Domain Matching Epitaxial Growth of High-quality ZnO Film on Si Using a Y_2O_3 Buffer Layer

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High quality ZnO epitaxial films were grown by pulsed-laser deposition on Si(111) substrates with a thin MBE grown Y_2O_3 buffer layer.[1] Radial scan along surface normal of the sample of a 0.2 μm thick ZnO layer, not shown, reveals c-plane oriented ZnO layer was observed on the Si(111) substrate with the cubic Y_2O_3 beffer layer also (111) oriented. The azimuthal ϕ-scans across non-specular reflections of ZnO{10-11}, Y_2O_3(440) and Si{220} reflections, shown in Fig. 1, were performed and yielded the in-plan epitaxial relationship of ZnO{10-10}||Y_2O_3{22-4}||Si{4-2-2}. Cubic Y_2O_3 has a bixbyite structure, which can be described as a vacancy-ordered fluorite. Viewing along the [111] direction of Y_2O_3, the O sub-lattice in Y_2O_3 consists of two-dimensional defective hexagonal lattices stacking with ABC sequence along the [111] direction, as shown in Fig. 2(a), in which the filled circles denote O atoms and open circles represent O vacancies. The hexagonal unit cell has a lattice constant equal to $a(Y_2O_3)\cdot\sqrt{2}/4$ = 3.750 Å and its axes are aligned with the Y_2O_3<10-1> directions, identical to the axes in ZnO basal plane. This elucidates the ZnO lattice is aligned with the O sub-lattice in Y_2O_3, as illustrated in Fig. 2(b). The lattice mismatch between ZnO and O sub-lattices in Y_2O_3 and in sapphire are -13.5% and 18.1%, respectively. For systems with such a large lattice mismatch, the well established lattice matching epitaxy (LME), where films grow by one-to-one matching of lattice constants or pseudomorphically across the film-substrate interface, is not the favorable mechanism. Instead, domain matching epitaxy (DME) [2], where integral multiples of lattice planes containing densely packed rows are matched across the interface, provides a nice description of the interfacial structure of these systems. The planar spacing ratio of ZnO(11-20) to parallel Y_2O_3(4-40), which coincides with the (11-20) planes of O sub-lattice inY_2O_3 falls between 6/7 and 7/8; this implies a matching of 7(8) planes of ZnO with 6(7) planes of Y_2O_3 across the interface along this direction. The large lattice mismatch is thus accommodated by the misfit dislocations localized at the interface. To verify this interfacial structure, we performed cross-sectional TEM measurements. Figure 3(a) is the TEM micrograph along Si[11-2] projection which shows atomically sharp ZnO/Y_2O_3 and Y_2O_3/Si interfaces; no intermediate reaction layer is observed in both interfaces. The periodic contrast variation along the ZnO/Y_2O_3 interface with an average spacing of ~1.2 nm found in the high resolution TEM images, shown in Fig. 3(b), was attributed to the misfit dislocations induced strain field. The nearly periodically arranged extra ZnO(11-20) half planes with a spacing of 6 or 7 Y_2O_3(4-40) planes are clearly seen in the Fourier filtered image shown in Fig. 3(c); this confirms the DME of ZnO on Y_2O_3 (111).

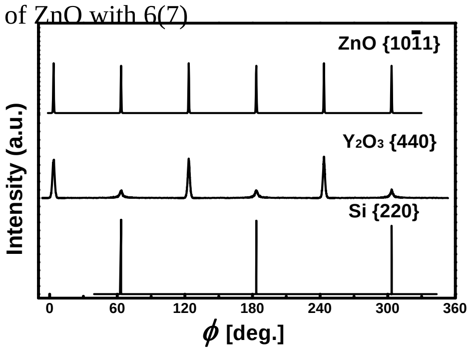

Fig. 1: ϕ-scan profiles across ZnO {10-11}, Y_2O_3{440}, and Si{220}off-normal reflections.

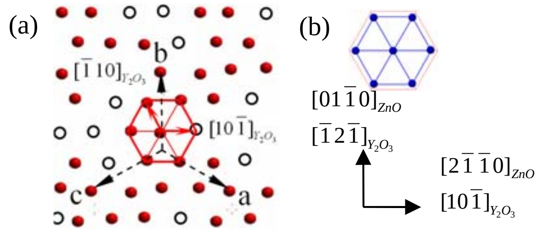

Fig. 2: (a) Schematic of atomic arrangement of O sub-lattice in Y_2O_3 (111) planes, where the filled circles are O atoms and the open circles denote O vacnacies. The dashed arrows are (111) projection of the basis vectors of Y_2O_3 cubic lattice. (b) Illustration of the lattice alignment of ZnO basal plane (small hexagon) with O sub-lattice in Y_2O_3 (large hexagon).

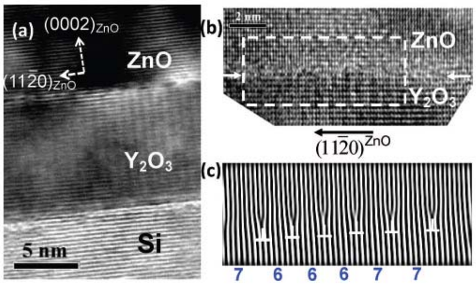

Fig. 3: (a) Cross-sectional TEM micrograph recorded along Si[11-2] projection. The high resolution image of the ZnO/Y_2O_3 interface is shown in (b). The Fourier filtered image of the area enclosed by the dashed rectangle in (b) is displayed in (c), on which the number of Y_2O_3(4-40) planes between adjacent extra ZnO(11-20) half planes are marked below.

References

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