MICROSCOPIC DYNAMICS OF LIQUID METALS

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High frequency collective dynamics in liquid tellurium

**Motivation:**

- Study whether the macroscopic anomaly in the sound velocity (increases with T) has a microscopic correlate.
- Try to understand the propagation of excitations in disordered media

\[ T_m = 723 \text{ K} \]

Since \( v_s \sim 1000\text{ms}^{-1} \) in the studied temperature range, **THERMAL NEUTRONS** are required

**IN8 Configuration**

- \( \text{Cu}(200)-\text{Te}-\text{Cu}(111) + \text{tight collimations, } k_f = 4.1 \text{ Å}^{-1} \)
- \( \Delta E = 0.9 \text{ meV} \)
- Max energy transfer \( \sim 9 \text{ meV} \)
High frequency dynamics in liquid tellurium

Study of 2 thermodynamic states:
- Just above melting ($T_m = 723 \text{ K}$)
- At $\sim 1000 \text{ K}$, where $v_s$ displays its maximum

High quality spectra:
Presence of clear excitations in both stokes and anti-stokes sides

Measured intensity:
$$I(Q,\omega) \propto S(Q,\omega) \otimes R(Q,\omega) + \text{bcgr}$$

$$\downarrow$$

$$S_{q,el}(Q,\omega) + S_{in}(Q,\omega)$$

$\mathcal{L}(Q,\omega)$

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The estimates for the sound velocity are above those found using macroscopic methods.

The response of a liquid sample to a probe of high frequency (thermal neutrons) is better understood in terms of that corresponding to an elastic medium, as described by the viscoelastic model.
Study of microscopic dynamics of alloys of geophysical interest
Data treatment of FeNi is in progress
Interest of measuring FeNiS in the future

Study of single-particle dynamics in molten transition metals
Liquid Nickel ($T_m = 1728$ K) IN5

Molecular dynamic simulations in liquid Tellurium
VASP code + nMoldyn

$T_m = 1650$ K
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