

m21.o03**Structural change wide-gap semiconductor in reconstructive phase transitions: AlN, BN and B_xAl_{1-x}N solid solutions**

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Of the greatest interest are semiconductors of row AlN, GaN, InN, BN, SiC, diamond, etc., that are widely used for the fabrication of optical and electronic devices. In the last years significant number of work, devoted study of structural, electronic and optical of properties wide-gap of semiconductors, is published. However to the present moment of the characteristic and the electronic nature of their properties even for the most widespread semiconductors are insufficiently investigated. By us with use large cluster (more than 250 atoms), shipped in an infinite crystal, are investigated peculiarities of a power spectrum electrons in B_xAl_{1-x}N solid solutions, in comparison with binary AlN and BN, in a wide range of change of concentration boron [1-3]. The electronic energy structure of 2H and 3C AlN and BN crystals and B_xAl_{1-x}N solid solutions in calculated on the basis of the local coherent potential method using the cluster version of the MT approximation and the theory of multiple scattering. The features of the electronic structure of 2H AlN crystals are compared with X-ray K and L absorption and emission spectra of aluminum and nitrogen. An interpretation of these feature is given. The concentration dependences of the width of the upper subband of the valence band and the band gap in B_xAl_{1-x}N solid solutions ($x = 0.25, 0.5, 0.75$) are investigated. Existence of carry charge from atoms of aluminium to atoms of nitrogen is shown, the size of which grows on a measure doping boron in both crystal updatings. It is shown, that the electronic power structure w-AlN and c-AlN, alongside with distinctions, has general laws, which are displayed in presence on a curve TDOS characteristic for AlN of peculiarities, in particular (personally) of peaks B and E, describing basic condition of nitrogen and aluminium in a crystal. The offered interpretation basic and for the first time revealed peculiarities on a curve TDOS w-AlN does not contradict experimental dat& and explains a nature of their formation.

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m21.o04**High pressure x-ray absorption study of BaTiO₃ and SrTiO₃ at the Ti K edge**A. Polian[#], J.P. Itié[&], A.M. Flank[&], P. Lagarde[&], B. Couzinet[#]*[#]Physique des Milieux Denses, IMPMC, CNRS-UMR 7590, Université P. et M. Curie, 140 Rue de Lourmel, 75015 Paris & Synchrotron SOLEIL, L'Orme des Merisiers, Saint-Aubin - BP 48 91192 GIF-sur-YVETTE CEDEX***Keywords: high-pressure phase transitions, X-ray absorption spectroscopy, perovskite oxides**

ATiO₃ perovskites exhibit often distortions from the ideal cubic structure due to instabilities related to the off centre position of the Ti atom with respect to the oxygen octahedron (BaTiO₃, PbTiO₃) or the tilt of the octahedra (CaTiO₃). SrTiO₃, cubic under ambient conditions, is supposed to be undistorted.

Under pressure, phase transformations occur corresponding to the vanishing of the ferroelectricity (BaTiO₃: tetragonal (cubic) or to the onset of the antiferrodistorsive (AFD) distortion (SrTiO₃: cubic (tetragonal)). These transitions have been determined by x-ray[1] or neutron diffraction[2], by Raman[3,4] and Brillouin[5] spectroscopies. Some questions about the local order around the Ti atom (local ferroelectric distortion) and the existence of broad Raman modes in the cubic structure (not allowed by the selection rules) remain open.

High pressure X-ray absorption spectroscopy at the Ti K edge is well adapted to answer these questions.

The main results are:

- BaTiO₃
 - The Ti remains off centre in the cubic phase up to 10 GPa
 - Above this pressure, the local structure is *cubic* with the Ti atom at the centre of the oxygen octahedron
 - The remaining intensity of the B feature is due to the quadrupolar term and to the thermal contribution
- SrTiO₃
 - At room pressure the Ti atom is slightly off centre (disordered)
 - Above 5 GPa the Ti atom is at the centre of the oxygen octahedron
 - AFD instability occurs
 - A strong modification of the structure occurs above 14 GPa with a redshift of the t_{2g} band while the e_g is stable

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