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Report:

AIM OF THE EXPERIMENT

The present work concerned x-rays investigations of the $BaTiO_3$ perovskite in the diamond anvil cell (DAC) up to 40 GPa between 20 and 295 K. These investigations aimed 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. 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 ($BaTiO_3$ 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 Rl line. The cell was placed either in a cryostat for the experiment at low temperature. 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 avaraging. A silicon powder standard was used to determine the wavelength and sample-to-plate distance.

RESULTS I

We investigated the four isotherms 294,225, 80 and 24 K up to 45, 18, 32, 8 GPa respectively and the two isobars 0.5 and 2.5 GPa between room temperature down to 24 K. The locations of the various transitions (cubic-tetragonal, tetragonal-orthorhombic, orthorhombic-rhomboedral) determined during the present work are given in Fig. 1.

Our present conclusions are the following :

i) The transition domains of the orthorhombic-rhombohedral transformation were very spread out but can be located close to the results of Ishidate et al.'.

ii) The orthorhombic-tetragonal transition locus was in agreement with Ishidate results in the temperature range 200-300 K. At low temperature we obtained larger transition pressures.

iii) The latter remark applied for the tetragonal-cubic transition.

4i) The fit of our room temperature data with a Murnaghan equation provided a bulk modulus B_0 close to 150 GPa in agreement to that deduced from Brillouin scattering experiment.[2] It is to be noted that $BaTiO_3$ is more compressible than $KNbO_3$ for which B_0 = 170 GPa.[3]

5i) At low temperature our cell volume data vs pressure did exhibit anomalous concavities (curves with no concavity or concave downward). This was due to the poor quality of the pressure transmitting medium. Silicon oil is too rigid at low temperature as compared to the sample. This in fact may explain the discrepancy with the Ishidate results.

Experiments with a better transmitting medium (argon or helium) must be undertaken.

REFERENCES

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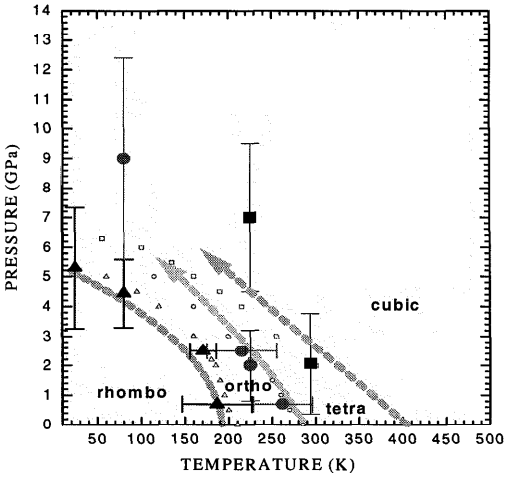

Fig.1 Phase diagram of $BaTiO_3$ (present status)

▫ , ○ , △ dielectric data : Ishidate et al

▲ , ● , ■ respectively ortho-rhombo, ortho-tetra, tetra-cubic transition locus (present work)

horizontal and vertical bars : widths of the transition zone

dash broad lines : trends according to this work