

Observation of Umklapp Processes in Non-Crystalline Materials

Umklapp processes (U-processes) are scattering processes among elementary excitations in crystals where *momentum conservation* is fulfilled by a contribution from the lattice. Their existence has fundamental consequences on transport properties such as the finite thermal conductivity, the electrical resistivity via the electron-phonon coupling, and the electronic contribution to the heat capacity. These U-processes are understood for crystals, where they are associated with the lattice periodicity. Their existence in a topologically disordered system is a matter of debate. They are unexpected because of the absence of *long-range* order, but, one could also imagine that just the *local* order could support them, at least for those phonon-like excitations observed in disordered systems at wavelengths comparable to the inter-particle separation.

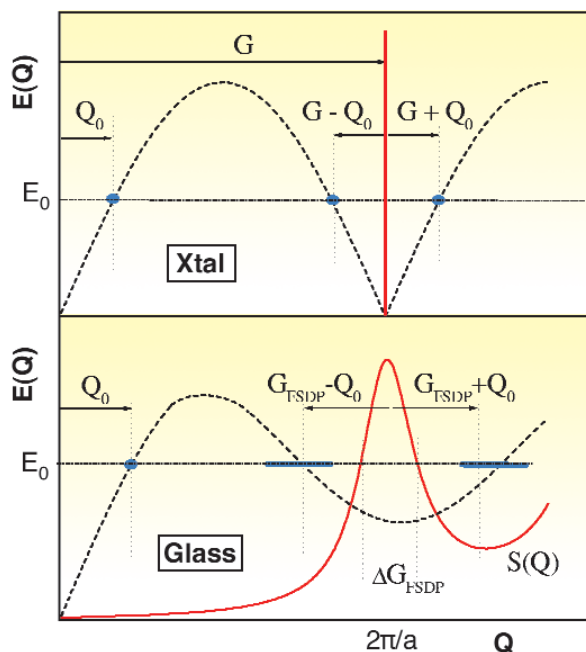


Fig. 1: Sketch of the dispersion relation $E(Q)$ (dashed lines) and of the static structure factor $S(Q)$ (red lines) of a one dimensional system. a) reports the case of an ordered chain; b) that of a disordered chain.

In **Figure 1a** we report the one-dimensional case of an acoustic phonon dispersion relation $E(Q)$ in a perfect chain with lattice constant a (dashed line). In such a system the dispersion relation repeats itself with a period $G = 2\pi/a$, while the static structure factor $S(Q)$ corresponds to Bragg peaks at Q -values $G_n = 2\pi n/a$ (full vertical line). If we now perform a scattering experiment at the fixed energy E_0 , we would observe a sharp Brillouin peak, at $Q = Q_0 \approx \hbar E_0/v$ where v is the sound velocity. This peak will also be observed at $Q = G \pm Q_0$, where G is any of the reciprocal

