

Liquid Indium real and virtual experiment

Liquid Indium:

- Very low scattering cross section
- Very high absorption
- Never measured with neutrons

Proposal includes both real and virtual experiment:

Simulation showed we would be able to measure the quasi-elastic line
Around the first structure peak in $S(q)$.

Experiment:

Levitation furnace (gas flow+laser)

T=450 K

IN22 $E_i=30.8$ meV

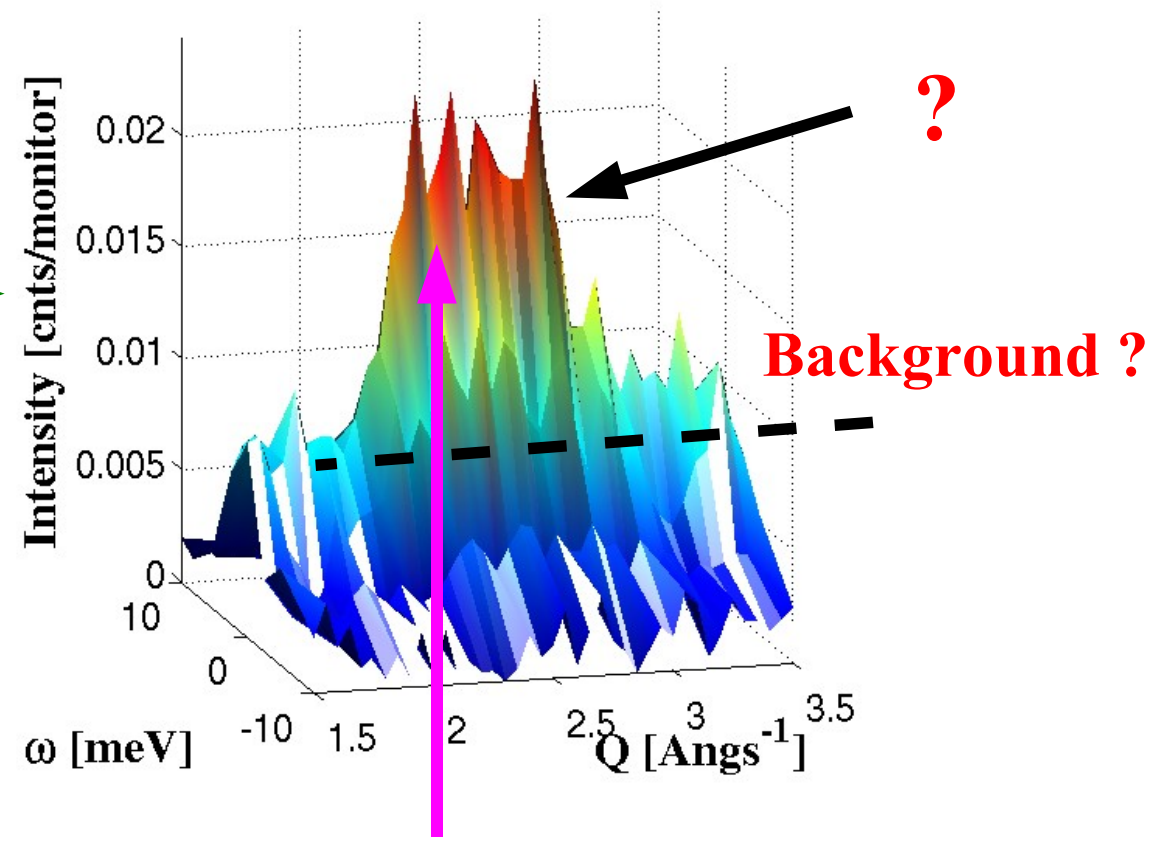
Team: E. Farhi, P. Willendrup, L.P.Regnault, McStas <mcstas.org>

Data includes contribution from the furnace and the B4C nozzle.
 Sample is a $\phi=4\text{mm}$ diameter sphere

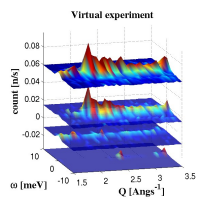
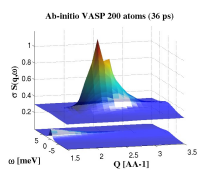
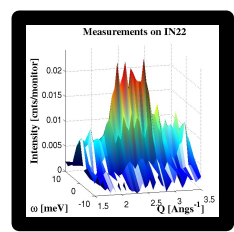
Experiment produces...



