

## Structure of liquid SnSe under pressure

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### Introduction

IV-VI compounds are regarded as average group V material. In crystalline group V elements and IV-VI compounds, the Peierls distortion occurs. Strong bonds with short bond length and relatively weak bonds with long bond length coexist in the crystal. Therefore anisotropic contraction of the local structure is expected under pressure [1]. In crystalline SnSe, atoms form two dimensional networks of covalent bonds with coordination number of three at the normal pressure. No pressure-induced transition in the crystalline phase has been reported.

In liquid SnSe, the local structure at the normal pressure is known to be similar to that of crystalline phase: The coordination number is about three and layer structure remains upon melting [2]. On the other hand, the local structure of liquid GeSe and liquid GeTe and its pressure dependence are different from those of the crystalline phase [3].

### Experimental

X-ray diffraction patterns were taken by an energy-dispersive method using the synchrotron radiation. Pressure was generated by using the multi-anvil high-pressure apparatus, MAX80, installed at AR-NE5C.

### Results and discussion

Figures 1 show the static structure factor  $S(Q)$  of liquid SnSe at various pressures.  $S(Q)$  changes its shape with increasing pressure. If the local structure contracts uniformly,  $S(Q)$  expands towards higher  $Q$  without changing its height. The change in the shape of  $S(Q)$  indicates an anisotropic structural change with pressure. The height of the first peak increases with changing its position towards higher  $Q$  value. On the other hand, the height of the subpeak decreases with changing its position towards lower  $Q$  value. Figure 2 shows the pair distribution function  $g(r)$  of liquid SnSe at various pressures. The main peak consists of two subpeaks. The sharp subpeak around 2.8 Å indicates the presence of the covalent bonds between atoms in the liquid. With increasing pressure, it shifts towards larger  $r$  in spite of the volume contraction, although its rising position does not shift. The subpeak at larger  $r$  shifts towards smaller  $r$ . This change suggests the shortening of the long bonds between the atoms on the adjacent layer with increasing pressure. The  $r_2/r_1$  ratio decreases with increasing pressure. If the peak positions indicate the intralayer atomic distances, the bond angle changes from 93° at 1.0 GPa to 81° at 7.0 GPa. These pressure dependences of the local structure of liquid SnSe are different from those of the crystals.

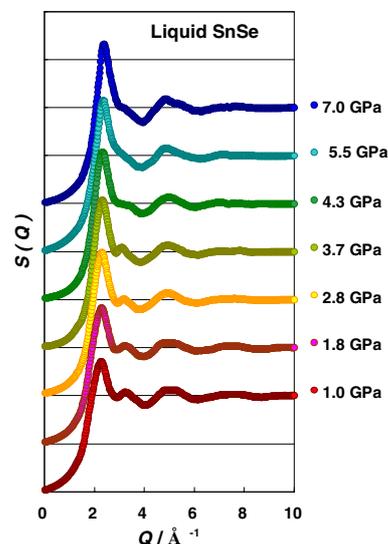


Figure 1.  $S(Q)$  of liquid SnSe at various pressures

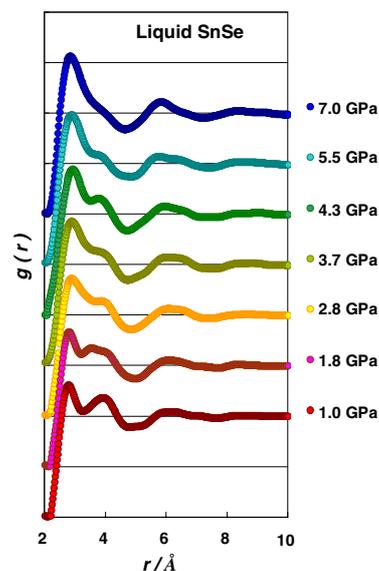


Figure 2.  $g(r)$  of liquid SnSe at various pressures

### References

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- [2] A. Onodera *et al.*, Phys. Rev. B **56**, 7935 (1997).
- [3] M. Tomomasa *et al.*, Proc. 21<sup>st</sup> AIRAPT conference, Catania, 2007, in press.

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