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CHARACTERISTICS OF THE SHOCK INDUCED TRANSFORMATION IN BaF_2

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I. INTRODUCTION

Two of the several structure types commonly displayed by the solids with the formula AB_2 , in which B is fluorine at room temperature and one atmospheric pressure, are quasi-six-coordinated rutile and eight-coordinated fluorite. The rutile structure is tetragonal and the fluorite structure is cubic. In situ high pressure x-ray diffraction studies and related post mortem analyses of quenched materials of the AB_2 compounds have revealed a large number of polymorphic transitions in these compounds at high pressures.¹ Most of these studies have been carried out at room temperature and the transition pressures have been only roughly established. The situation is further complicated by varying rates of transformation in the different AB_2 compounds, which has made the study of these compounds by static high pressure methods difficult. Since the shock compression method had been successful in determining the pressure of transition in various materials,² it prompted us to use this technique to establish transition pressures in these compounds.

The starting material chosen was barium fluoride because the pressure of transition for it is one of the lowest among the fluorides studied so far.³ The shock compression experiments reported in this work were performed on the gas gun facility at Washington State University.

In order to make this paper self-contained, we first summarize the information available on barium fluoride from static compression studies and then present the results of our shock compression work.

II. RESULTS OF STATIC COMPRESSION IN BARIUM FLUORIDE

Phase transformations in barium fluoride (BaF_2) at elevated pressure under static conditions have been studied by several investigators.^{1,4,5,6,7,8,9,10} Of these, the investigations of Seifert,^{5,6} and of Dandekar and Jamieson⁹ consisted in analyzing the quenched specimens of BaF_2 subjected to high pressure and temperature by the x-ray diffraction technique. The rest pertain to in situ high pressure investigations of BaF_2 . Both types of investigations established that (1) BaF_2 , which crystallizes in the fluorite structure (from now on identified as $\beta\text{-BaF}_2$) at ambient condition, transforms to the orthorhombic $\alpha\text{-PbCl}_2$ structure (from now on also identified as $\alpha\text{-BaF}_2$) at elevated pressures.¹¹ (2) The transition from $\beta\text{-}$ to $\alpha\text{-BaF}_2$ is extremely sluggish at room temperature, i.e. the transition is characterized by a large hysteresis. (3) $\alpha\text{-BaF}_2$ is 10% to 11% denser than the fluorite phase at the ambient conditions.

The results of these investigations vary in three respects: (1) with regard to recovery of the high pressure polymorph of barium fluoride on release of pressure; (2) with regard to the magnitude and direction of change in pressure of transition with increasing temperature; and, (3) with regard to the pressure of transition at room temperature. These differences are described below in that order.

Under hydrostatic pressure, $\alpha\text{-BaF}_2$ transforms back to $\beta\text{-BaF}_2$ on release of pressure.⁸ In anvil type pressure generating systems, $\alpha\text{-BaF}_2$, once formed, is metastably recovered.^{1,5,9}

Samara⁸ reports that the pressure of transition decreases with increasing temperature. For example, whereas the transition pressure at 22°C is 26.8 kbars, the transition pressure at 200°C is around 20 kbars. The values of dP/dT are $\sim -2.6 \times 10^{-2}$ kbars/°C below 100°C and $\sim -2.2 \times 10^{-2}$ kbars/°C between 100° and 300°C. The results of ref. 9 indicate that the transition pressure tends to decrease with increasing temperature. However, Seifert's work⁵ indicates that the pressure of transition tends to increase with increasing temperature. He reports an increase of 22 kbars in transition pressure when temperature is increased from room temperature to 200°C. It is not clear if the increased pressure is an equilibrium pressure.

Values of transition pressure at room temperature reported by various investigators are listed in Table 1. It is seen that variations in transition pressure are quite large.