

High spectral density of XFEL:

- allows for x-ray spectrograph with energy resolution of ~ 0.1 meV and scanning energy range ± 1000 meV.
- This will allow to measure complete and exact DOS (density of phonon states).
- Exact DOS may describe lattice dynamics better than dispersive relations.
- Exact DOS may describe structure better than x-ray diffraction

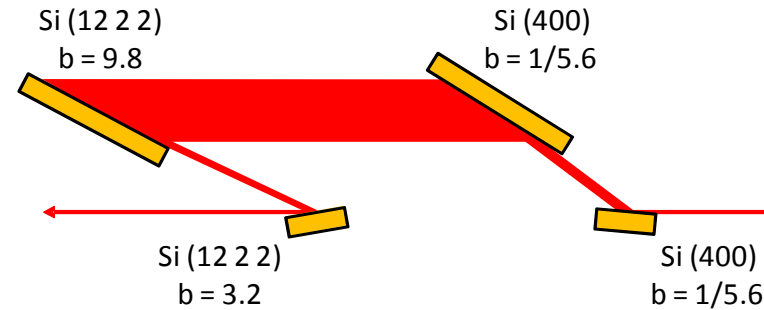
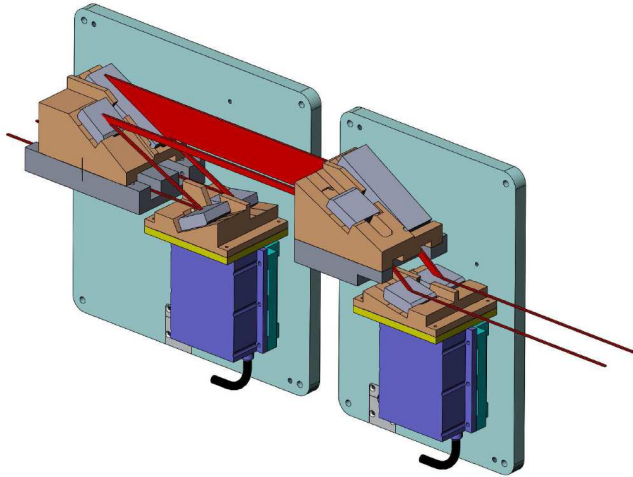
Aleksandr Chumakov, ESRF

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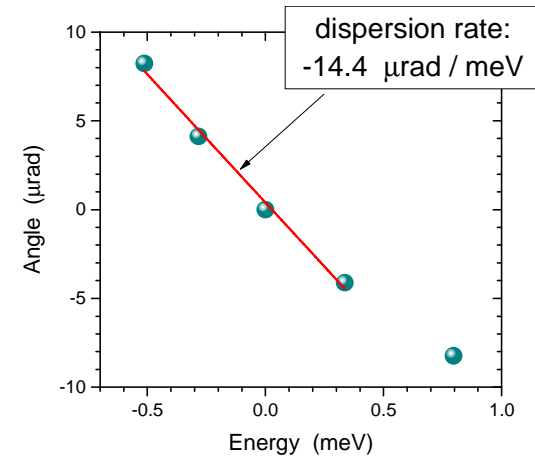
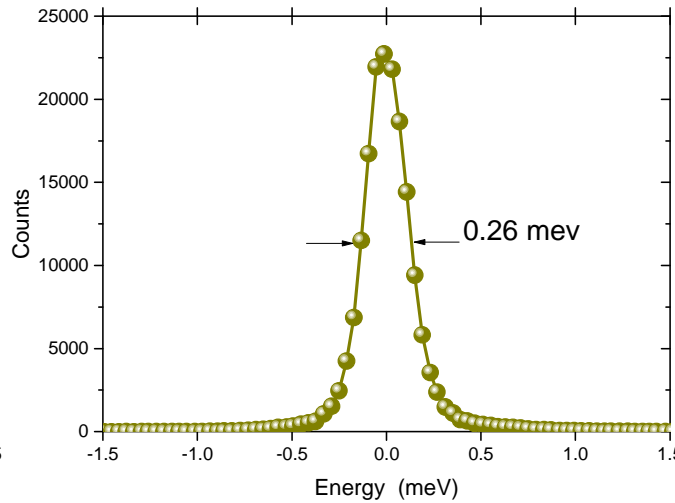
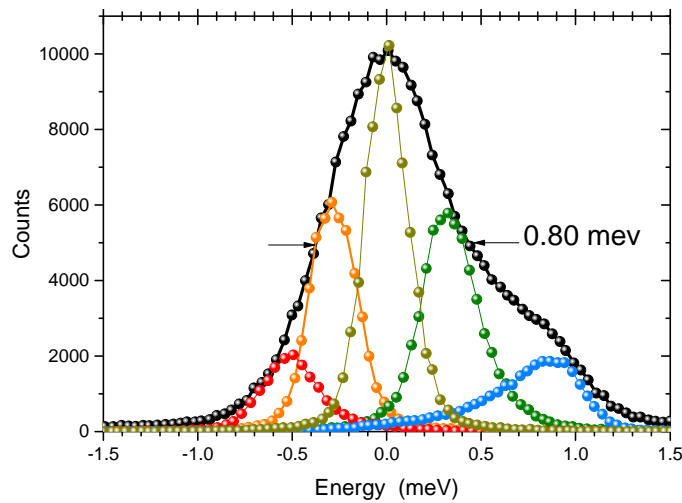
- allows for high statistical accuracy even if we use much smaller (~0.1 meV) energy bandwidth
- what we need is an x-ray spectrograph with energy resolution of ~0.1 meV and scanning energy range ± 1000 meV.
- then we may measure complete and exact DOS