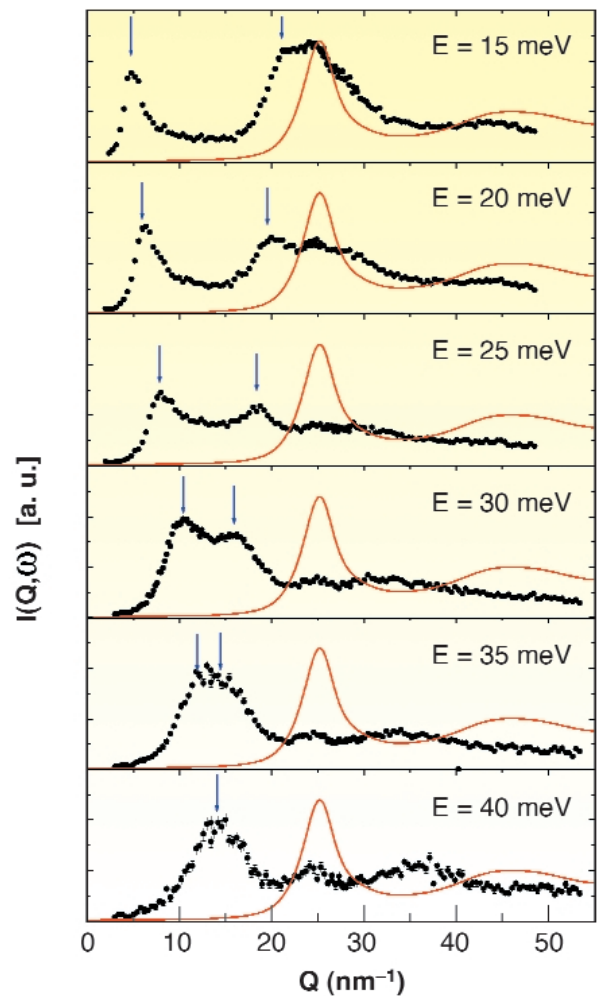


Fig. 2: IXS spectra of liquid lithium at $T = 475$ K (full circles) taken at the indicated constant energy as a function of Q . The blue arrows mark the position of the main spectral features (Brillouin peaks at low Q and Umklapp peaks around the FSDP). The red line in each panels is the $S(Q)$ reported on an arbitrary intensity scale.

lattice vectors: naively, one can say that the phonon of momentum Q_0 is "reflected" by the lattice (or by the Bragg peak at $Q = G$). In **Figure 1b**, we report an attempt to translate such scattering experiment from a periodic array into a disordered chain. In this case, the sharp Bragg peak is replaced by a feature, the so called First Sharp Diffraction Peak (FSDP), centered at $Q = G_{\text{FSDP}} \approx 2\pi/a$ (a is the average near neighbor distance). This feature has a finite width, ΔG_{FSDP} , determined by the distribution of nearest-neighbour distances that typically is an important fraction of G_{FSDP} . In analogy to the crystal case, one may expect that this FSDP is also capable of "reflecting" the phonons. However, with respect to the peak at Q_0 , the peaks at $Q = G_{\text{FSDP}} \pm Q_0$ will have a width increased by ΔG_{FSDP} .

IXS spectra of liquid Lithium, measured as a function of Q on the horizontal spectrometer of the **ID16** beamline at the indicated constant E values, are reported in **Figure 2** (full circles). In the same figure the static structure $S(Q)$ is also shown as a red line, and the FSDP is found at $G_{\text{FSDP}} \approx 25 \text{ nm}^{-1}$ with a width of $\Delta G_{\text{FSDP}} \approx 4 \text{ nm}^{-1}$.

In the small Q region a Brillouin peak that increases its Q position and width with increasing energy is observed. More importantly, the spectra show also other inelastic peaks at higher Q values (marked by the arrows). This ensemble of inelastic features can be interpreted within the same framework as the one sketched in Figure 1b. In fact, one observes, at low energy transfer E , not only the Brillouin peak at $Q_0(E)$, but also a second peak at approximately $G_{\text{FSDP}} - Q_0(E)$. Moreover, one clearly observes that, with increasing E , the peaks at $Q_0(E)$ and $G_{\text{FSDP}} - Q_0(E)$ get closer and, at the energy $E \approx 40$ meV, they merge together at a Q value correspondent to $G_{\text{FSDP}} / 2$.

In conclusion, we have shown that in a system without any periodic order such as a monatomic liquid, one observes inelastic excitations that can be interpreted as the non-crystalline counterpart of Umklapp peaks. These peaks are no longer sustained by the periodicity of the lattice –as in crystals– but are due to the “reflection” of the wave-like (Brillouin) excitations from the short range order that still exists in the disordered material.

Principal Publications and Authors

T. Scopigno (a), M. D’astuto (b), M. Krisch (b), F. Sette (b) and G. Ruocco (c), *cond-mat / 0010048*; T. Scopigno, U. Balucani, A. Cunsolo, C. Masciovecchio, G. Ruocco, F. Sette and R. Verbeni, *Europhys. Lett.* **50**, 189 (2000); T. Scopigno, U. Balucani, G. Ruocco and F. Sette, *Phys. Rev. Lett.* **85**, 4076 (2000).

