

Acoustic dispersion in liquids with Peierls distortions

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So far, we have conducted inelastic X-ray scattering (IXS) experiments on liquid Bi [1], liquid GeTe [2], liquid Sb [3], and liquid Ge₂Sb₂Te₅ [4] using the spectrometer at BL35XU/Spring-8. We have observed the dynamic structure factor $S(Q,E)$ and investigated the excitation energy associated with the collective motion of atoms. Bi, Sb, and GeTe, which have a crystal structure with Peierls distortion, have a local structure in which shorter and longer bonds appear alternately even on melting. Ge₂Sb₂Te₅ has a rock salt structure with pores, but in the liquid state, it is thought to have a local structure with Peierls distortion like the other liquids. When $S(Q,E)$ is analyzed using a model function consisting of a quasi-elastic component and two inelastic excitation components, the Q dependence of the excitation energy of the longitudinal acoustic mode in these liquids shows a flat-topped curve. The second excitation energy shows values smaller than the excitation energy of the longitudinal acoustic mode and we have regarded this low-energy excitation as the excitation originating from transverse waves in the liquids and have called it a transverse acoustic mode.

In this talk, we will mainly present the results of liquid phase-change material Ge₂Sb₂Te₅. Ge₂Sb₂Te₅ has been applied to a nonvolatile memory because of fast phase change between crystalline and amorphous states. We found that $S(Q,E)$ of ternary liquid Ge₂Sb₂Te₅ contains the third inelastic excitation component. The third excitation energy at the flat-topped Q region agrees with the energy at the corresponding Q in liquid GeTe. Because it is inferred that the vibration frequencies of the Sb-Te pair are different from those of the Ge-Te pair, the result suggests that they are observed separately. More interestingly, the third excitation energy behaves like an optical mode with decreasing Q towards 0. The destination seems to correspond to the vibration energy of four-fold coordinated Ge sites with an octahedral order in the amorphous state obtained by ab initio molecular dynamics (AIMD) simulations. The result suggests that four-fold coordinated Ge sites in the amorphous state are originated from those in the liquid state. These results indicate that $S(Q,E)$ obtained by IXS can provide important information on structural properties in the liquids.

[1] M. Inui et al., Phys. Rev. B. **92**, 054206 (2015).

[2] M. Inui et al., Phys. Rev. B **97**, 174203 (2018).

[3] M. Inui et al., submitted to J. Phys.: Condens. Matter.

[4] M. Inui et al., Phys. Rev. B. (2021) in press.

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