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Theoretical investigation of polarity determination for c-plane InN grown on yttria-stabilized zirconia (111) substrates

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An yttria-stabilized zirconia (YSZ) (111) substrate is a promising candidate for the growth of c-plane InN due to its small lattice mismatch of 2.7%. Polarity control of InN (0001) films on YSZ substrates is a crucial issue for device fabrication because mixture of In-polar and N-polar InN will degrade device performance. We have recently found that thermal annealing of the YSZ (111) substrates leads to the formation of In-polar InN films. This phenomenon is probably caused by segregation of the Y atoms at the surfaces of the YSZ substrates [1]. In this presentation, we will discuss the polarity determination of c-plane InN films grown on YSZ (111) substrates based on the calculated adsorption energies for the In atom on the N-covered YSZ (111) surface.

A cubic zirconia (111) slab is employed as the Y-segregation free substrate. For the Y-segregated substrate, all Zr atoms in the upper half of the zirconia in the cell were replaced with Y atoms. Firstly, adsorption energies of the In and N atoms on the YSZ surfaces are calculated. The large adsorption energy for N atoms compared with that for In atoms suggests that the first layer on the Y-segregated YSZ (111) surfaces should consist of N atoms. Calculations of the adsorption energies of an In atom on the N adatoms covering the surfaces was performed to investigate the polarity dependence of the stability of InN on YSZ. As shown in Fig.1, an In atom at the center of three N atoms (“Hollow N”) leads to In-polar InN, whereas an In atom on the top of a N atom (“Top N”) results in N-polar InN. According to the calculations shown in table 1, In-polar InN is more stable on the Y-segregated surfaces. On the other hand, the energy difference between the In-polar and N-polar InN on the segregation-free cubic zirconia surfaces is quite small. These data are quite consistent with the experimental results.

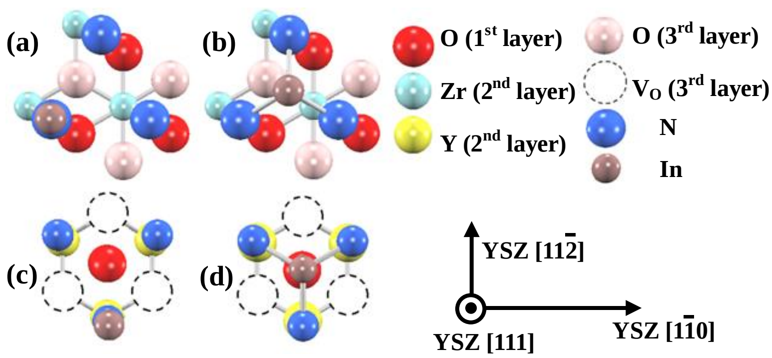

Fig. 1 Schematic illustration of structures during the initial stages of (a) N-polar and (b) In-polar InN growth on pure cubic zirconia, and (c) N-polar and (d) In-polar InN growth on Y-segregated YSZ.

Table 1 Adsorption energies (in eV) of an In atom on the nitrogen adlayer covering YSZ (111) surfaces.

Substrate	Adsorption energy of In	
	In-polar	N-polar
Y-segregated	**7.86**	**5.24**
Cubic zirconia	**3.28**	**3.27**

[1] A. Kobayashi, K. Okubo, J. Ohta, M. Oshima and H. Fujioka, Phys. Status Solidi A **209**, 2251 (2012).