

High-pressure phase transition in BaSe

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A new high-pressure phase transition in BaSe has been found to occur at a pressure of 60 ± 2 kbar using both direct visual and x-ray-diffraction high-pressure techniques. The phase transition, from a NaCl(*B1*) to the CsCl(*B2*) structure, has an associated volume decrease of 13.9% and produces a color change in the specimen from yellow to a deep red.

BaSe has been found to undergo a structural phase transition from the NaCl(*B1*)-type structure at ambient pressure to the CsCl(*B2*)-type structure at 60 ± 2 kbar with an associated volume decrease of 13.9%. Visual observation of the specimen under pressure revealed a change from its characteristic light yellow color at pressures below 60 kbar to a deep red color at pressures above 60 kbar. Upon unloading, the specimen returned to its original yellow color.

The high-pressure phase was studied utilizing a Ruoff-Baublitz-type gasketed opposed diamond anvil cell described elsewhere.¹ A fine ground powder of BaSe as well as a 4:1 methanol-ethanol mixture and a small ruby chip were loaded into the 150- μ m gasket hole and pressurized. The pressure was obtained from the shift of the ruby fluorescence lines,² while a hydrostatic environment is obtained by the use of the methanol-ethanol mixture.³

The BaSe compound was obtained from CERAC Inc.,⁴ and was of purity greater than 99.5%. The as-received BaSe powder (-20 mesh) was a deep red in color but took on a light yellow color upon heating to 600°C in hydrogen gas for 36 h. X-ray diffractometer measurements taken on the hydrogen-treated BaSe powder revealed its NaCl-type crystal structure and a lattice constant of 6.593 ± 0.016 Å, consistent with its American Society for Testing and Materials card designation.

X-ray studies of the new high-pressure phase utilizing CHESS (Cornell High Energy Synchrotron Source) and energy-dispersive x-ray-diffraction techniques revealed new peaks which were consistent with a cubic high-pressure structure. Comparison of the x-ray peaks for the new high-pressure phase with those of CsBr at room pressure (CsCl structure) reveals many similarities in their peak intensity ratios as shown in Table I. This should be expected due to the nearly equivalent scattering factors of Ba^{2+} and Cs^{1+} , and of Se^{2-} and Br^{1-} . The prominence of the (110) reflections, as well as the near absence of the (111) and (210) reflections, are consistent with assigning the CsCl structure to the new phase of BaSe.

Data taken at a pressure of 82.5 kbar gave a lattice parameter of 3.795 Å with a standard deviation of 0.007 Å for the seven observed peaks of the new phase. A more detailed intensity calculation is being prepared and will be published in the future along with data on the bulk modulus and its variation with pressure.

This CsCl-type structure found for BaSe at high pressure is expected from earlier work on BaS by Yamaoka *et al.*,⁵ BaO by Liu and Bassett,⁶ and the alkali halides⁷ which undergo similar structural transitions to a CsCl or a closely related structure.

Similar work is currently being performed on BaTe in which a similar structural transition is expected. Bridgman⁸ has already observed a discontinuity in his compressibility data at approximately 50 kbar, and optical observation by us has revealed an optical transition at a similar pressure when observed in an ungasketed diamond cell.

BaTe, assuming it is fully ionic, is a closed-shell system which is isoelectronic with xenon. It is predicted that BaTe will become metallic at a pressure of 300 kbar,⁹ a pressure much below that which was

TABLE I. Comparison of observed peak intensities of BaSe and CsBr.

<i>hkl</i>	BaSe	CsBr
100	Not observable ^a	Weak
110	Very strong	Very strong
111	Not observable ^b	Very weak
200	Medium	Medium
210	Very Weak	Weak
211	Strong	Strong
220	Medium	Medium
310	Medium	Medium
321	Medium	Medium

^a Obscured by Se fluorescence peak.

^b Obscured by (220) reflection of the remaining *B1* phase of BaSe. No indication for a strong or medium (111) reflection was noted.

required to metallize xenon.^{10,11} The study of the band-gap variation with pressure in BaTe is under way.

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