Experiment title: Dynamic structure factors of liquid Ge and Si	Experiment number: HS1155
Beamline: ID28	**Date of experiment**: from: 1 March 2000 to: 8 March 2000	**Date of report**: 1 Sept. 2000
Shifts: 21	**Local contact(s)**: Dr. Michael Krisch	*Received at ESRF:*

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Report:

Liquid (*l*-) Ge shows many unusual properties, which in the past have stimulated intensive experimental and theoretical investigations. Upon melting it 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 state to about 6.5 in the liquid [1]. Despite its metallic nature, the structure of *l*-Ge is more complicated than that of typical liquid metals like liquid alkalis. Besides the undercoordination, the structure factor $S(Q)$ of *l*-Ge has a shoulder on the high-Q side of the first peak, a feature that cannot be reproduced using a simple hard-sphere model. These features were interpreted as indications that covalent structures persist in the liquid state [1]. In this report we present the first results of the dynamic structure factor $S(Q,\omega)$ for *l*-Ge.

The sample was located in a single-crystal sapphire cell [2], placed in a high-pressre vessel equipped with Be windows capable to cover scattering angles of 0°-55° [3]. The vessel was filled with 2 bar of high-purity grade He gas. The temperatures of 980 °C and 1500 °C were achieved using a W resistance heater and measured using two W-5%Re:W-26%Re thermocouples. The experiments were performed for nine Q values between 2-28 nm^{-1}. A resolution correction was performed by fitting the convolution between a model function and the experimental data. As the model function, a Lorenzian was chosen for the central line and a damped harmonic oscillator [4] for the inelastic peaks.

Fig.1 shows the results of $S(Q,\omega)$ at 980 °C normalized to $S(Q)$ at Q = 2-12 nm^{-1}, where inelastic peaks can clearly be identified. Full circles represent the experimental data with error bars and the solid line is the best fit of the convolution integral to the data with the

experimental resolution function (a dashed line). At $Q = 2$ nm^{-1}, the sharp phonon peaks located at $\omega = \pm 3.8$ meV superimpose the central quasielastic line. With increasing Q, the width of both the elastic and inelastic peaks broaden, and especially the phonon peaks get to be highly damped. At $Q = 12$ nm^{-1}, which is about a half the Q value of the first maximum in $S(Q)$ (25 nm^{-1} [1]), the phonon peaks are located at ± 17.2 meV. The spectra in Fig. 1 demonstrate that the dynamics of l-Ge is dominated by longitudinal propagating modes, analogous to liquid alkali metals where phonon excitations are well known [5].

The excitation energy Ω_Q and the peak width Γ_Q as a function of Q are depicted in Fig. 2 by squares and triangles, respectively. The dashed line represents the dispersion of hydrodynamic sound obtained from recent measurements of the adiabatic sound velocity (2682 m/s). Of particular interest in this dispersion relation is the observation that within the experimental error, the positions of the phonon peaks lie on the hydrodynamic line in the low Q range up to 6 nm^{-1}. Namely, the so-called *positive* dispersion relation observed in liquid alkali metals [6] is not found in l-Ge. Almost the same results were also obtained at 1500 °C. Detailed scientific discussions are given elsewhere [6].

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[2] K. Tamura, M. Inui, and S. Hosokawa, Rev. Sci. Instrum. **70**, 144 (1999).
[3] S. Hosokawa and W.-C. Pilgrim, Rev. Sci. Instrum., submitted.
[4] B. Fak and B. Dorner, ILL Report No. 92FA008S, 1992.
[5] W.-C. Pilgrim *et al.*, J. Non-Cryst. Solids **250-252**, 96 (1999), and references therein.
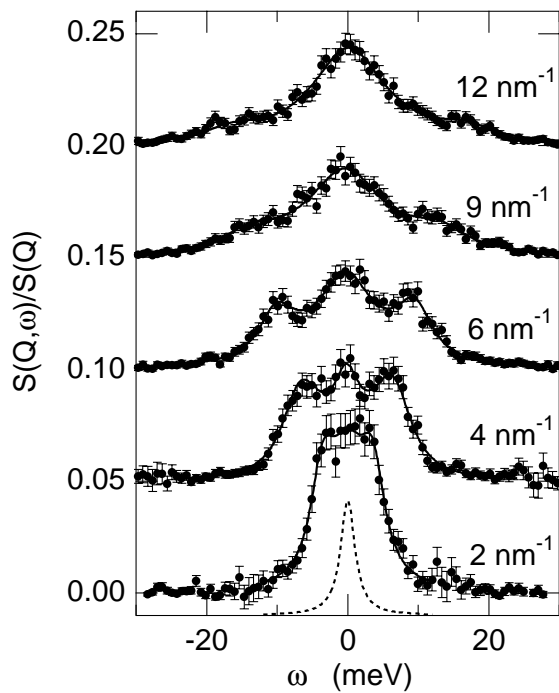[6] S. Hosokawa, Y. Kawakita, W.-C. Pilgrim, H. Sinn, M. Lorenzen, and M. Krisch, Phys. Rev. E, submitted.
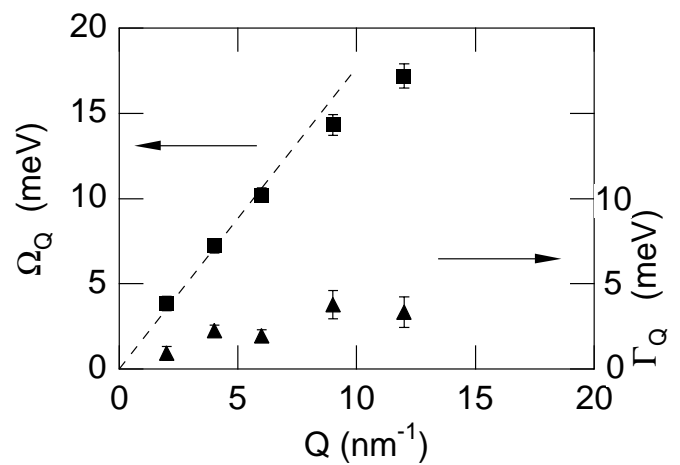
Fig. 1

Fig. 2