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

***S. Endo(3065), Y. Kobayashi(3078), M. Nishino(3087), H. Katoh(3071) and T. Tsukawake(3088)**

Research Center for Materials Science at Extreme Conditions, Osaka University, Toyonaka, Osaka 560, Japan

Lead Zirconate ($PbZrO_3$), produces the most important piezoelectric material known as PZT, is antiferroelectric and crystallized in the orthorhombic structure (phase I) under ambient condition. It transforms to paraelectric cubic phase II above 230℃. Samara reported the transition temperature, T_C, between them using a dielectric measurement up to 1.2 GPa. We have tried to determine T_C by 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 have the triangle front face with 8 mm edge. A powdered sample with in a teflon cell was filled inside a graphite tube heater in an octahedral magnesia with 14 mm edge. Pressure was determined from the lattice parameter of NaCl. Diffracted X-rays were detected by an SSD.

Each diffraction peaks in the cubic phase are separated into a few closely adjacent peaks in the orthorhombic phase. In the previous experiment (1998A0138-ND-np), the latter peaks overlapped each other and became gradually only one broad peak with increasing pressure, we regarded as the pressure gradient and the strain caused in the sample by the use of a solid pressure medium. So in this time it was tried to measure under hydrostatic pressure. But we could not detect the transition, too. Therefore we have estimated the full width at half maximum (FWHM) of the peaks corresponding to the 240+004 in the orthorhombic phase and the 200 in the cubic phase in the same way as the previous experiment. The temperature dependence of FWHM is plotted in Fig. 1. T_c are considered to be 265℃ at 1.4 GPa. The *P-T* phase diagram for $PbZrO_3$ is shown in Fig. 2 in which the boundary between the phase I and the phase II, that is, T_c of phase I, determined by Samara is shown together with the results obtained in the our study on SPring-8 as astarisk(∗). The result indicates the existence of the maximum of critical point, between 1.4 GPa and 6 GPa. It is necessary to examine whether this phenomenon is related to the obtained anomaly of Raman scattering and dielectric constant at around 3 GPa at room temperature.

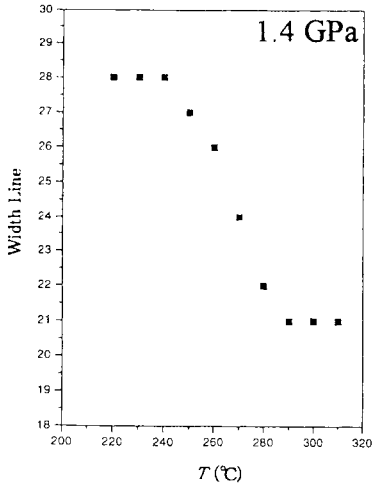

Fig. 1

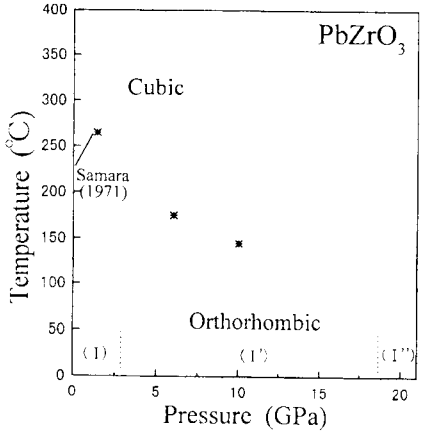

Fig. 2