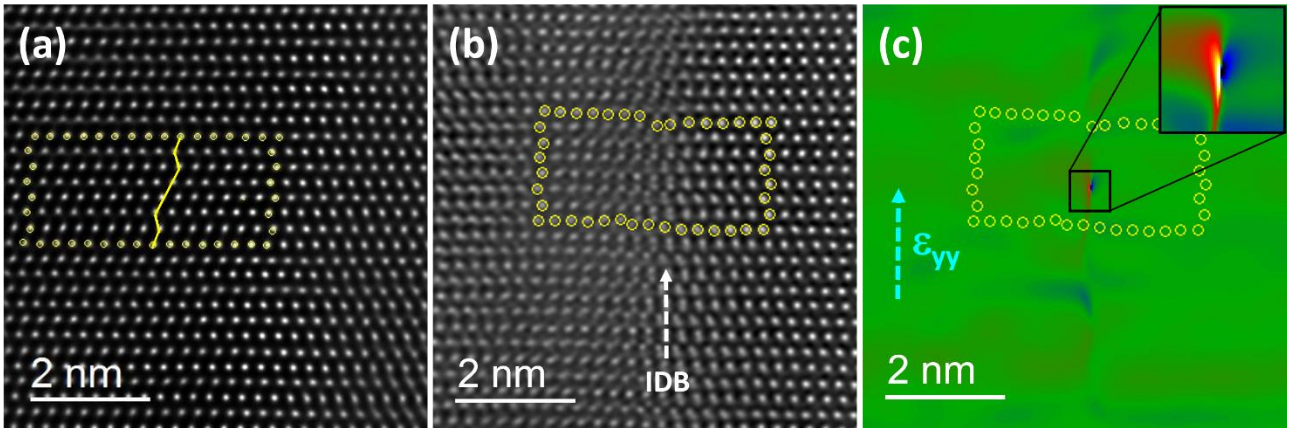

Figure 1. (a) HAADF-STEM image of an I2 SF in the 200°C sample, (b) interaction of a different SF with an inversion domain boundary and (c) strain map of the image (b), Shockey partial dislocation has been enlarged in the figure.

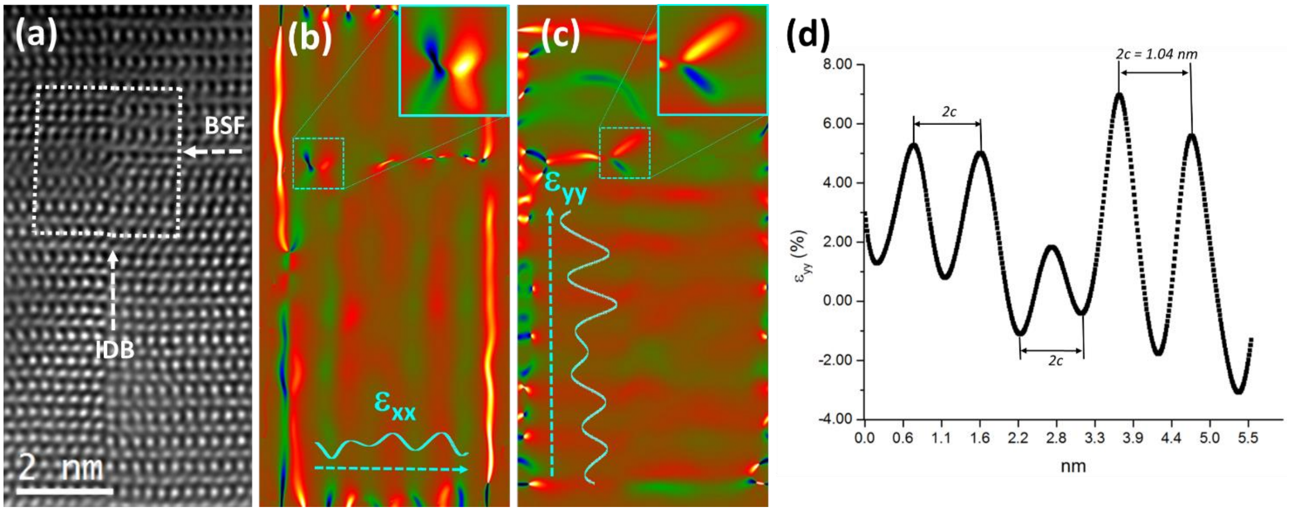

Figure 2. Interaction of an inversion domain boundary and a basal stacking fault: (a) HAADF-STEM image from the 150°C film, (b) exx strain map, (c) eyy strain map and (d) strain profile (eyy=±6.0%) along the [0001] direction.

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