ESRF	**Experiment title:** Fine structure of the dynamic structure factor of the free electron gas	**Experiment number:** HE-2266
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Shifts: 9	**Local contact(s):** S. Huotari	*Received at ESRF:*

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Report:

An experiment to study the dynamic structure factor $S(q,\omega)$ of valence electrons in metallic sodium was performed at beamline ID16. The experiment was performed using a prototype of the recently inaugurated 9-element spectrometer designed for electronic excitations in the non-resonant inelastic x-ray scattering regime in the photon energy range of 9.7–10.0 keV. We used two analyser crystals, which were bent Si(110) wafers with a bending radius of 1 m and wafer diameter 100 mm. The analyser crystals had a difference in scattering angle of 6°, giving the possibility to measure the $S(q,\omega)$ for two different momentum transfers at a time.

The studied momentum transfer range was $q = 0.6 - 2\text{Å}^{-1}$ to study the regime where the plasmon enters the particle-hole continuum, and $q = 12$ Å^{-1} to measure the Compton lineshape. The spectra were measured with resolutions 1.0 eV and 1.5 eV depending on the momentum transfer. The sample was prepared in a miniature helium-flow cryostat in a glove box filled with argon, transported to the beamline within argon atmosphere and pumped to a vacuum of 10^{-6} mbar. All spectra were taken both in room temperature (RT) and at 6 K to observe if finite temperatures have an effect on the dynamic structure factor. This was believed to have an important effect since sodium is near to its melting point in RT, and the Debye-Waller factor changes dramatically between RT and 6 K. Thus temperature might broaden all band-structure related features in the dynamic structure factor.

The measured spectra in the plasmon/particle-hole regime are plotted in Figure 1 and in the Compton regime in Figure 2. The most important results can be preliminary summarised as follows. 1) There is no double-peak structure in the $S(q,\omega)$ of Na, which suggests that it is not a universal property of the electron gas. 2) The spectra are not affected largely by finite temperature since there is very little difference between the data between RT and 6K except for a small change in plasmon energy due to density difference. 3) The tail of the valence electron Compton profile exists also in low temperatures. Calculations within the TDDFT are currently being done for comparison with the experimental results. Most importantly we will obtain in near future a theoretical prediction for the non-existence of the double peak structure when band structure effects are also taken into account.

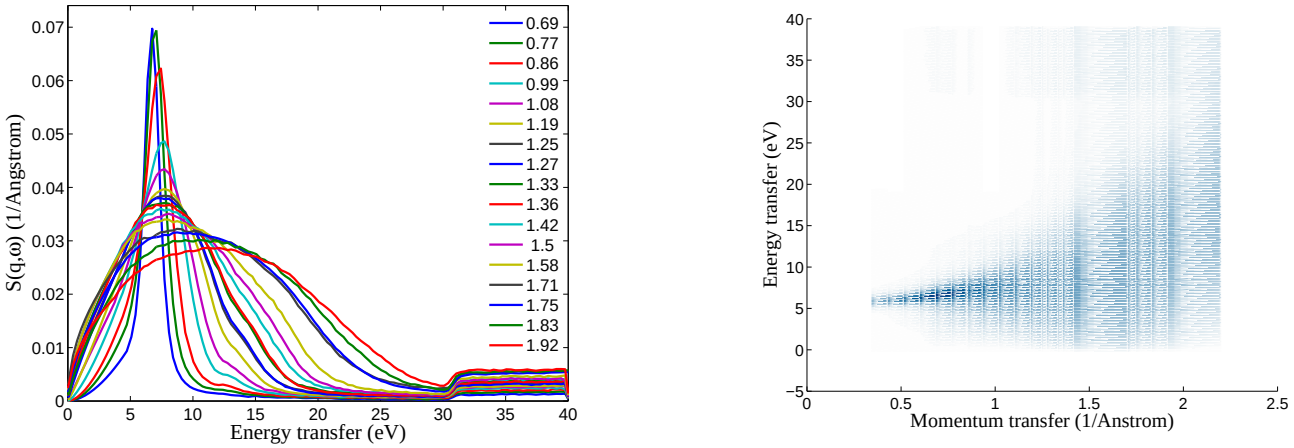

Figure 1. Left: $S(q,\omega)$ for Na at $T = 6K$ for momentum transfers mentioned in the legend in units of Å^{-1}. Smallest momentum transfer corresponds to the sharpest and highest peak, and largest to the broadest and lowest peak. The jump at 30 eV energy transfer is the Na $L_{2,3}$ edge. Right: $S(q,\omega)$ measured in RT, where slightly higher momentum transfer values were also measured (up to 2.2 Å^{-1}).

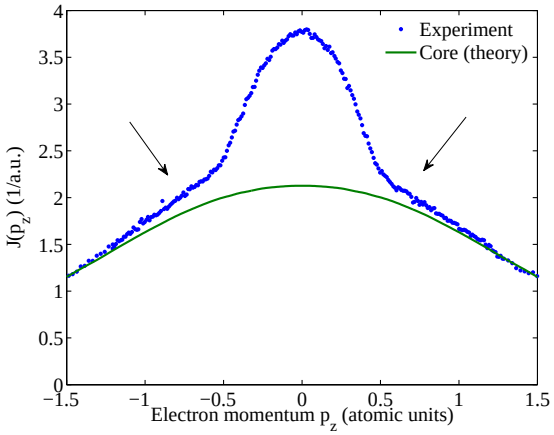

Figure 2. Measured high-resolution Compton profile at $T = 6$ K. It has been always observed that the valence contribution on top of the core electron contribution has much larger tails (marked by arrows) than explained by any electron theory. The fact that it exists also at 6 K shows that it cannot be explained by finite-temperature effects (e.g. by incorporating the Debye-Waller factors into the pseudopotential scheme) and other explanations must be sought.