

## Structure of liquid GeSe under pressure

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### Introduction

In crystalline GeSe, atoms form two dimensional networks of covalent bonds with coordination number of three at the normal pressure and the room temperature and at high temperature it transforms to a rocksalt (B1) structure with coordination number of six. In liquid GeSe, the local structure at the normal pressure is known to be different from the rocksalt structure but similar to the ternary coordinated structure [1]. The presence of the Peierls distortion was reported and the strong covalent bonds between intralayer atoms and the relatively weak bonds between interlayer atoms coexist. An anisotropic local contraction is expected in the liquids with increasing pressure.

### 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 GeSe 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 hands, the height of the subpeak decreases. The pressure dependence of  $S(Q)$  changes around 6 GPa. In the low  $Q$  region of  $S(Q)$  of liquid GeSe, there is a small peak around  $1.2 \text{ \AA}^{-1}$ . It was observed up to 1.7 GPa and its height decreases with increasing pressure. This peak suggests that the networks of the covalent bonds similar to the crystal with two dimensional zigzag planar structure remains in the low pressure region. Figure 2 shows  $g(r)$  of liquid GeSe at several pressures. The main peak consists of two subpeaks. The sharp subpeak around  $2.8 \text{ \AA}$  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 and the weakening of the Peierls distortion. The  $r_2/r_1$  ratio changes from 1.47 at 0.7 GPa to 1.33 at 8.0 GPa. If the peak positions indicate the intralayer atomic distances, the bond angle changes from

$94^\circ$  to  $84^\circ$ . These pressure dependences of the structure of liquid GeTe are different from those of the crystal.

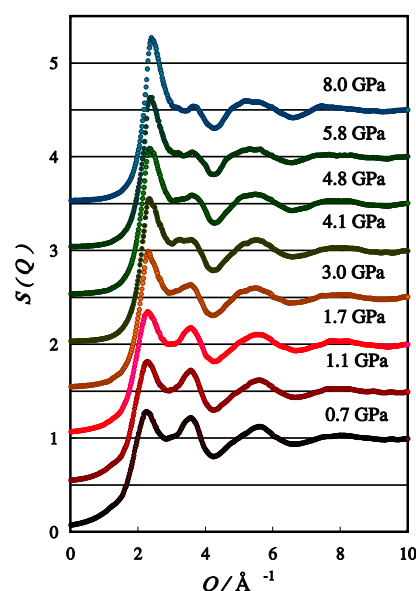


Figure 1.  $S(Q)$  of liquid GeSe at various pressures

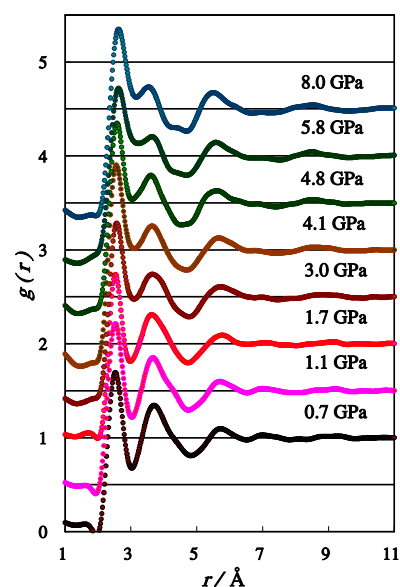


Figure 2.  $g(r)$  of liquid GeSe at various pressures

### References

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  - [2] A. Onodera et al., 1997 Phys. Rev. B 56 7935 (1997).
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