SHOCK INDUCED TRANSFORMATION IN BaF

$$t = \tau_1 \text{ or } \tau_2 \qquad (a_p)^2 \cdot (1/\rho_0) \cdot (\partial u/\partial h)_{t,h=0} = F \qquad (11b)$$

$$\tau_1 < t < \tau_2$$
  $(a_p)^2 \cdot (1/\rho_0) \cdot (\partial u/\partial h)_{t,h=0} > F$  (11c)

In the derivation of the conditions expressed by Eq. (11), it has been assumed that particle velocity decreases with increasing propagation distance. These conditions do not seem to violate any fundamental relations. In terms of the rate of change of density, the above sets of conditions imply that during the time interval 0 and up to  $\tau_1$ , the rate of change of density at the interface may be positive or negative. In the case it is positive, its magnitude must be less than the value of F/a<sup>2</sup>. During the time interval  $\tau_1$  and up to  $\tau_2$ , the rate of change of density must be positive and its magnitude must be larger than the value of F/a<sup>2</sup>. At the time points  $\tau_1$  and  $\tau_2$  either both the rate of change of density must be positive and F are identically zero or the rate of change of density must be positive and balance with the value of F/a<sup>2</sup>. None of the situations described above violates any physical conditions, especially since a negative rate of change of density is observed in an elastic-plastic relaxing material as a shock compression wave propagates in it.

In BaF<sub>2</sub>, the situation may be more complicated if above 25 kbars it behaves both plastically and starts to transform to its  $\alpha$ -phase. We plan to pursue the present study of polymorphic behavior of BaF<sub>2</sub> further by performing the following experiments. (1) Experiments where stresses generated would be such that  $\beta$ -BaF<sub>2</sub> would almost instantaneously transform to  $\alpha$ -BaF<sub>2</sub>, i.e., probably at stresses in excess of 70 kbars; (2) experiments on the samples at high temperatures; (3) experiments measuring stress profile at various depths in the specimens of BaF<sub>2</sub> at varying initial temperatures; and (4) the above type of experiments will permit us to build a model for the behavior of BaF<sub>2</sub> under shock compression.

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## REFERENCES

1. D. P. Dandekar and J. C. Jamieson, <u>Proceedings of Symposium on</u> <u>Crystal Structures at High Pressures</u>, American Crystallographic Association (1969) pp. 19, and the references in the article.

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- O. E. Jones and R. A. Graham, <u>Accurate Characterization of the High-Pressure Environment</u>, National Bureau of Standards Special Publication 325, U.S. Government Printing Office, Washington, D.C., 1971, pp. 229 and references therein.
- 3. Lead fluoride which is isostructural to BaF<sub>2</sub> transforms at 4.8 kbars at 23°C. Hence, lead fluoride would have been the ideal material to start with, but for the unavailability of a good large single crystal of the same. On the other hand BaF<sub>2</sub> crystals are readily available and economical to perform experiments with.
- 4. S. Minomura and H. G. Drickamer, J. Chem. Phys. <u>34</u>, 670 (1960).
- 5. K. F. Seifert, Ber. Bunsenger, Physik. Chem. 70, 1041 (1966).
- 6. K. F. Seifert, Fortschrift Miner. 45, 214 (1968).
- J. H. Chen and H. I. Smith (Report AFCRL-66-601), (1966) and Bull. APS <u>11</u>, 414 (1966).
- 8. G. A. Samara, Phys. Rev. B1, 4194 (1970).
- 9. D. P. Dandekar and J. C. Jamieson (Unpublished).
- 10. J. R. Kessler and M. Nicol, Bull. APS II, 17, 123 (1972).
- 11. Both structures contain 4 molecules per unit cell. In the fluorite structure (space group Fm3m-05) barium atoms are in a cubic close-packed type of arrangement with fluorine atoms occupying all the tetrahedral sites. Each fluorine atom is surrounded by 4 barium atoms disposed tetrahedrally, and each barium atom by 8 fluorine atoms disposed toward the corners of a cube. In the  $\alpha$ -PbCl<sub>2</sub> structure (space group Pbnm-v<sup>16</sup>) each barium atom is surrounded by 9 fluorine atoms, but all of these atoms are not equidistant from the cation they surround. This structure may be considered as a distorted close-packing of fluorine atoms with the barium atoms accommodated in the same plane with them. For details see: R. W. Wyckoff, Crystal Structures, Vol. 1, (Interscience, New York, 1963). Chapter IV.
- 12. B. F. Naylor, J. Am. Chem. Soc. 67, 150 (1945).
- 13. A similar transition has been observed in SrCl<sub>2</sub>, BaCl<sub>2</sub>, SrBr<sub>2</sub> below their respective melting points. These compounds are isostructural to CaF<sub>2</sub> and BaF<sub>2</sub>. The possible nature of this transition may be inferred from the x-ray diffraction work of Croatto and Bruno on SrCl<sub>2</sub>. They suggested that the resulting high temperature structure shows a disordering in the anion

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