

experimental data to perform a three-dimensional bond density refinement of the Si(111)-7x7 surface. These two experimental techniques are quite complimentary as electron diffraction is rather more sensitive to the core-screening effects of bonding, while only the x-ray dataset is three dimensional (and is a direct transform of the local charge density). By utilizing a combinatorial ab initio Density Functional Theory (DFT) approach, we have developed a parameterized model for fitting valence charge density in silicon to experimental diffraction data which enhances performance, but adds no additional adjustable parameters. When bonding effects are properly accounted for, the improvement to the refinement of the overall structure is significant to >99% confidence (using a degree-of-freedom reduced Chi figure of merit), and site-specific perturbations due to adatom bonding at the surface are also possible. The experimental results will be compared to a full-potential, all-electron DFT structural relaxation of the Si(111)-7x7 surface slab.

Keywords: surface diffraction, charge density, density functional theory

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Phonon and electronic properties of crystals and chirality studied with resonant X-ray diffraction

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Recent theoretical and experimental results on the diffraction of x-rays near absorption edges of atoms (resonant diffraction) will be presented together with application to electronic and phonon properties of crystals (a review of earlier results can be found in [1]). In comparison with EXAFS, the resonant diffraction is more sensitive to the symmetry of atomic environment and to distortions of the electronic states of atoms in crystals. For example, the resonant forbidden reflections can be caused by opposite chirality of atomic positions in centrosymmetric crystals (observed in Fe₂O₃ and Cr₂O₃), or by phonon displacements of atoms (studied in detail for Ge and ZnO), or by the quantum jumps of hydrogen atoms in KH₂PO₄-type crystals. Symmetry consideration is accompanied by results of the muffin-tin and ab initio simulations. Experimental studies have been done in collaboration with synchrotron groups from Tsukuba, Grenoble, Hamburg, Daresbury, Oxfordshire, and Moscow. This work was supported by the Russian Foundation for Basic Research (project 07-02-00324).

[1] V. E. Dmitrienko, K. Ishida, A. Kirfel, E. N. Ovchinnikova, Polarization anisotropy of X-ray atomic factors and 'forbidden' resonant reflections, *Acta Crystallographica A* 61 (2005) 481-493.

Keywords: resonant scattering, phonon properties, chirality

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The structure and dynamics of GaN(0001) surface during HVPE GaN growth — *Ab initio* study

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The conditions for the reliable simulation of semiconductor surface structure and processes are formulated for GaN growth by Hydrogen Vapor Phase Epitaxy. The chemical state of the system is formulated within kinetic and thermodynamic picture. The GaN(0001) surface in ammonia-rich (N-rich and H-rich) environment is analyzed. The equilibrium state of GaN(0001) surface is considered using both formulations. Using ab-initio quantum mechanical density functional theory (QM DFT) SIESTA and VASP codes, it is proved that the thermodynamic approach, suggesting the mixed NH₃-NH₂ coverage is in accordance with the dynamic results, which show that ammonia is adsorbed molecularly on the surface. The resulting NH₃ coverage is dynamically unstable with respect of creation of molecular hydrogen (H₂). These molecules move away from the surface, overcoming small, 0.14 eV high energy barrier. The remaining H adatoms move along the surface, jumping between neighboring NH₂ radicals with relatively small (0.15 eV) energy barrier. It is also shown that GaCl is attached on the NH₂-covered surface without any energy barrier. The chlorine adatoms is removed by reaction with the mobile H adatoms creating HCl molecules which leaves GaN(0001) surface.

Keywords: gallium nitride, hydride vapor phase epitaxy, density functional theory

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Hydride vapor phase epitaxy of AlN and AlGaN

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Realization of bulk wafers related to AlN must attract considerable attention for expanding the applications such as optical and electronic devices using the group III nitride semiconductors. Up to now, ultraviolet light emitting devices (UV-LEDs) are fabricated using GaN-template substrates grown on sapphire wafers. Unfortunately, the thermal conductivity of sapphire is very poor compared to AlN and GaN. From the viewpoint of high-power UV optical devices, AlN and/or AlGaN bulk crystal is a promising substrate material for their devices. Vapor phase epitaxy (VPE) is generally done using MOVPE (metalorganic vapor phase epitaxy) or HVPE (hydride vapor phase epitaxy). The MOVPE method is versatile and thus used for several materials, while HVPE is well developed for GaN wafer fabrication. In the past, HVPE has been thought unsuitable for the growth of Al-containing semiconductors such as AlN and AlGaN, because the major Al-precursor in HVPE is AlCl₃ which cause the reaction between AlCl₃ and the quartz reactor (SiO₂). However, HVPE of AlN has proved successful using AlCl₃, which does not react with the quartz reactor at the growth temperatures [1]. In addition, we have reported that AlGaN ternary alloy can be grown by HVPE using GaCl-AlCl₃-NH₃ system [2]. In the presentation, a thermodynamic analysis of the HVPE of AlN using AlCl₃ and AlGaN using AlCl₃ and