

## Equation of state for B1 and B2 KBr

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Pressure-induced phase transformation of alkali halides is the structural change from the rock salt structure (B1) to the cesium chloride structure (B2) during which the coordination number changes from six to eight. It has been argued that the bulk modulus  $K_T$  would drop when the phase transformed from B1 to B2, in association with weakening of bond strength [1]. It has been, however, controversial whether the  $K_T$  increases or decreases during the phase transition [2, 3, 4]. Almost all experimental volume measurements have been conducted under non-hydrostatic conditions, so that the volume data would be expected to be collected under hydrostatic condition. We determined the volume-pressure relationships for B1 and B2 structured potassium bromide at hydrostatic pressures by in-situ X-ray observation.

**Experimental**

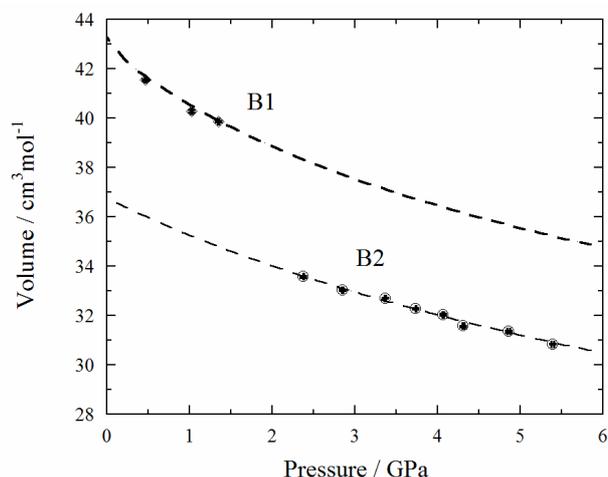
High pressure experiments were conducted using the MAX80 system installed at the PF-AR NE5C. The KCl powder and the NaCl pressure marker were sealed in a Teflon capsule with a mixture of methanol and ethanol (4:1 in volume) to generate a hydrostatic condition. X-ray diffraction patterns were taken by an energy dispersive method using a Ge-SSD up to 5.4 GPa at a room temperature

**Results and Discussion**

Volume data of B1 and B2 phases of KBr are shown in Fig.1 as a function of pressure. The data have been fitted to 3rd order Birch-Murnaghan EOS based on the finite strain analysis [5]. The bulk moduli, their pressure derivatives and molar volumes at ambient pressure are listed in Table 1. As the pressure range of the B1 stability field is small and we have only three data points, only the  $dK_T/dP$  was evaluated with the fixed  $V_0$  and  $K_{T0}$ . The  $dK_T/dP$  is slightly larger than the ultrasonic value. The  $G$  vs  $g$  plot for B2 KBr can be fitted by a straight line, so that the  $dK_T/dP$  is assigned the common value of four. The least squared fitting yields the molar volume and bulk modulus of the B2 KBr at ambient pressure equal to

Table 1. Equation of state parameters.

	$V_0$ cm <sup>3</sup> /mol	$K_{T0}$ GPa	$dK_T/dP$
B1	43.28 <sup>*</sup>	14.8 <sup>#</sup>	6.2 (2)
B2	36.77 (1)	22.0 (1)	4 (fixed)

<sup>\*</sup> Calculated from JCPDS.<sup>#</sup> Ultrasonic data [6].**Figure 1.** The pressure-volume relation of KBr.

36.77 cm<sup>3</sup>/mol and 22.0 GPa. These values are different from the previous estimation of  $V_0 = 37.9$  cm<sup>3</sup>/mol and  $K_{T0} = 17.0$  GPa [7].

We calculated the bulk moduli of both the B1 and the B2 KBr at the pressure of the phase boundary at ambient temperature (1.74 GPa). The bulk modulus of the B1 phase equal to 25.0 GPa is apparently smaller than that of the B2 (28.7 GPa) at 1.74 GPa. This is opposite to Hofmeister's results based on the IR spectroscopy [1]. Sims et al [8], however, pointed out her analysis was inadequate because of her model ignoring the second neighbor shell effect. Combined with the recent compression studies [2, 4, 6], our results support the common concept that the dense high pressure form is more rigid than the low pressure one.

**References**

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