(a) *Universita’ di Trento (Italy)*

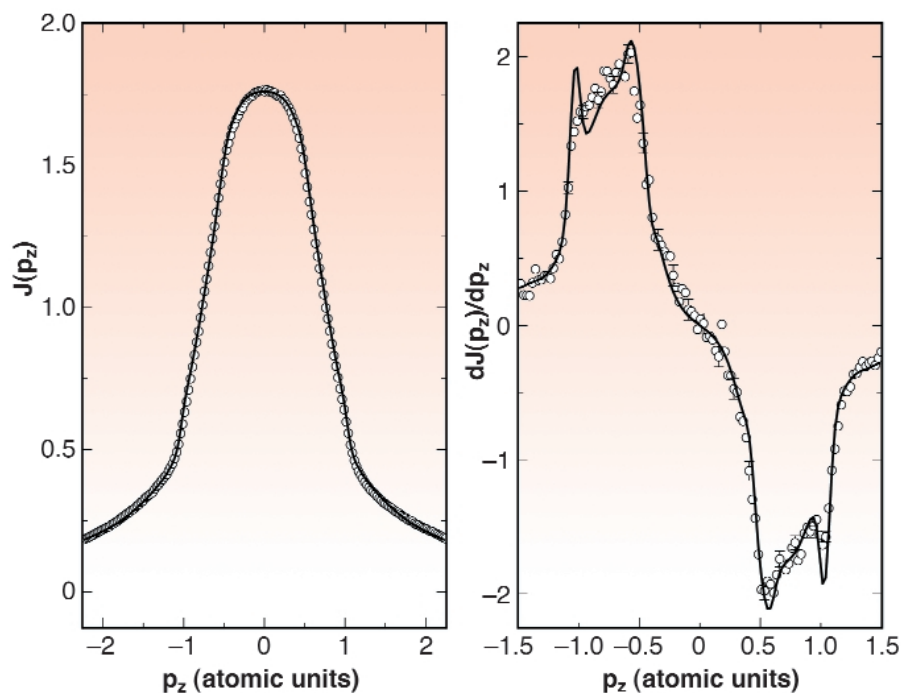
(b) *ESRF*

(c) *Universita’ di L’Aquila (Italy)*

Inhomogeneous Electron Gas: a Compton Scattering Study on Beryllium.

Compton scattering experiments aim to the determination of the three-dimensional momentum density distribution of the electronic system under study. Quite generally, in solids, the electrons of interest are the valence electrons, and fundamental questions one can address are,

Fig. 1: Left panel: the measured (circles) and theoretical (solid line) Compton profiles of Be with the scattering vector along the [110] reciprocal lattice vector. Right panel: the corresponding first derivative.



among others, the electron-electron and the electron-ion interactions. Practically, most methods for calculating valence electron wave functions in solids are based on the one-electron picture, and the so-called correlation effects are often neglected [1,2]. In the Compton scattering theory, the correlation effects are usually taken into account by the Lam-Platzman correction (LPC) [2], which is adequate in the case of a homogeneous electron gas. This correction has been shown to work reasonably well in the alkali metals Li, Na, K, and Rb, which are metals with one valence electron per primitive unit cell and therefore are the solid systems that approach the most a nearly homogeneous electron gas. In other metals the validity of the LPC has not been yet extensively studied.

We have studied the incident energy dependence of the Compton scattering cross-section and the momentum density of Be single crystals at **ID15B** and **ID16**. We measured the Compton scattering cross-section using incident photon energies of 10 (ID16), 29 and 56 keV (ID15B). The momentum space resolution in the experiments was 0.02, 0.08 and 0.16 atomic units, respectively. The measured Compton profiles are compared to an accurate local density approximation (LDA) based calculation of the momentum density in Be, the correlation effects being incorporated using the LPC.

An example of the measured and calculated Compton profiles is presented in **Figure 1**. The left panel shows the Compton profile taken with the scattering vector along the reciprocal lattice vector [110], and with the incident photon energy of 29 keV. The right panel shows the corresponding first derivative. Along are plotted the calculated profile and the corresponding derivative, both broadened to reflect the finite experimental resolution. The fine structure in the derivative arises directly from the complicated Fermi surface structure of Be, consisting of well-known “cigars”