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Report:

INTRODUCTION

The ferroelectric perovskites $KNbO_3$ and $BaTiO_3$ is a very important class of materials exhibiting on cooling, at room pressure and from the Curie temperature T_c, the phase transition sequence :

***cubic** (paraelectric)→ **tetragonal** (ferro) → **orthorhombic** (ferro) → **rhombohedral** (ferro)* (C-T, T-O, O-R). As pressure increases a lowering of the various transition temperatures is observed.' However despite the very interesting physical features of these compounds, their phase diagrams and their equations of state are hardly known. Recent investigations under pressure using dielectric measurements on $BaTiO_3$ [2] and XAFS on $KNbO_3$ and $PbTiO_3$ [3], are worth mentioning.

The present work concern x-rays investigations of the $KNbO_3$ perovskite in the diamond anvil cell (DAC) up to 35 GPa between 95 and 520 K. These investigations aim at obtaining, first the stability range of the ferroelectric domains, and secondly information on the high pressure structures and the equation of state.

EXPERIMENTAL

The high-pressure devices used were membrane diamond anvil cells (DAC) designed in our laboratory.[4] The diamond culet diameters were around 500 μm and the full (48) x-ray aperture was 56°. A preindented stainless-steel gasket confined the sample ($KNbO_3$ powder + silicon oil as pressure transmitting medium) into a 150 μm diameter hole. Small ruby pellets were placed into the hole for *in situ* pressure measurement according to the shift of the ruby luminescence R_1 line. The cell was placed either in a cryostat or a thermostat for the experiments at low and high temperature respectively. Powder diffraction was performed in an angle-dispersive method on station ID09 with image plate detector. The monochromatic x-ray beam ($\lambda \sim 0.4$ A), parallel to the symmetry axis of the DAC, was collimated down to 50x50 μm^2 and cleaned up close to the cell to avoid gasket signal. During exposure times, the cell was rocked through ± 3 ° in order to improve the crystallite averaging. A silicon powder standard was used to determine the wave-length and sample-to-plate distance.

RESULTS AND CONCLUSIONS

We investigated the four isotherms 520, 300, 200 and 95 K up to 35 GPa and the isobar 1GPa. The locations of the various transitions (C-T, T-O, O-R) determined during the present work are consistent with our Raman results?

Our present conclusions are the following :

i) The ferroelectric-paraelectric transition temperature T_c undergoes a slight non-linear drop suggesting only a « classical » regime for the transition in all the temperature range, specifically we have not observed a rapid drop at low temperature assigned to a quantum regime as claimed for $BaTiO_3$.[2]

ii) The above remark holds for the tetragonal-orthorhombic and orthorhombic-rhombohedral transitions, in other words no regime change was observed at low temperature.

iii) The pressure dependence of the cell volume fits well with a Murnaghan equation, i.e. the bulk modulus B writes :

$B = B_0 + B'p$; assuming $B' = 4$, B_0 is found close to 170 GPa. $KNb0_3$ is found less compressible than $BaTi0_3$ for which $B_0 = 140$ GPa.

We must point out that, contrary to other reports,[6] $KNbO_3$ is not amorphous above 15 GPa, moreover after each pressure run -more than 10 pressure runs were performed along the x-ray and the Raman investigations- we always observed a recovered product unchanged compared to the initial sample.

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