

**PS18.01.10 HIGH PRESSURE STRUCTURES OF GROUP V ELEMENTS AND GROUP IV-VI COMPOUNDS.**

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Using two-dimensional data collection techniques combined with synchrotron x-ray powder diffraction, similar high-pressure phases have been observed to exist in the group V elements Sb and Bi, and the group IV-VI compounds PbS, PbSe, and PbTe.

Our high-resolution angle-dispersive data, collected using image plates from samples within diamond anvil high-pressure cells, has shown that one high-pressure structure type is common to all five materials we have studied. The structures offer a transition route to a body-centered cubic phase in Sb and Bi, and to a CsCl-type structure in the Pb-chalcogenides.

The final structure solutions were aided by a new technique involving a MonteCarlo algorithm. This method, originally used in studies of molecular crystals, was modified to allow us to locate atomic positions accurately enough to be used in conventional Rietveld refinements.

**PS18.01.11 STRUCTURAL SYSTEMATICS OF THE PRESSURE-INDUCED PHASE TRANSITIONS IN P, As, Sb AND Bi.**

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Based on the results of a series of our diffraction studies on the title elements on laboratory X-ray and synchrotron radiation sources and the results recently reported, it is possible to express the sequence of structural phase transitions observed in them in a unified form as follows:

<b>P</b>	A17---	A7 ----	PSC		
<b>As</b>		A7 ----	PSC ----	dist.BCC(II)----	BCC
<b>Sb</b>		A7 ----	----	dist.BCC(I) ----	BCC
<b>Bi</b>		A7--	mod.PSC--	dist.BCC(I)----	BCC

Abbreviations used are A17 (orthorhombic layered structure), A7 (rhombohedral layered structure), PSC (primitive-simple-cubic) and BCC (body-centered-cubic). dist.BCC(I) represents the tetragonal structure, which is regarded as a distorted BCC (Iwasaki & Kikegawa, 1990; Chen et al, 1994), dist. BCC(II) the orthorhombic structure regarded as another kind of distorted BCC (Greene et al., 1995) and mod.PSC the monoclinic structure reinterpreted as a modified PSC (Chen et al., 1996).

The table suggests that the dist.BCC and BCC phases will form in **P**, though relevant pressure is extremely high.

Chen, J. H., Iwasaki, H., Kikegawa, T. (1996). High Pressure Research, in press.  
Chen, J. H., Iwasaki, H., Kikegawa, T., Yaoita, K. & Tsuji, K. (1994). AIP Conf. Proc. No, 309, 421-424.

Greene, R. G., Luo, H. & Ruoff, A. L. (1995). Phys. Rev. **B51**, 597-600.  
Iwasaki, H. & Kikegawa, T. (1990). High Pressure Research **6**, 121-132.

**PS18.01.12 PHASE TRANSITION OF CeAuGe UNDER PRESSURE.**

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We have characterized the pressure induced structural phase transition of CeAuGe from a layer type structure at ambient pressure into a high pressure polymorph with a three dimensional anion framework by means of full profile refinement of x-ray powder data.

A large number of binary intermetallic phases  $RE M_2$  ( $RE =$  rare earth metal;  $M = Cu, Ag, Au, Ga$ ) crystallize in  $A1B_2$  varieties. Ternary phases like  $RE Au Ge$  ( $RE = Sc, Ce, Lu$ ) form closely related crystal structures. Substituting the rare-earth metal causes a change of the  $[AuGe]$  polyanions from two dimensional fragments in CeAuGe to a three dimensional network in ScAuGe [1]. Hydrostatic pressures induce similar changes of the gallium framework in binary  $RE Ga_2$  compounds. Thus, the investigation of the ternary intermetallic compound CeAuGe is performed in order to compare the effects of pressure on the chemical bonding in these two classes of compounds.

At ambient pressure CeAuGe crystallizes in the NdPtSb type structure (ordered  $CaIn_2$  variety,  $P6_3mc$ , no. 186) [2]. At a pressure of 9(1) GPa we observe a structural phase transition and data sets of the high pressure modification can be indexed and refined assuming an orthorhombic  $TiNiSi$  type ( $Pnma$ , no. 62) crystal structure. Calculation of the Au-Ge bond lengths reveal that the phase transformation is associated with a change of the anion coordination from trigonal to distorted tetrahedral.

[1] R. Pöttgen et al., J. Alloys Comp., in press.

[2] R. Pöttgen et al., J. Magn. Magn. Mat. 152 (1996) 196.

**PS18.01.13 STRUCTURAL CHANGE IN MOLTEN KCl AND KBr UNDER PRESSURE.**

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Pressure-induced structure change in the molten KCl and KBr has been extensively studied by the X-ray diffraction analysis. Energy dispersive X-ray diffraction experiments were conducted up to 4 GPa by using the cubic type high pressure apparatus, MAX90, and the synchrotron radiation. The derived radial distribution functions show that the molten KCl and KBr transform from a NaCl-like structure into a CsCl-like structure. The structure change in both melts starts at the atmospheric pressure and continues with increasing pressure, accompanied by the gradual increase of the coordination number of the nearest neighbor ions. The phase transition in melt is completed at 1.5 GPa for KCl and at around 2 GPa for KBr. The dense CsCl-like high pressure melts are stable above these pressures. In the solid state, both alkali halides take the NaCl structure below 1.8 GPa, and they take the CsCl structure above this pressure. The phase transition pressure in molten KCl is clearly lower than that in solids. In these materials, the structural change in melt precedes the phase transition in solid.