

certain distance from the interface. But, the increase of the NWR diameter by far exceeds the lattice mismatch of 6 %. Lateral growth is observed when the NWR length exceeds the path length of the surface diffusion. A portion of the diffusing atoms is consumed for lateral growth. This effect leads to the well-known tapering of NWRs. The expected formation of a Cd-rich shell in the buckled region is not found. Hence, the buckling is not due to a lateral growth. Conclusively, only a variation of either the size or shape of the catalyst droplet can cause the buckling. By altering growth parameters like temperature or droplet composition the properties of the liquid droplet are modified. This can cause a different diameter or even an ellipsoidal shape of the droplet leading to an enlarged liquid/solid interface area.

Keywords: semiconductor; nanowire; axial heterostructure

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X-ray Absorption Spectroscopy: A Powerful Tool to Probe the Zr Shift Towards the Centrosymmetric Position in PZT ($\text{PbZr}_{0.52}\text{Ti}_{0.48}\text{O}_3$) Under High Pressure and High Temperature.

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Ferroelectrics materials with the perovskite structure have drawn considerable attention for many years. $\text{PbZr}_{1-x}\text{Ti}_x\text{O}_3$ (PZT) ceramics have been the subject of numerous studies due to their exceptional ferroelectric properties. These solid solutions exhibit their highest electromechanical responses for compositions ($x \sim 0.48$) lying at the so-called morphotropic phase boundary between the rhombohedral or monoclinic and tetragonal phases. PZT adopts an ABO_3 perovskite-type structure with chemical disorder on the B site (occupied by Zr and Ti). Intrinsic short range dynamical disorder has been experimentally observed [1] and theoretically predicted [2]. The presence of diffuse X-ray/neutron scattering is clearly observed in $\text{PbZr}_{0.52}\text{Ti}_{0.48}\text{O}_3$ diffraction patterns which is an evidence of local lattice deformations with respect to the average structure [3]. Simultaneous high pressure at high temperature X-ray absorption and X-ray diffraction experiments were carried out on BM29 at ESRF to follow the changes in short range order around Zr at the ferro- to para-electric phase transition. Measurements on the 300K isotherm indicate a clear change in the EXAFS signal, between 5.3GPa and 6.1GPa, as well as a decrease of the intensity of the prepeak (observed in spite of a short lifetime of the excited state, 3.83eV). Changes in the XANES in the same pressure range can be reproduced by calculations with the FDMNES code [4]. A noticeable decrease in the Debye-Waller factor

(DWF) is observed above 6GPa, in agreement with DWF for the centrosymmetric BaZrO_3 [5]. All these features indicates that Zr atoms shift toward the centrosymmetric position between 5.3 and 6.1GPa, corresponding to the ferro-paraelectric transition. Moreover, this pressure range corresponds to the value of the Curie pressure P_c obtained by neutron diffraction and resonant Raman spectroscopy [3]. Similar results are observed for the 450K isotherm. X-ray absorption is thus the technique of choice to probe the ferro-paraelectric transition at the local scale. It has been possible to observe, through the decrease of the DWF, a very small displacement of the Zr ($\sim 0.06 \text{ \AA}$) from an off-center to a centrosymmetric position.

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