

## Structure of liquid GeTe under pressure

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### Introduction

In crystalline GeTe, 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 GeTe, 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. Although the transition pressure in the crystalline phase is 18 GPa in GeTe [2], an anisotropic local contraction is expected in the liquids with increasing pressure below the transition pressure of the crystal.

### 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 GeTe 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 around  $3.2 \text{ \AA}^{-1}$  decreases.

The second peak consists of at least two subpeaks. With increasing pressure, the subpeak at the low  $Q$  side becomes higher with shifting its position towards lower  $Q$  and the subpeak at high  $Q$  side becomes lower. These suggest that the pressure-induced structural transformation occurs around 3 GPa. This behavior is different from those of liquid III-V and II-VI compounds [3, 4].

Figure 2 shows  $g(r)$  of liquid GeTe 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  $r$ . The height of  $g(r)$  at the first minimum increases with increasing pressure. With increasing pressure the Peierls-

type distortion becomes small and the bond angle decreases. A sharp change in  $S(Q)$  and  $g(r)$  was observed in liquid GeTe between 1.8 GPa and 4.0 GPa. These pressure dependences of the structure of liquid GeTe are different from those of the crystal.

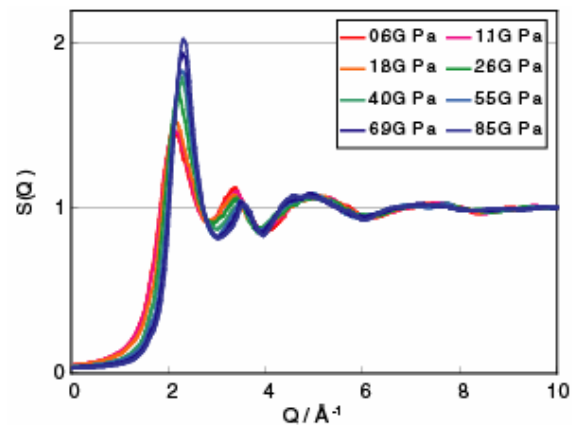


Figure 1.  $S(Q)$  of liquid GeTe at various pressures

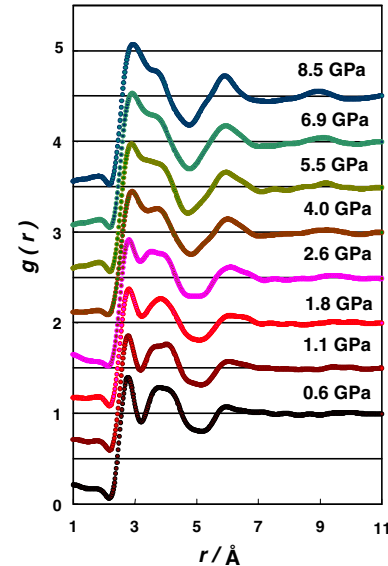


Figure 2.  $g(r)$  of liquid GeTe at various pressures

### References

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