The determination of the *P-T* phase diagram of $PbZrO_3$

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$PbZrO_3$ is an end member of the most practical piezoelectric material PZT. At ambient conditions it exists in an orthorhombic perovskite-type structure and has an antiferroelectric property. Pressure-induced transitions were studied up to 80 GPa at room temperature by us. On the other hand, it transforms to the cubic structure and turns to paraelectric at 230℃ at ambient pressure. The pressure dependence of this transition temperature (*Tc*) was studied up to only 0.8 GPa by Samara using a dielectric measurement; *Tc* once increases slightly and then becomes almost constant.

We have tried to determine *Tc* to higher pressure by an X-ray diffraction experiment. A multianvil driven by a 1,500 ton hydraulic press was used to obtain powder X-ray diffraction patterns at high pressure and high temperature. The cubic anvils made of WC-Co alloy has the triangle front face with 8 mm edge. A powdered sample was filled inside a graphite tube heater in an octahedral magnesia with 14 mm edge length. Pressure was determined from the lattice parameter of NaCl powder placed adjacent to the sample. X-ray diffraction was detected by an SSD.

Each diffraction peak in the cubic phase is separated into a few closely adjacent peaks in the orthorhombic phase. However, the latter became gradually only one broad peak with increasing pressure due to the pressure gradient and the strain caused in the sample by the use of a solid pressure medium. As a result, we did not detect the orthorhombic-cubic transition by the peak shape. Then, we have estimated the halfwidth (FWHM) of the peak corresponding to the 240+004 in the orthorhombic phase and the 200 in the cubic phase. The temperature changes of FWHM are plotted in Fig. 1. The temperatures at which the width abruptly decreases on heating, that is, 175℃ and 145℃ are considered to be *Tc* at 6 GPa and 10 GPa, respectively.

The obtained *Tc* is plotted as asterisk(*) in the P-T diagram shown in Fig. 2, in which the pressure-induced phase transitions observed at room temperature by our previous measurements. The present results clearly indicate that the boundary between the orthorhombic and cubic phases decreases rapidly at high pressure. The elongation of this boundary is necessary to determine the relation with the other high pressure phases found at room temperature.

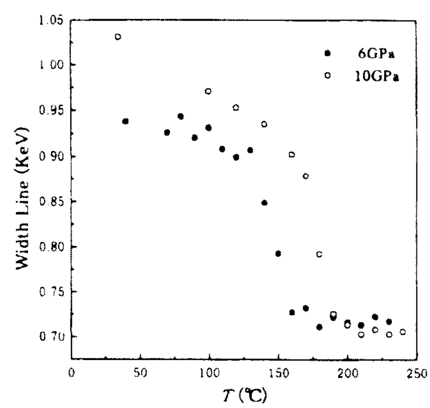

Fig. 1

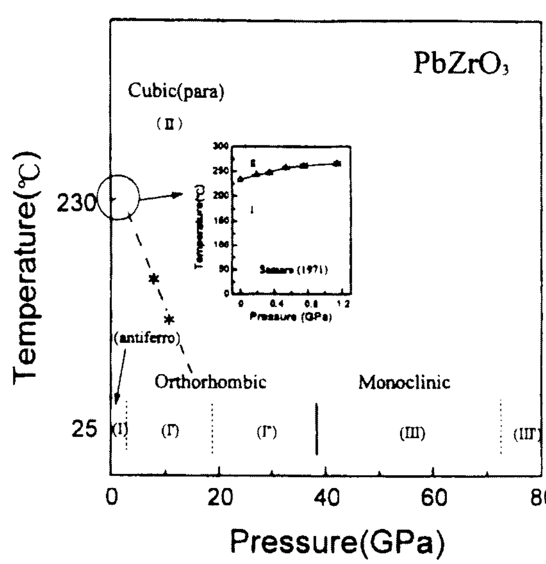

Fig. 2