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Atomic Resolution Z-Contrast Imaging of the Interface Between Non-Polar *a*-ZnO Grown on *r* -Cut Al_2O_3 by Pulsed Laser Deposition

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Epitaxial growth of non-polar ZnO is of significant technological importance owing to its absence of spontaneous polarization. The spontaneous polarization, for example, in LED applications, generates an internal electric field leading to a lowered electron-hole recombination and a reduced photon generation efficiency [1]. High quality non-polar ZnO films, such as *a*-ZnO (with growth direction normal to ZnO $(11\bar{2}0)$), have been successfully grown on *r*-cut Al_2O_3 substrates (with surface parallel to Al_2O_3 $(1\bar{1}02)$), where the large lattice mismatch (as high as 18.3 % along ZnO $[01\bar{1}0]$ direction) was relaxed by misfit dislocations [2-3]. The effect of misfit dislocations on epitaxial film electronic and optical properties has drawn major research interest in the past decades [4-9]. However, the role of dislocations has not been completely understood, partially due to the difficulty of studying the dislocation core structures, especially in systems with complex crystal structure. In this study, we have employed aberration-corrected STEM-Z, where sub-angstrom resolution can be achieved, to study the interface between *a*-ZnO and *r*-Al_2O_3 along two in-plane orthogonal zone axes ZnO $[0001]$ and ZnO $[01\bar{1}0]$, with the focus on misfit dislocations. The $(11\bar{2}0)$ ZnO // $(1\bar{1}02)$ Al_2O_3 with in-plane epitaxial orientation relationship determined to be $[0001]$ ZnO // $[1\bar{1}0\bar{1}]$ Al_2O_3 is consistent with earlier studies [2-3]. Misfit dislocations can be seen in both projections with extra planes lying on the Al_2O_3 side. Seen from the ZnO $[01\bar{1}0]$ zone axis, misfit dislocations are distributed far apart due to the extremely small lattice misfit along the ZnO $[0001]$ direction (1.5 %) and were mostly found on substrate steps as shown in Fig. 1 (a), suggesting the important role played by substrate steps in misfit dislocation nucleation in systems with such small lattice misfit. Seen from the ZnO [0001] zone axis, on the other hand, misfit dislocations ($b = 1/3\langle 2\bar{1}\bar{1}0\rangle$ Al_2O_3) are closely and uniformly spaced, which is consistent with the domain matching epitaxy paradigm [2,10] to accommodate the large lattice misfit along the ZnO $[01\bar{1}0]$ direction (18.3%) (Fig. 1 (b) and (c)). The core structure of this set of misfit dislocations is characterized by two extra Al_2O_3 planes as well as a compact strained region on the ZnO side of the interface (Fig. 1 (b) and (c)). The characteristics of the core structures are related to the thin film growth conditions and the extent of rearrangements of atoms during thermal annealing [11][12].

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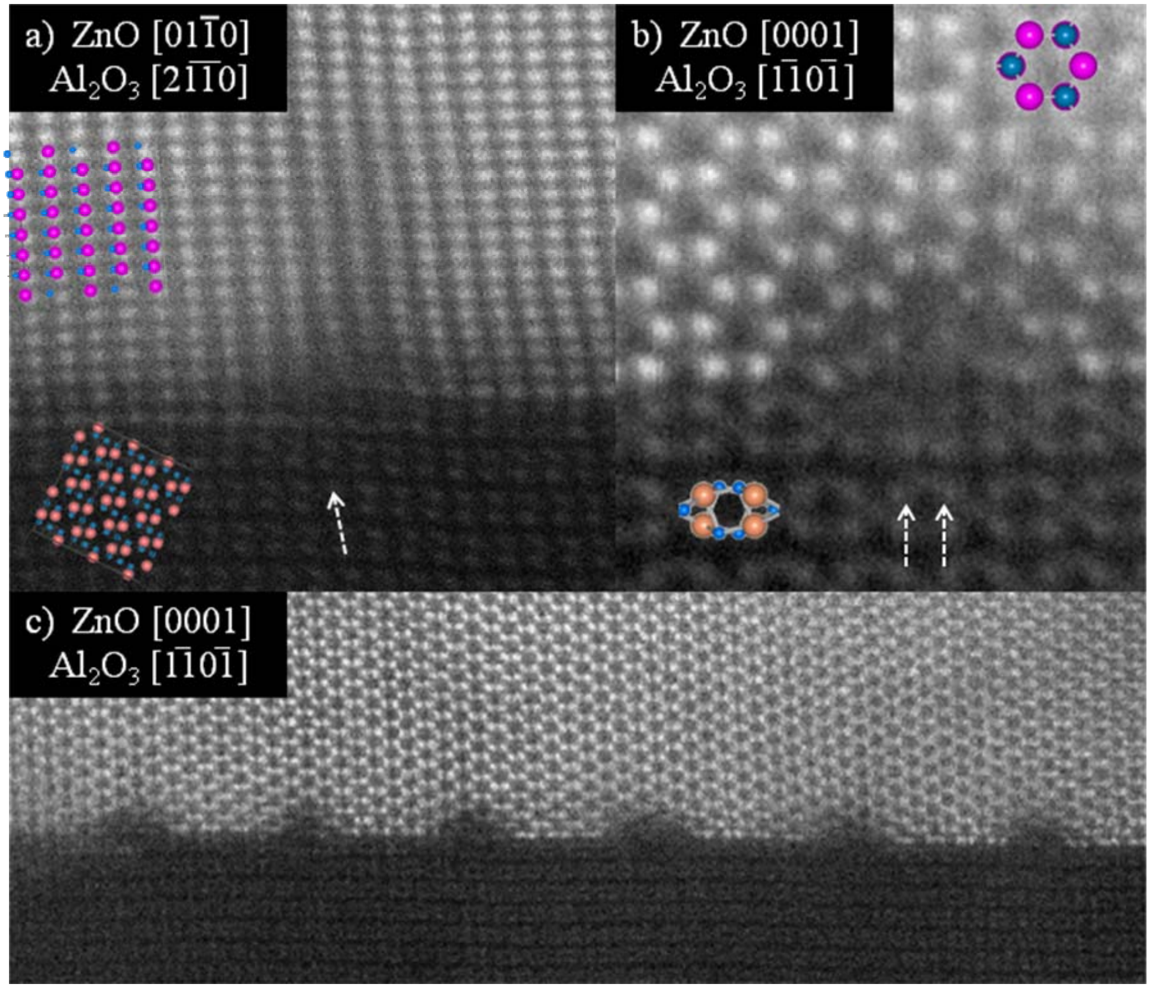

FIG. 1. Cross-sectional HAADF (High Angle Annular Dark Field) images of the interface between *a*-ZnO and *r*-Al_2O_3 along two in-plane orthogonal zone axes. (a) a misfit dislocation lies on a substrate step seen from the ZnO $[01\bar{1}0]$ zone axis. (b) a high magnification image of (c), which shows an array of misfit dislocations (b = 1/3$\langle 2\bar{1}\bar{1}0\rangle$ Al_2O_3) with uniform spacing on the interface seen from ZnO [0001] zone axis. The core structure of this set of misfit dislocations is characterized by two extra Al_2O_3 planes as well as a compact strained region at ZnO side of the interface. Orange, pink and blue balls in schematic drawing indicates the position of Al, Zn, and O atoms, respectively. Dashed arrows indicate extra planes.