



	<b>Experiment title:</b> Inelastic X-ray scattering of liquid Rb at high pressures and temperatures.	<b>Experiment number:</b> HD 443
<b>Beamline:</b> ID 28	<b>Date of experiment:</b> from: 13/04/2011 to:19/04/2011	<b>Date of report:</b>
<b>Shifts:</b> 18	<b>Local contact(s):</b>	<i>Received at ESRF:</i>
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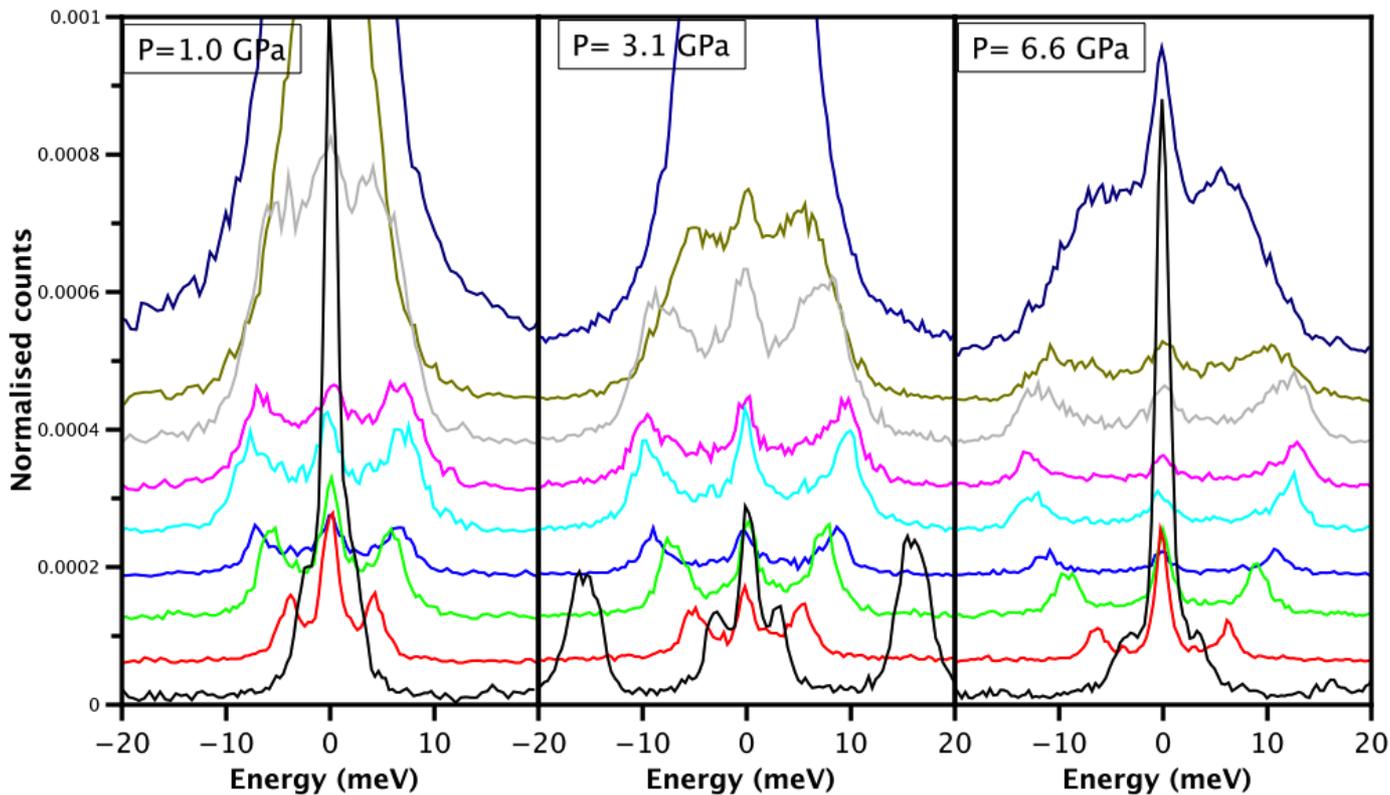
**Report:**

Rb was loaded in a Re gasket in a membrane diamond anvil cell. The IXS spectrum of liquid Rb at 573 K has been measured at 1.0, 3.1 and 6.6 GPa. The sound speed at the three pressures has been compared with the one obtained with ab initio simulations and published in:

T. Bryk, S. De Panfilis, F. A. Gorelli, E. Gregoryanz, M. Krisch, G. Ruocco, M. Santoro, T Scopigno, and A. P. Seitsonen Phys. Rev. Lett. 111, 077801 (2013)

**Abstract:** Density-driven phase transformations are a known phenomenon in liquids. Pressure-driven transitions from an open low-density to a higher-density close-packed structure were observed for a number of systems. Here, we show a less intuitive, inverse behavior. We investigated the electronic, atomic, and dynamic structures of liquid Rb along an isothermal line at 573 K, at 1.2–27.4 GPa, by means of ab initio molecular dynamics simulations and inelastic x-ray scattering experiments. The excellent agreement of the simulations with experimental data performed up to 6.6 GPa validates the overall approach. Above 12.5 GPa, the breakdown of the nearly-free-electron model drives a transition of the pure liquid metal towards a less metallic, denser liquid, whose first coordination shell is less compact. Our study unveils the interplay between electronic, structural, and dynamic degrees of freedom along this liquid-liquid phase transition. In view of its electronic nature, we believe that this behavior is general for the first group elements, thus shedding new light into the high-pressure properties of alkali metals.

<http://link.aps.org/doi/10.1103/PhysRevLett.111.077801>



**Figure caption: IXS spectra of liquid Rb at 573 K and 1.0, 3.1 and 6.6 GPa. The spectra at 1.0 and 6.6 GPa are relative to the same sample, while the spectra at 3.1 GPa are relative to another sample. The intense peaks at the smallest Q at 3.1 GPa are the transverse acoustic phonons from the diamond anvils.**