Static structure of liquid germanium alloys

by
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Abstract: Static structure of liquid germanium and alloys was measured by using the neutron scattering technique. The latest data of liquid structures measured by our research project are shown in this section.

1. Introduction

The liquid state can be regarded as a dense and disordered state. An atom migrates in the liquid with interaction to other atoms in the liquid. Therefore, for the understanding of the tracer atom of diffusion in liquids, it is important to know the configuration of its surrounding neighboring atoms in detail. The diffusion in liquid germanium is one of the main targets in this research project. The diffusion model of liquid germanium is being developed based on the hard sphere model coupled with actual liquid structures and molecular dynamics simulations. It is well known that the liquid germanium and liquid silicon show the characteristic liquid structures, in which a clear shoulders are observed at just beyond the first peak of Q (wave number) for the static structure factor, S(Q). The origin of these shoulders has been studied from the theoretical and experimental points of view. However, it has not been identified clearly. In this research project, the structure of liquid germanium alloys was measured carefully with the use of neutron scattering techniques. The obtained data are important references for molecular dynamics simulations and model construction. In this section, the experimental method and data obtained are described briefly.

2. Crucible for the neutron scattering experiments in the high temperature

The neutron scattering technique is useful for the measurement of structure of liquid metals because of high transparency of neutron beam for the most of materials. This merit provides us that the wide variety of materials can be applied as the crucible material for the neutron scattering experiment of high temperature melts. In the case of liquid germanium alloys, the liquidus temperatures are higher than 1200K. Therefore, the crucible materials must be selected carefully and a few kinds of ceramic materials have been used for the neutron scattering experiments. In this project, the grassy carbon which has been used for shear cell in our project was for the first time applied to the crucible material for the neutron scattering experiments. The grassy carbon is a hard material and resists the corrosion by high temperature metallic melts. We made the cylindrical shape of crucible, whose diameter was 10 mm and wall thickness was 0.5 mm by using the glassy carbon. The diffraction pattern of glassy carbon is observed as amorphous-like halo pattern. Therefore, the neutron diffraction of sample can be obtained without obstacle Bragg peak of crucible material, as can be seen in figure 1. This is the great merit for the observation of characteristic liquid structure of germanium alloys because the Bragg peaks of the most of crucible materials are positioned near the first peak of Q for the S(Q) of liquid matters.

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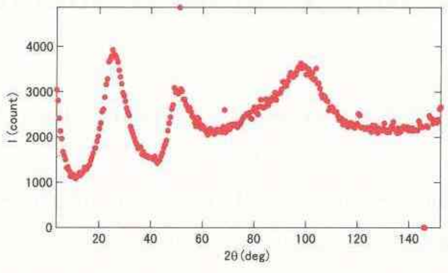

Figure 1 Diffraction pattern of glassy carbon crucible

3. Brief summary of experimental results

The neutron scattering experiments of liquid Ge-Sn and liquid Ge-Si alloys were performed at the Japanese Research Reactor 3 (JRR3) in Japan Atomic Energy Research Institute (JAERI) with the use of glassy carbon crucible. In this research project, members used two kinds of different diffractometers, HERMES for Ge-Sn and HRPD for Ge-Si. The crucibles containing samples were installed in a radiation heating furnace with Nb foil heater and were heated under a high vacuum condition. The details of experiments and correction procedures (absorption, normalization, etc.) were described in the previous report of our research project [1].

3.1 Static structure of liquid germanium-tin alloys

The S(Q)'s of liquid Ge-20 atomic%Sn were measured by using the neutron scattering technique at the temperatures of 1273K, 1523K and 1773K. The obtained S(Q)'s were shown in figure 2 together with those of liquid Ge and liquid Sn. The characteristic feature of S(Q) of liquid Ge remains to be present in the S(Q) of liquid Ge-Sn alloy, in which the shoulder shape was observed at the high Q side of the first peak of S(Q). The temperature dependence of S(Q) of Ge-Sn is not so large. However, the height of first peak decreases slightly with increasing the temperature.

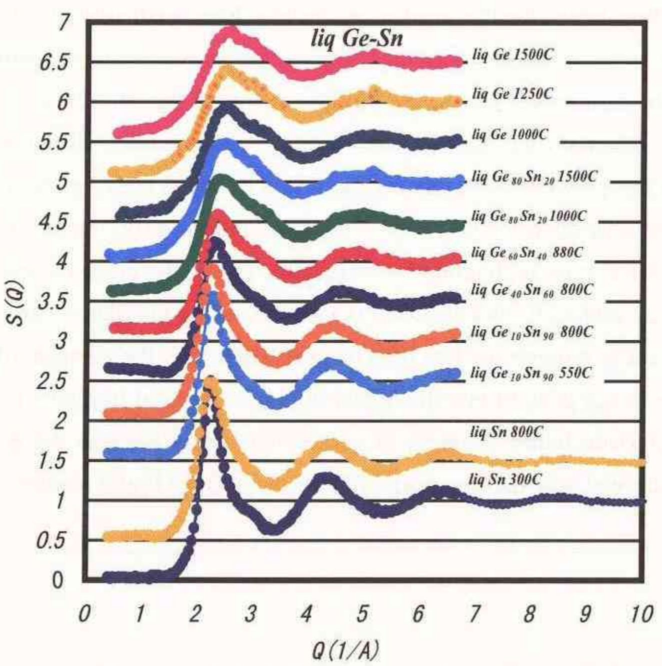

Figure 2 Static structure factor of liquid Ge-Sn alloys

3.2 Static structure of liquid germanium-silicon alloys

The S(Q) of liquid Ge-50 atmic%Si was measured by using the neutron scattering technique at the temperature of 1583 K. The obtained S(Q) was shown in figure 3. The shoulder of S(Q) was clearly observed for the liquid Ge-Si alloy. This particular feature of S(Q) for liquid Ge-Si alloy is same as that of liquid Ge.

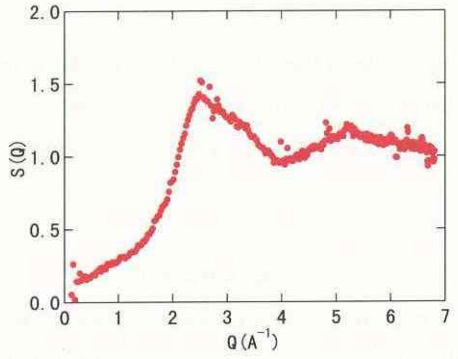

Figure 3 Static structure factor of liquid Ge-50 atomic% Si

4. Summary

The liquid structures of Ge-Sn alloys and Ge-Si alloy were measured by using the neutron scattering technique. The glassy carbon can be applicable for the crucible materials for neutron scattering experiments of reactive materials at high temperature. The shoulder of the first peak of S(Q) was able to be observed in both liquid Ge-Sn alloys and liquid Ge-Si ones.

Reference

[1] "Modeling and Precise Experiments of Diffusion Phenomena in Melts under Microgravity" Annual Reports 2001, NASDA-TMR-020025E.