Measurements on IN22



Structure peak position



Liquid Indium: Ab-Initio Molecular Dynamics

We use *VASP*

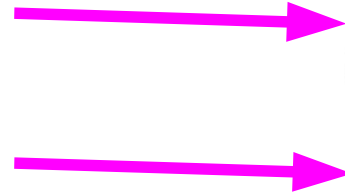
200 atoms in a 17 Å cube

Record atoms dynamics for 36 ps

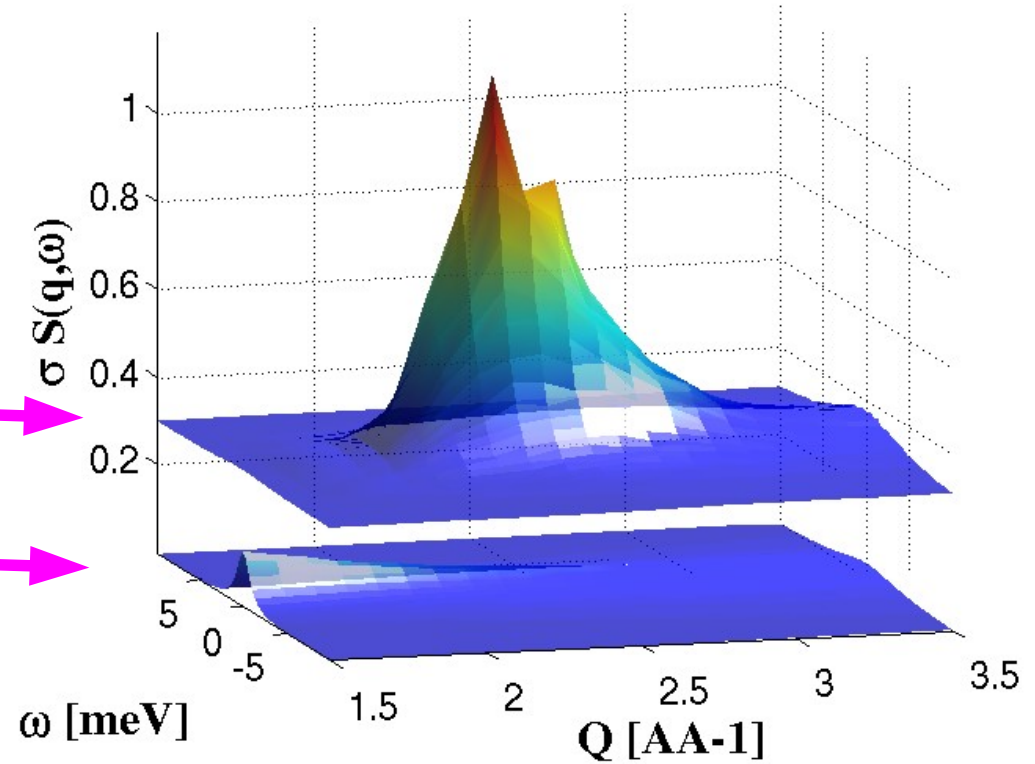
Compute $S(q, \omega)$ using *nMoldyn*

Coherent part

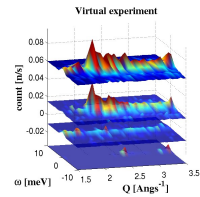
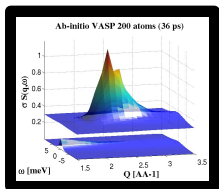
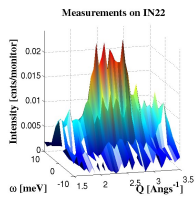
Incoherent part



Ab-initio VASP 200 atoms (36 ps)