WE ALREADY ALMOST HAVE A SUCH SPECTROGRAPH

ac, I. Sergeev, Yu. Shvyd'ko,
D. Bessas, R. Ruffer, June 2016



Our (ID18, ESRF) standard in-line 0.5 meV monochromator works as a spectrograph:



EXACT DOS MAY DESCRIBE LATTICE DYNAMICS BETTER THAN DISPERSION RELATIONS

dispersion relations:

momentum-differential (+)

but:

for selected momentum transfer (-)

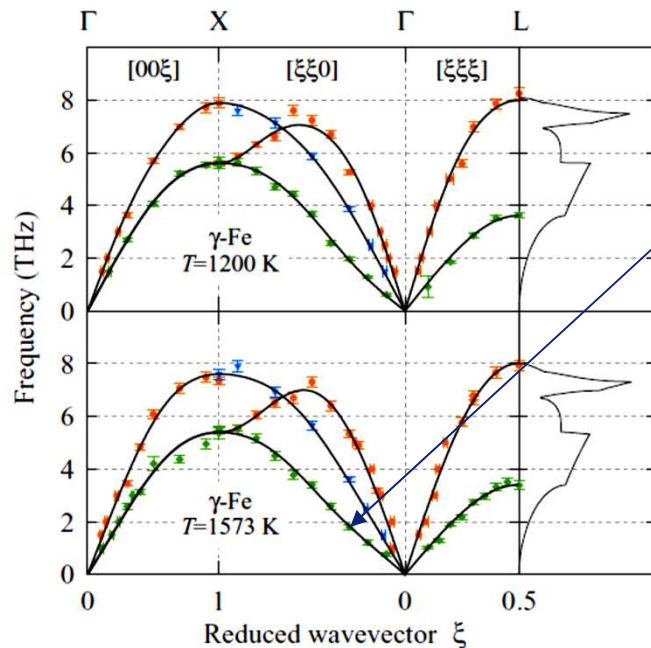
DOS:

momentum-integrated (-)

but:

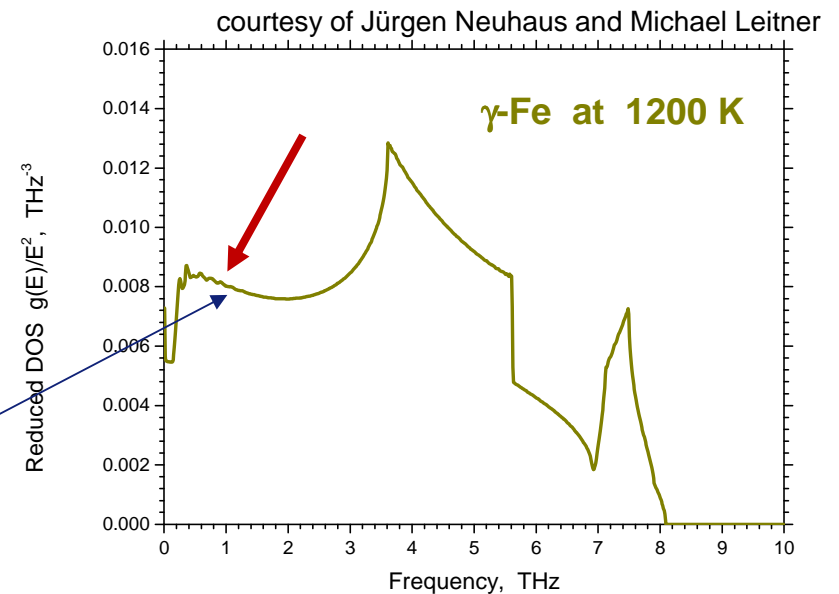
for all momentum transfers (+)

