



國家同步輻射研究中心年度實驗報告

NSRRC Annual Experiment Report

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報告題目 Report Title	High Quality ZnO Epitaxial Films		
計畫主持人 Principal Investigator	姓名 Name	*****	單位 Affiliation
			****大學*****學系

年度實驗報告須以英文概述利用本中心設施之年度實驗成果。格式採單行距、英文字型 Times New Roman、12 號字，篇幅以 2 頁為限。

Please summarize the research results associated with NSRRC facilities in English. Use single line spacing and Times New Roman font, at 12 point size. Do NOT exceed 2 pages.

High quality ZnO epitaxial films were grown by pulsed-laser deposition on Si(111) substrates with a thin MBE grown Y₂O₃ 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 Y₂O₃ beffer layer also (111) oriented. The azimuthal ϕ -scans across non-specular reflections of ZnO{10-11}, Y₂O₃(440) and Si{220} reflections, shown in Fig. 1, were performed and yielded the in-plan epitaxial relationship of ZnO{10-10}||Y₂O₃{22-4}||Si{4-2-2}. Cubic Y₂O₃ has a bixbyite structure, which can be described as a vacancy-ordered fluorite. Viewing along the [111] direction of Y₂O₃, the O sub-lattice in Y₂O₃ 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 $a(\text{Y}_2\text{O}_3) \cdot 2/4 = 3.750 \text{ \AA}$ and its axes are aligned with the Y₂O₃ <10-1> directions, identical to the axes in ZnO basal plane. This elucidates the ZnO lattice is aligned with the O sub-lattice in Y₂O₃, as illustrated in Fig. 2(b). The lattice mismatch between ZnO and O sub-lattices in Y₂O₃ 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 Y₂O₃(4-40), which coincides with the (11-20) planes of O sub-lattice in Y₂O₃ falls between 6/7 and 7/8; this implies a matching of 7(8) planes of ZnO with 6(7) planes of Y₂O₃ 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, M. Hong, and J. Kwo, *Cryst. Growth Design* 9, 239 (2009).
 [2] J. Naraya, and B. C. Larson, *J. Appl. Phys.* 93, 278 (2003).

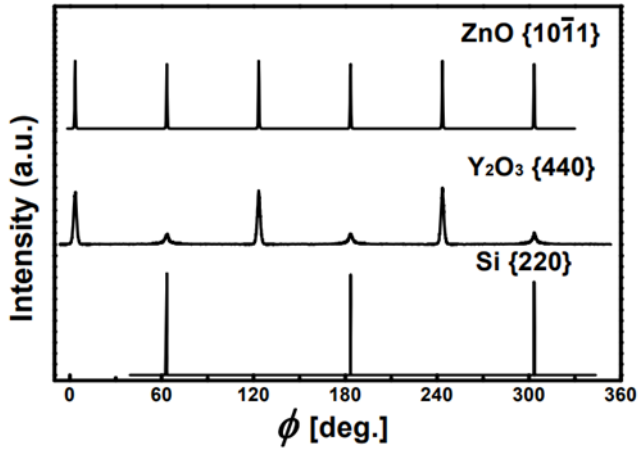


Fig. 1: ϕ -scan profiles across ZnO $\{10\bar{1}1\}$, $Y_2O_3\{440\}$, and Si $\{220\}$ off-normal reflections.

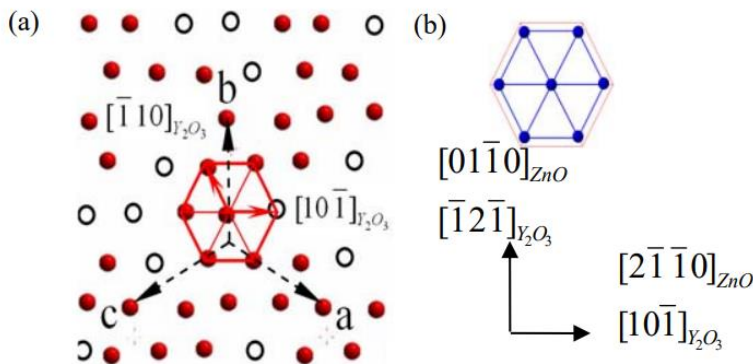


Fig. 2: (a) Schematic of atomic arrangement of O sub-lattice in Y_2O_3 (111) planes, where the filled circles are O atoms and the open circles denote O vacancies. The dashed arrows are (111) projection of the basis vectors of Y_2O_3 cubic lattice. (b) Illustration of the lattice alignment of ZnO basal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