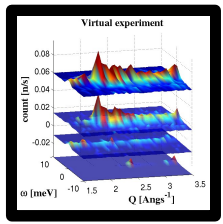
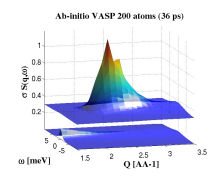
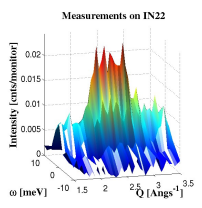
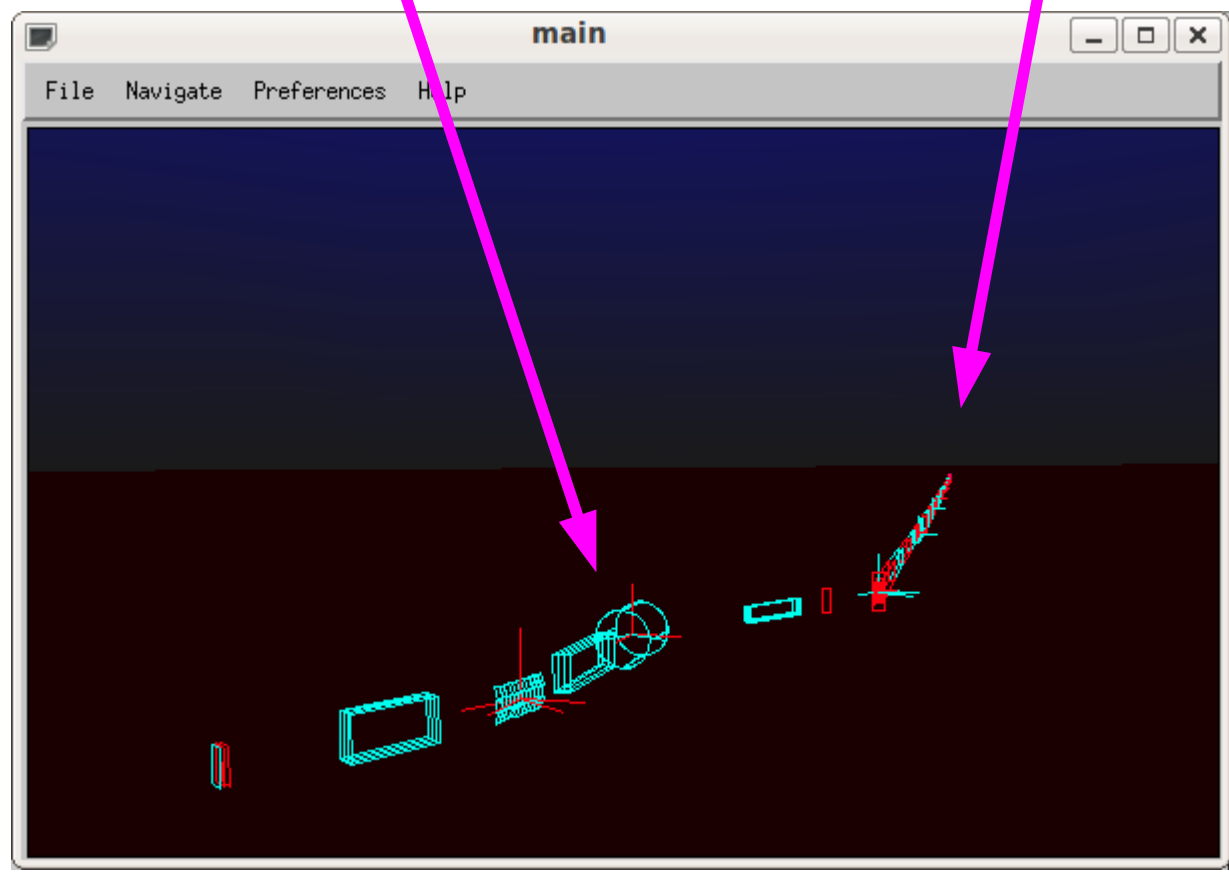


*We show here the measurement range
Compared to experiment,
computed $S(q, \omega)$ is very clean*



Liquid Indium: Virtual experiment

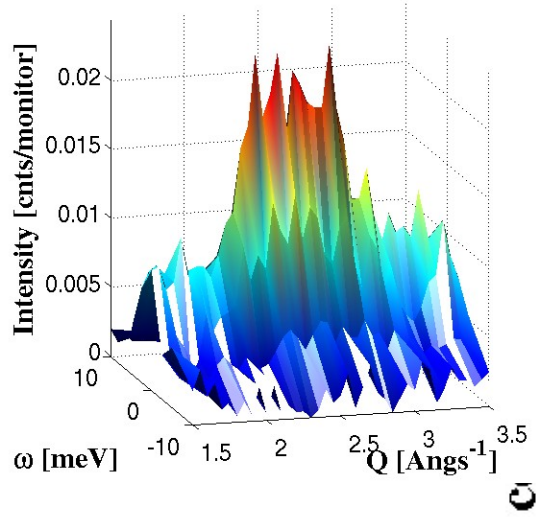
We use *McStas* <mcstas.org> to model the reactor, the H25 supermirror Guide and the IN22 triple-axis spectrometer. Model includes levitation furnace and nozzle.



