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Pressure-Induced Structural Change in Liquid Ge-Te alloys

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Introduction

In liquid Ge-Te alloy, temperature-induced structural change was reported from atomic volume measurements [1]. In this liquid, atoms are covalently bonded with anisotropic interaction, and pressure is expected to cause microscopically anisotropic contraction similar to liquid Te and liquid GeTe [2, 3].

Experimental

X-ray diffraction patterns were taken by an energy-dispersive method using the synchrotron radiation. From the measured diffraction intensities, the static structure factors *S(Q)* and the pair distribution function *g(r)* of liquid metals were deduced.

Results and discussion

We have studied the pressure dependence of the structure of liquid $Ge_{33}Te_{67}$ and found a gradual but large change in *g(r)* with increasing pressure [4]. We confirm that the structure does not take the $Ge(Te_{1/2})_4$ tetrahedral network structure in any pressure up to 9 GPa, which is in contrast to liquid $Ge_{33}Se_{67}$ and $Ge_{33}S_{67}$.

Figures 1 shows the *S(Q)* of liquid $Ge_{0.15}Te_{0.85}$ at several *PT* conditions [5]. At 0.5 GPa, the height of the second peak decreases and the first peak position slightly shifts towards higher *Q* values with increasing temperature. Also with increasing pressure, the height of the second peak decreases and the height of the first peak increases. Simultaneously, the first peak position slightly shifts towards higher *Q* values similar to the change with increasing temperature.

Since the heights of the first and the second peaks of *S(Q)* change remarkably with temperature and pressure, the ratio of the heights of the first and the second peaks of *S(Q)* is investigated as a function of temperature at several pressures. At 0.5 GPa the slope of the ratio changes around 700 K. On the other hand, no change of the slope was observed at 1.8 GPa and 2.4 GPa. This implies that a temperature-induced liquid-liquid transformation occurs in liquid $Ge_{15}Te_{85}$ at 0.5 GPa.

Figure 2 shows a *P-T* diagram of $Ge_{15}Te_{85}$. The diamond shows the *P-T* conditions where *S(Q)* in Fig. 1 was obtained. The closed and open circles show the points where the high-temperature liquid and the low-temperature liquid exist, respectively. The dashed line shows the temperature where the kink was observed, which corresponds to the end temperature of the temperature-induced liquid-liquid transformation. The boundary between the low-temperature and the high-temperature phases has a negative slope in a P-T phase diagram. Since the high-temperature (high-pressure) phase has a smaller volume than that of the low-temperature (low-pressure) one, it is concluded from the Clausius-Clapeyron equation that the high-temperature (high-pressure) phase has larger entropy than the low-temperature (low pressure) one.

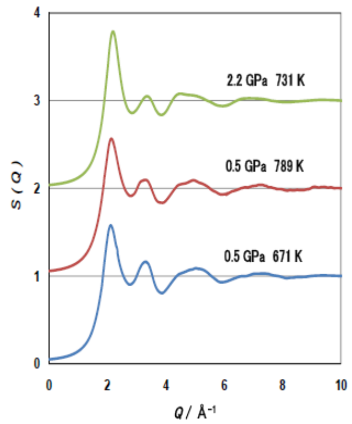

Figure 1. *S(Q)* of liquid $Ge_{15}Te_{85}$ at several *PT* conditions.

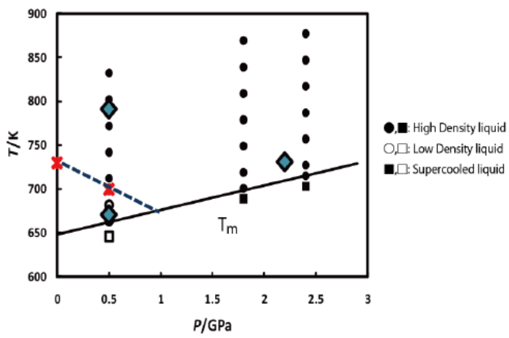

Fig.2 P-T phase diagram of $Ge_{15}Te_{85}$. The red asterisks show temperatures where the kink was observed in the ratio of the peak heights in *S(Q)*.

References

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