

## Structure of Liquid InAs under Pressure

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### Introduction

In order to elucidate the effects of the ionicity in chemical bonding on the structure of covalent liquids, we have investigated the structure of liquid III-V compounds. Recently we reported the structure of liquid GaSb [1] and liquid InSb [2] under pressure, which are relatively less ionic among III-V compounds. Succeeding to the study, we have investigated the structure of liquid InAs, which is more ionic than the liquids.

### Experimental

X-ray diffraction patterns were taken by an energy-dispersive method using the synchrotron radiation source and the multi-anvil high-pressure apparatus, MAX80, installed at AR-NE5C. The pressure and temperature conditions of the measurements are shown in Fig. 1. Here, the phase diagram determined in this study is shown together.

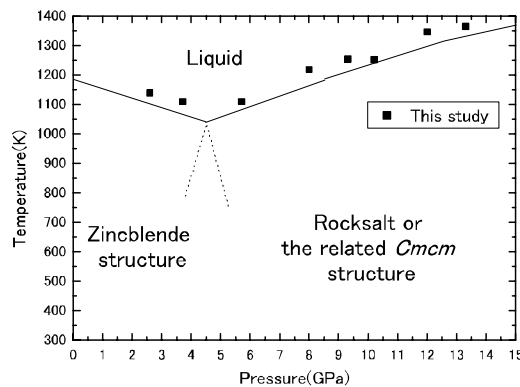


Fig.1 PT conditions for the data collection of liquid InAs.

### Results and Discussion

The structure factors,  $S(Q)$ , at high pressures are shown in Fig. 2. Throughout whole pressure region of the present study, the hump is observed at the right-side of the first peak ( $Q=3.3 \text{ \AA}^{-1}$ ). It implies the existence of a non-simple local structure in the liquid.

With increasing pressure up to 9 GPa, the shape of the profile does not change markedly and the  $S(Q)$  only shifts toward a large  $Q$  value. On the other hand, at pressures above 9 GPa, the first peak becomes higher and the hump becomes smaller with increasing pressure. These results suggest that the contraction behaviour changes from a uniform one into a non-uniform one at about 9 GPa, and that the local structure gradually changes above 9 GPa. To reveal the local structure and the pressure-induced change, we analyzed pair distribution function,  $g(r)$ , which is obtained by the Fourier transformation of  $S(Q)$ , by the two-species model in conjunction with a distorted crystalline model [1]. The results show that the structure of the liquid InAs is explainable by the mixture of the

beta-tin-like and bcc-like local structures, rather than the previously reported crystalline forms, zincblende-type or NaCl-type structures [3], and also that the ratio of the bcc-like local structure gradually increases above 9 GPa (Fig. 3). From these results, we conclude that the non-uniform contraction above 9 GPa is due to the gradual change in the local structure from the beta-tin-like one into the bcc-like one. The detail results and discussion are reported in Ref. [4].

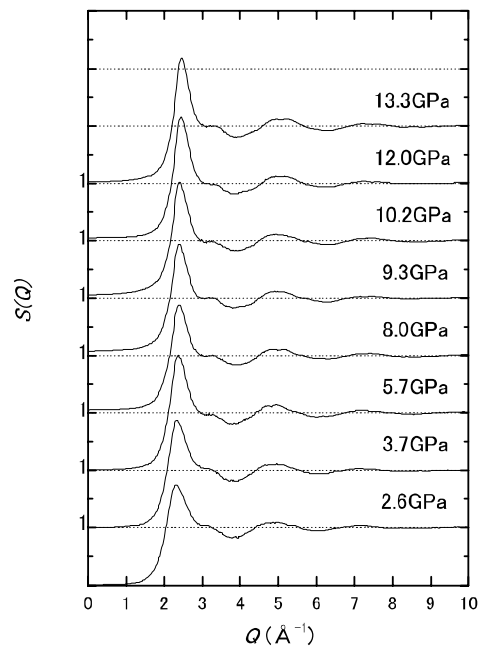


Fig. 2  $S(Q)$  of liquid InAs at various pressures.

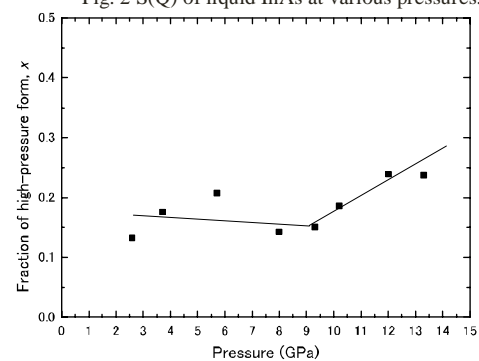


Fig. 3 Fraction of the bcc-like local structure at various pressures.

### References

- [1] T. Hattori et al., PRB **68**, 224106 (2003).
- [2] T. Hattori et al. (in prep.)
- [3] Vohra et al., PRB **31**, 7345 (1985), and references therein.
- [4] T. Hattori et al., J. Phys.: Condens. Matter **16** S997 (2004).

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