國家同步輻射研究中心年度實驗報告

NSRRC Annual Experiment Report

Form: ER1

計劃編號 (Proposal no.)	2011-1-021		所有光束線編號 (All BL no.)	BL13A, BL17B1		
計畫題目 (Proposal title)	High quality ZnO epitaxial films					
計畫主持人 (Principal Investigator)	姓名 (Name)	徐嘉鴻	單位 (Affiliation)	NSRRC	職稱 (Position)	

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 m 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.

References

[1] W.-R. Liu, Y.-H. Li, W. F. Hsieh, C.-H. Hsu, W. C. Lee, Y. J. Lee, and M. Hong, and J. Kwo,

Cryst. Growth Design **9**, 239 (2009).

[2] J.Naraya, and B. C.Larson, J. Appl. Phys. **93**, 278

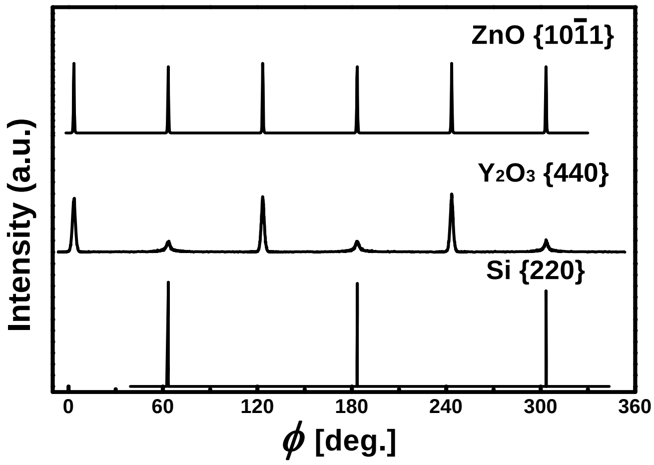

Fig. 1 ϕ-scan profiles across ZnO {10-11}, Y_2O_3{440}, and Si{220}off-normal reflections.

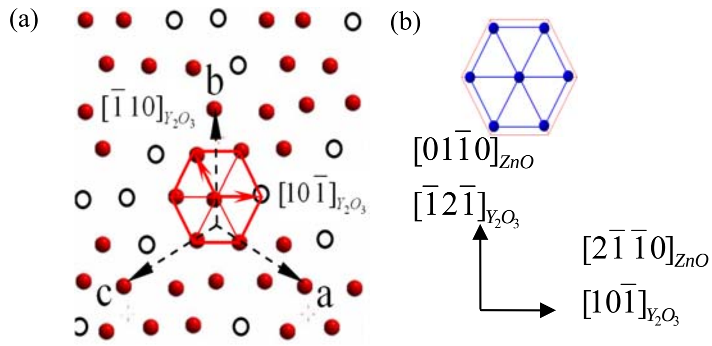

Fig. 2 (a) Schematic of atomic arrangement of O sub-lattice in Y_2O_3 (111) planes, where the filled circles are O atoms and the open circles denote O vacnacies. The dashed arrows are (111) projection of the basis vectors of Y_2O_3 cubic lattice. (b) Illustration of the lattice alignment of ZnO basal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