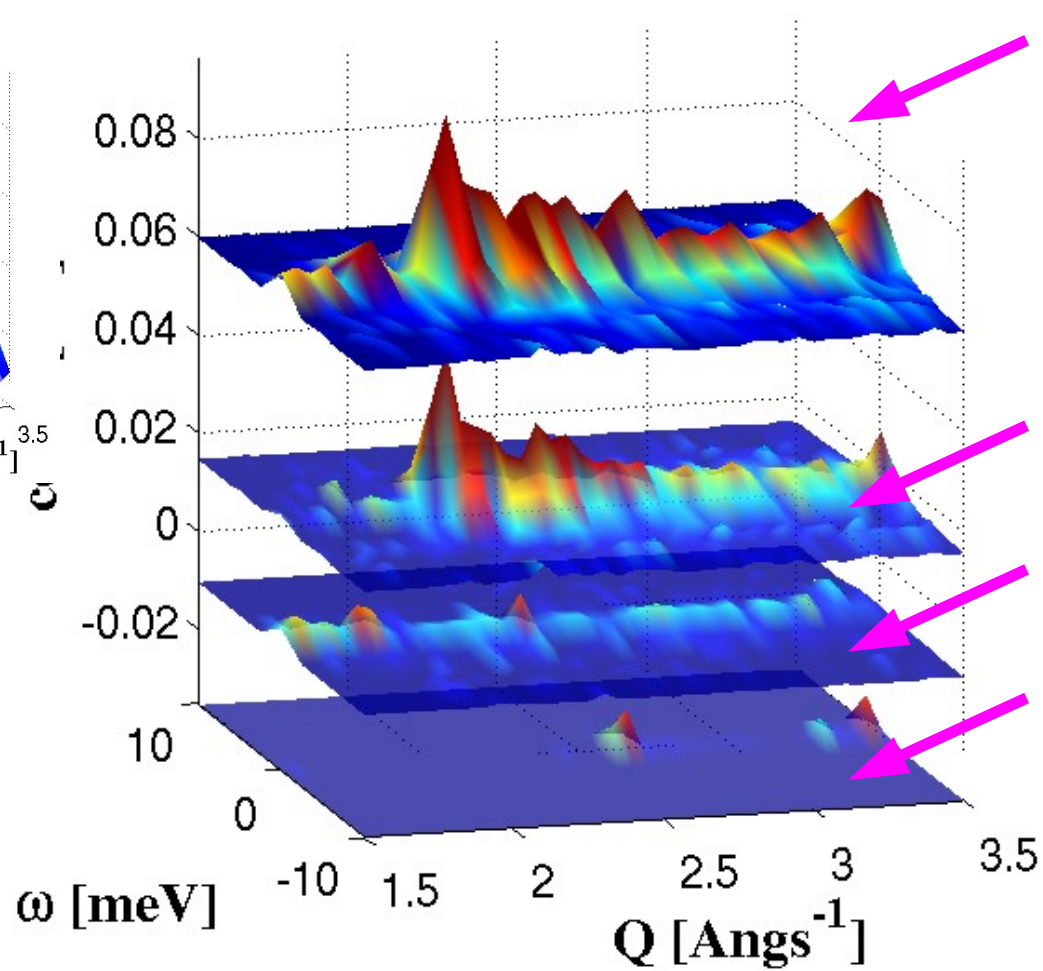
We run on 80 cores for 4 hours to simulate all q -energy scans.

Liquid Indium: Virtual experiment (cont'd)

Measurements on IN22



Virtual experiment



Total signal shows a tail after the structure peak

Coherent part

Incoherent part

Furnace contribution

Virtual experiment enables to **prepare and understand** the measurement.

***l*-In measured with neutron**

