ESRF	**Experiment title:** Dynamic structure factor of liquid Ge	**Experiment number**: HS-849
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Report:

Liquid (l-) Ge has many unusual properties, which in the past have stimulated intensive experimental and theoretical investigations. Upon melting Ge undergoes a semiconductor-metal transition in which the density increases by about 4.7 % accompanied by significant structural changes: The coordination number grows from four in the solid to about 6.5 [1] in the liquid. Despite its metallic nature, the structure of l-Ge is more complicated than that of simple liquid metals. Besides a low coordination number, the structure factor $S(Q)$ has a shoulder on the high-Q side of the first peak. These features have been interpreted as indications that covalent bonds persist in the liquid states.

This interplay between metallic and covalent bondings makes l-Ge of particular theoretical interest. Most studies have been carried out using molecular dynamics (MD) techniques, and some of them [2] encompassed dynamic properties of l-Ge such as self-diffusion and collective motion. In contrast to the theoretical efforts, experimental studies for the dynamics have so far been limited to the measurements of diffusion coefficient [3]. In this article, we report the first results of dynamic structure factors $S(Q,\omega)$ of l-Ge from a high-resolution inelastic x-ray scattering experiment [4].

The experiments were carried out using a inelastic scattering spectrometer at ID28 in a transmission mode. The incident x-rays were chosen to be 17.794 keV obtained using an extreme backscattering geometry of Si(999). The energy resolution of the spectrometer was 2.98 meV. The sample was located in a single-crystal sapphire cell, which was placed in a

vessel equipped with Be windows and filled with He gas. High temperature of 980 °C was achieved using a W resistant heater and measured with two W-Re thermocouples.

Figure 1 shows the scattering intensity $I(Q)$ at Q = 13 nm^{-1}, which is almost a half Q value at the first maximum of $S(Q)$. Open circles indicate the experimental data, and the solid line shows the best-fit convolution of an enhanced-hydrodynamic-modes model with the experimental resolution function, which is shown as a dashed line in the figure. Although the data are fairly scattered, small but distinct phonon-peaks appear at ± 17-18 meV, which is the first indication of propagating modes in non-simple liquid metals. Each of the recent ab initio MD showed that the power spectrum of the velocity autocorrelation function has a strong shoulder around 20 meV, which is consistent with our data.

Figure 2 exhibits the Q dependence of the width z_0 of the central quasielastic peak (full circles), which are the results of the deconvolution. The dashed and dot-dashed lines indicate z_0-Q relations according to the well-known DQ^2 law using two results of the self-diffusion constants [3], respectively, and open circles the corresponding $S(Q)$ [1]. The present results show a strong *de Gennes* narrowing near the first maximum position in $S(Q)$. The solid line shows the theoretical results calculated according to an approximation for dense hard-sphere fluids on the basis of kinetic theory [5]. The present results show a narrower '*de Gennes* minimum' than the theory, which is probably due to the existence of the crystal fragments in l-Ge near the melting point.

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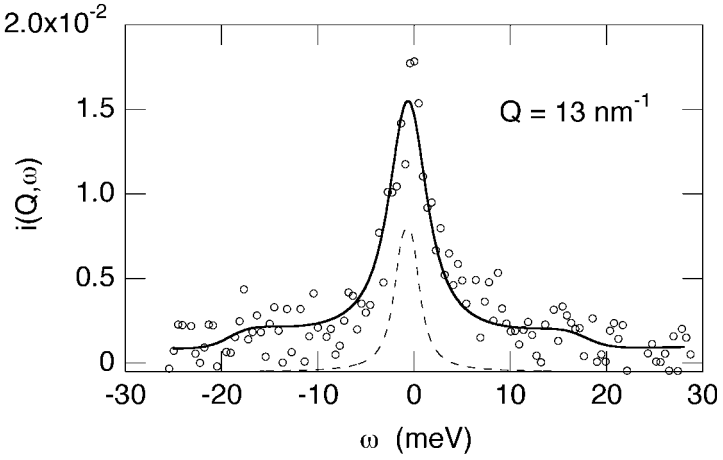

Figure 1

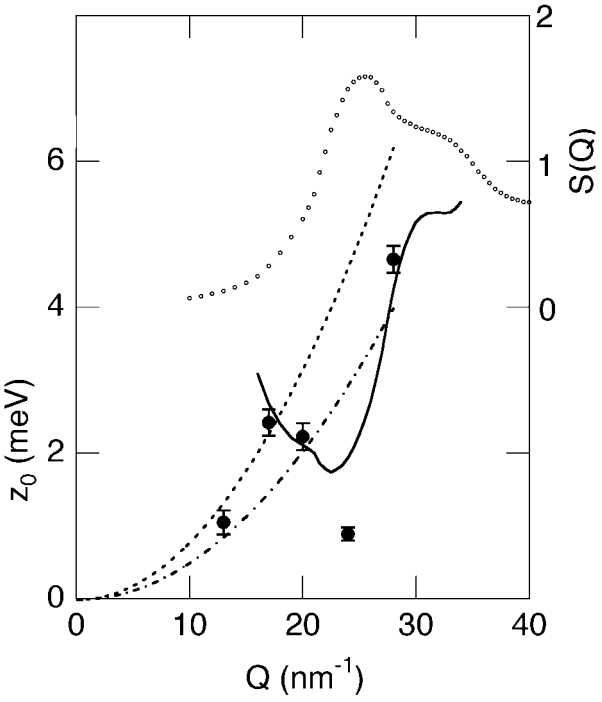

Figure 2