

Observation of Anisotropic Disorientation Grain Boundaries in Sn₂O₃ Nanobelts Using X-Ray Nanodiffraction*

Zhonghou Cai and Yanan Xiao

Advanced Photon Source, Argonne National Laboratory, Argonne, IL 60439

Molecules in a thermodynamic system have a spontaneous tendency to seek maximum interactions among themselves for lowering the free energy of the system via variation of density distribution. It is well known that the intensive parameters like temperature and pressure often limit the extent of the interactions and are responsible for the richness of phases that a system exhibits. However, the exploration of the extent of interactions due to the extensive parameters, such as the volume and the number of molecules in a system, and the effect on the density distribution is still in its infancy, due to the limited availability of such systems. A wire-like nanostructure synthesized through one-dimensional growth exhibits the effect due to its condensed phase, which enables molecules to significantly interact, while the small cross-section size limits the extent of the interactions. For instance, the energy needed to form a point defect at the growth front of a nanowire is much less than the energy needed to form the same defect in the bulk, since the lattice elastic deformation and associated strain field quickly die out when the boundary of the nanomaterial is reached. Once the energy can no longer counter the energy due to the change of the entropy associated with the formation of the point defect at the growth temperature, disorder starts to become the favorable configuration. This imposes a fundamental limitation on the smallest cross-section size of a perfect nanowire crystal that can be synthesized through one-dimensional growth. In order to observe the limitation, the internal structures of tin oxide (Sn₂O₃) nanobelts of various cross-section sizes, from 200 nm x 40 nm down to 22 nm x 8 nm, were individually investigated using x-ray diffraction with a focused beam (7 keV) obtained from advanced zone-plate optics. By mapping the diffraction intensity of the (030) reflection with a CCD area detector along the full length of the nanobelts, we observed disorientation boundaries in the belts of cross-section sizes of 100 nm x 30 nm and smaller. The lattice disorientation of grains inversely relates to the cross-section size of the belts. Moreover, the lattice disorientation boundaries are confined only in the plane of growth front and none of that out of the plane has been observed. Given the fact that a tin oxide nanobelt is bounded by faces of high density and low surface energy, all the observations obtained from the tin oxide nanobelts can be explained consistently with the limited extent of interactions among molecules at the growth front.

* This work was supported by U. S. Department of Energy, Office of Basic Energy Sciences, under Contract W-31-109-Eng-38.