Structure of liquid Ge-Te alloys under pressure

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Introduction

In Ge-Te alloys, the melting temperatures of GeTe compound and pure Te at ambient pressure are 724°C and 450°C, respectively. Between GeTe and Te concentration, the alloy is eutectic and the eutectic point locates at 85 at% Te and 365°C. In spite of the presence of GeO₂, GeS₂ and GeSe₂ compounds, the GeTe₂ compound does not exist. Pressure dependence of the local structure of liquid GeTe and liquid Te has been known [1, 2]. Both liquids show anisotropic contraction with increasing pressure indicating the change of the bonding between atoms. Relation of the local structure of liquid GeTe₂ and liquid Te is investigated.

Experimental

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

Results and discussion

Figures 1 show the static structure factor S(Q) of liquid GeTe₂ at various pressures. S(Q) changes its shape with increasing pressure. If the local structure contract 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. The subpeak around 3.4 Å⁻¹ also shifts towards higher Q value. Figure 2 shows g(r) of liquid GeTe₂ at various pressures. The main peak consists of two or three subpeaks. The sharp subpeak around 2.9 Å indicates the presence of the covalent bonds between atoms in the liquid. With increasing pressure, its position is kept almost constant. The peak at the right hand side approaches towards the first peak.

In the pressure region between 2.4 GPa and 5.7 GPa, S(Q) of liquid GeTe₂ is well reproduced by the simple model of the mixture of liquid GeTe and liquid Te. The discrepancy is large below 1.6 GPa and above 7.8 GPa. From these results, it is concluded that the local structure of liquid GeTe₂ is different from that of liquid GeO₂, GeS₂ and GeSe₂ compounds.

References

[1] M. Tomomasa et al., Proc. AIRAPT conference, 2007, in press.

[2] N. Funamori and K. Tsuji, Phys. Rev. B 65 (2001) 014105-1-5.



Figure 1. S(Q) of liquid GeTe₂ at various pressures



Figure 2. g(r) of liquid GeTe₂ at various pressures