**Effect of the Chemical State of the Surface on the Relaxation of the Near-Surface Layer**

The effect of the chemical state of the surface of nanoparticles on the relaxation in the near-surface layer was examined using the concept of the apparent lattice parameter \( \text{alp} \) determined for different diffraction vectors \( Q \). At low diffraction vectors the peak positions are affected mainly by the structure of the near-surface layer, while at high \( Q \) values only the interior of the grain contributes to the diffraction pattern. Theoretical \( \text{alp} \) relations were obtained from diffraction patterns calculated for models of nanocrystals with a strained surface. We studied nanocrystalline \( \text{SiC} \) and \( \text{GaN} \) with average crystallite size from 5 to 30 nm. Following the measurements of as synthesized powders we investigated powders annealed at 400°C under vacuum, and same powders wetted with water. A strong dependence of the experimental \( \text{alp} \)-\( Q \) plots on the grain size and purity was found. Evaluation of the strain at the surface shell was made by comparison of experimental \( \text{alp} \)-\( Q \) plots with those computed for the core-shell model. We estimated the thickness of the shell in \( \text{SiC} \) nanocrystals to be 4 – 6 Å, with the tensile strain of about 10%. In \( \text{GaN} \), the shell thickness is approximately 7 Å with the compressive strain in the range 10 - 15%. Annealing the powders at 400°C under vacuum, as well as wetting them with water leads to a strong change of the measured \( \text{alp} \) values. Fig. 1. We interpret this effect as a reconstruction of the atomic structure of the surface with simultaneous decrease of the surface strain.

**Keywords:**
- Nanocrystals, \( \text{SiC} \), \( \text{GaN} \)

---

**Surface and Interface Structure Beamline (BL13XU) at SPring-8**

O. Sakata1, Y. Furukawa1, S. Goto1, T. Mochizuki1, T. Uraga1, K. Takeshita1, H. Ohashi1, T. Ohata1, T. Matsushita1, S. Takahashi1, T. Ishikawa1, K. Sumitani1, T. Takahashi1, M. Nakamura2, M. Ito2, A. Saito2, T. Shimura1, M. Takahashi1

1Japan Synchrotron Radiation Research Institute Materials Science Kouto 1-1-1, 1, Mikazuki SAYO HYOGO 679-5198 JAPAN 2Riken Harima-Institute University of Tokyo 3Keio University 4Osaka University 5Japan Atomic Energy Research Institute

In order to elucidate the effects of the ionicity in chemical bonding on the structure and the high-pressure sequence in liquids, we have investigated the structure of liquid III-V compounds, such as GaSb and InSb, under pressure. Experiments are performed by means of the energy-dispersive (EDX) and angle-dispersive X-ray diffraction methods (ADX) using a synchrotron radiation source in conjunction with the high-pressure apparatus. The EDX experiment using the double staged high-pressure apparatus enables us to reveal the averaged structure of the binary liquid at high pressures and temperatures up to about 20 GPa and 1400 K. The ADX experiment with a multi-channel collimator using the anomalous dispersion effect give information on the chemical short-range order under pressure.

The EDX results show that the local structure of liquid III-V compounds with both covalent and ionic bonding does not contract uniformly unlike simple liquid metals. The nearest neighbor distance does not change markedly in spite of the volume contraction. An analysis of the pair distribution function has shown that the local structures in liquids can be described by the distorted local structures of their high-pressure crystalline phases. The local structure is found to change from a low-coordinated state to a high-coordinated state under one high pressure. The effects of the ionicity in chemical bonding are discussed from the experimentally determined local structures for the liquids of GaSb and InSb.