coupled technique, PArallel Recording Of Dark-field Images (PARODI). It is a new breed of convergent beam electron diffraction developed at Brookhaven to accurately determine structure factors of low-order reflections that are sensitive to valence electron distribution. The synchrotron based single-crystal x-ray diffraction was used to determine the structure factors of high-order reflections that are sensitive to atomic positions and Debye-Waller factors. The two sets of experimental data were combined and refined, and then compared with DFT calculations. Examples on charge density studies including $CaCu_3Ti_4O_{12}$ oxide that exhibits extremely high dielectric constant (~104) over a wide range of frequencies and temperatures will be given [1,2]. Our recent work on electron scattering amplitudes involving non-spherical orbitals (p and d orbitals) of transition-metal elements will also be reported. We demonstrate that it is possible to accurately measure valence electron distribution, electron orbitals and bonding characteristics of complex functional materials using quantitative electron and x-ray diffraction.

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Keywords: charge density, convergent-beam electron diffraction, perovskite oxides

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Bonding electrons visualization in photo-excited state using synchrotron X-ray powder diffractometry

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The synchrotron X-ray powder diffractometry has been recognized as one of powerful methods for materials science research. By using Maximum Entropy Method (MEM) as an analytical method for the powder diffraction data, bonding electrons can be visualized to reveal the structure-property relationship. The reliability of the MEM charge density depends on 'accuracy' and 'precision' of experimental data. In present studies, we have succeeded in visualizing bonding electrons in the photo-excited state [1]. So far the accuracy of structural analysis under photo irradiation has not reached bonding electrons level. That can be attributed to inhomogeneous excitation caused by large difference between probe light (X-ray) and excitation light (visible laser) energy. In order to overcome the difficulties, we designed sample packing method into a capillary and photo irradiation system for homogeneous excitation. As a result charge density analysis under photo irradiation was successfully achieved in one of spin crossover complexes, $Fe(phen)_2(NCS)_2$, which shows a dynamical photo-induced phase transition (PIPT). The bonding nature between Fe and N under photo irradiation is clearly suppressed compared with both ground low-spin phase and temperature induced high-spin phase. The bonding nature created by visible laser may characterize the faster relaxation process of the dynamical PIPT. In my talk, charge density study of persistent PIPT materials (transition metal cyanides [2, 3]) and transient PIPT materials (charge transfer organic materials) will be presented with the dynamical PIPT material.

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Keywords: synchrotron powder diffraction, maximum-entropy method, charge density distribution

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Structure based design of new thermoelectric materials

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There is an urgent need to develop new environmentally friendly energy sources and improving energy efficiency in many technologies and processes. One interesting possibility is thermoelectric energy conversion. Thermoelectric materials are functional materials, which are attracting huge attention due to their dual ability of electrical-thermal energy conversion. Thus, thermoelectric materials are used either for cooling or for energy production. In spacecrafts the preferred method of energy generation is conversion of heat from a radioactive plutonium source to electricity using multi-step thermoelectric converters. There are a vast number of waste heat sources in modern societies that could be harvested in similar ways. In the talk the interplay between structure and thermoelectric properties will be discussed for a range of new complex thermoelectric materials. The materials design has particular focus on lowering the lattice contribution to the thermal conductivity e.g. by introduction of rattling guest atoms or interstitial atoms. The talk will cover materials with applications in high temperature (inorganic clathrates [1-3]) and intermediate temperature (zinc antimonides [4-6]) energy conversion as well as low temperature cooling (iron antimonides [7]).

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Keywords: thermoelectrics, structure-property, clathrates

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Experimental measurements of bond density at the Si(111)-7x7 surface

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Measurement of valance charge density, the distribution of electrons important to bonding, in bulk materials is a rather well established technique in the diffraction community. In principle, the ability to directly measure the charge density at a surface is at least as interesting as in the bulk, if not more so. The exact structure of these surfaces dictates their usefulness and, in particular, the charge density determines the physical, chemical, and electronic properties important to building a device, or designing a catalytic reaction. We have used a combination of electron and x-ray diffraction 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 Fe_2O_3 and Cr_2O_3), or by phonon displacements of atoms (studied in detail for Ge and ZnO), or by the quantum jumps of hydrogen atoms in KH_2PO_4-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).

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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 NH_3-NH_2 coverage is in accordance with the dynamic results, which show that ammonia is adsorbed molecularly on the surface. The resulting NH_3 coverage is dynamically unstable with respect of creation of molecular hydrogen (H_2). 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 NH_2 radicals with relatively small (0.15 eV) energy barrier. It is also shown that GaCl is attached on the NH_2-covered surface without any energy barrier. The chlorine adatoms is removed by reaction with the mobile H adatoms creating HCl molecules which leaves GeN(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 AlCl which cause the reaction between AlCl and the quartz reactor (SiO_2). However, HVPE of AlN has proved successful using $AlCl_3$, 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-$AlCl_3$-NH_3 system [2]. In the presentation, a thermodynamic analysis of the HVPE of AlN using $AlCl_3$ and AlGaN using $AlCl_3$ and