

**P03.06.23***Acta Cryst.* (2008). **A64**, C225**Multi-resolution atomistic simulations and diffuse scattering in BaTiO<sub>3</sub>**

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The archetype perovskite BaTiO<sub>3</sub> is probably the most intensively studied compound in view of understanding ferroelectric phase transitions, both from theory and experimentally. Despite many efforts there are still some unclear issues concerning the character of the phase transition, particularly in connection with understanding local atomic displacements. In 1970, based on diffuse scattering (DS) experiments on a similar compound - KNbO<sub>3</sub>, the 8 site order-disorder model was proposed by Comes et al. In our study we address the question of the adequacy of order-disorder model by performing molecular dynamics and Monte Carlo simulations, combining the atomistic resolution of the former with the statistical flexibility of the latter. We extract patterns of Ti displacements from constant pressure - constant temperature molecular dynamics runs performed on systems of moderate size. From this we calculate displacement correlation coefficients, which are used to build a spin-like model of Ti shifts. This allows us to dramatically scale up the simulation size and to perform Monte Carlo simulations on large, adequate systems for accurate DS pattern determination. Our results for different temperatures compare very well with experiments. Along this line, realistic domains are obtained separated by domain walls. The study allows us to shed light on the relationship between macroscopic features (macroscopic polarization, unit cell deformation) and microscopic mechanism of the disorder and the phase transformations in BaTiO<sub>3</sub>.

Keywords: diffuse scattering, ferroelectrics, atomistic simulation

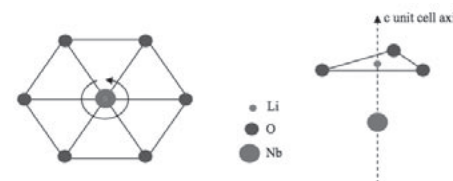
**P03.01.24***Acta Cryst.* (2008). **A64**, C225**Structural investigation of lithium niobate between 293 and 100K**

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A comparative study have been carried using X-ray diffraction investigation on a single crystal of LiNbO<sub>3</sub> at 120 K and ambient temperature. The Lithium Niobate (LiNbO<sub>3</sub>) is a ferroelectric inorganic compound largely used in the integrated and guided optical waves. The LiNbO<sub>3</sub> compound is a also known for its interesting properties in the in the non-linear optical field. The components of the first hyperpolarizability present large values compared to the known inorganic compounds in the non linear optical domain. The according field transparency extends from 350 to 5000 nm and its manufacturing process is well controlled. The experimental data were obtained from high resolution x-ray diffraction experiment. The data processing was carried using the formalism as described by Blessing in 1989. The structure refinement was carried out using the program MOLLY taking into account the contribution of the non spherical electron distribution. The reliability factors obtained at the end of the refinement are 6 % for ambient experiment and about 3 % for the

low temperature investigation. This present investigation has shown clearly a small displacements of 1 % (figure-1) of the Oxygen atoms around the Li-Nb axis. However, the crystal structure of Lithium Niobate seems to be stable in the large temperature investigated domain.



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Keywords: monocristal, linbo<sub>3</sub>, refinement

**P03.06.25***Acta Cryst.* (2008). **A64**, C225**Computer modelling of local structure, properties and stability of NaCl-KCl solid solution**

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Computer modelling of NaCl-KCl (halite - sylvite) solid solution was accomplished by atomistic pair potentials with using of GULP program [1], which is based on search of energy minimum. The mixing properties of NaCl-KCl solid solution (enthalpy  $\Delta H$ , interaction parameter  $Q$ , deviations from additivity of unit cell volume  $\Delta V$  and bulk modulus  $\Delta K$ ) are in quite good agreement with the recent experimental data [2] and essentially confirm the main conceptions of crystal chemical theory of solid solutions [3]. Calculated vibrational entropy  $\Delta S$  which is nearly independent on temperature plays important role in the mixing Gibbs energy. The latter allows us to obtain stability boundaries of solid solution, which are in good agreement with experimental decomposition diagram. Analysis of solid solution structure relaxation leads to conclusion that both anionic and cationic sublattices are distorted, but anionic one is distorted much more. Calculations of local valence balance on all types of ionic sites reveal the deviations from valence balance on cationic sites, whereas the general balance is maintained. The values of electrostatic potential in ionic positions display the reduction of bonding force in solid solution in comparison with pure crystals NaCl and KCl.

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Keywords: solid solutions, mineral crystal structures, computer modelling solids