J. Neuhaus *et al*, PRB 89 (2014) 184302



Occasionally, this can be missed

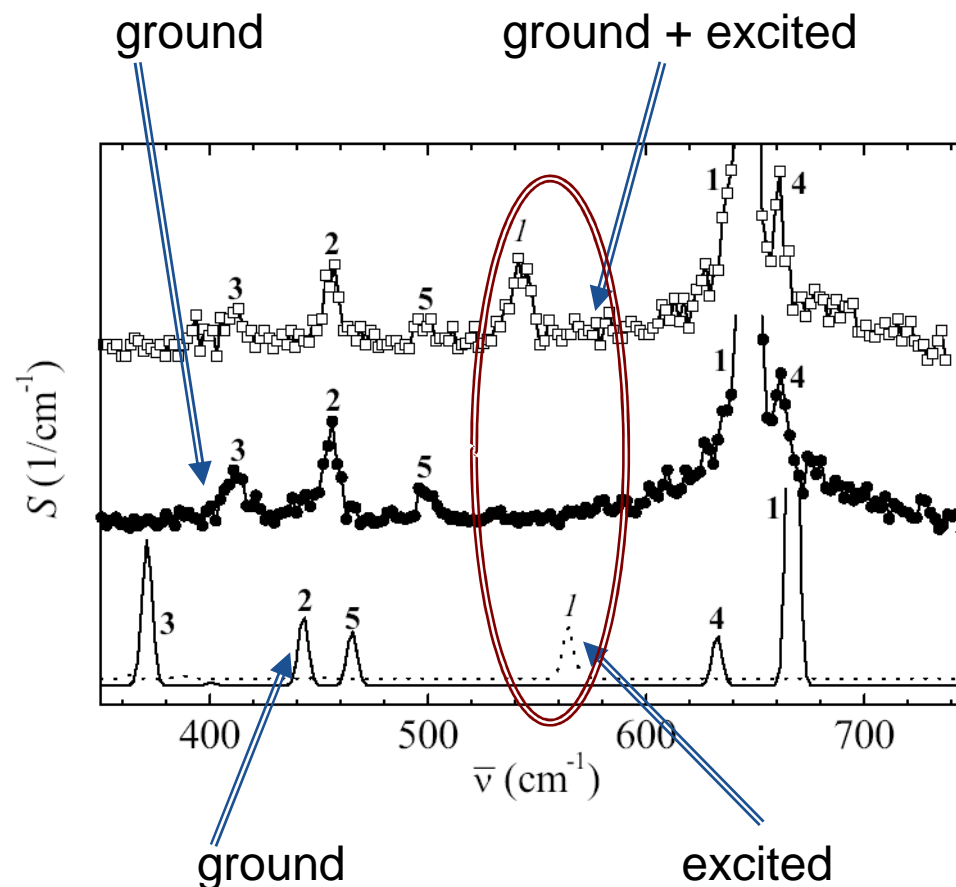
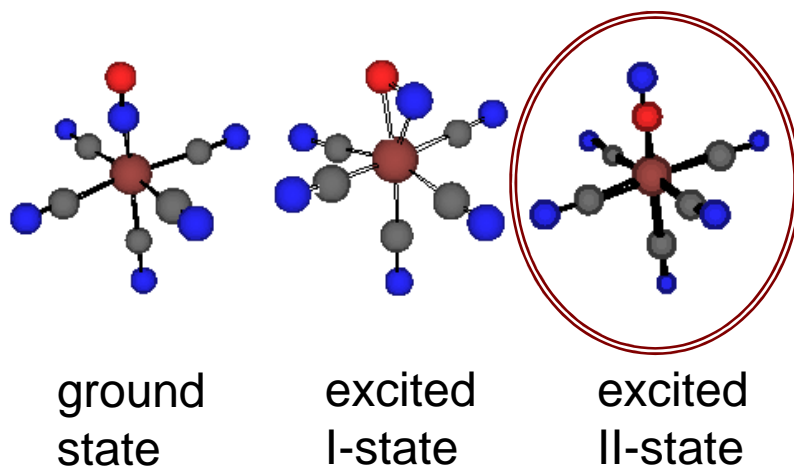
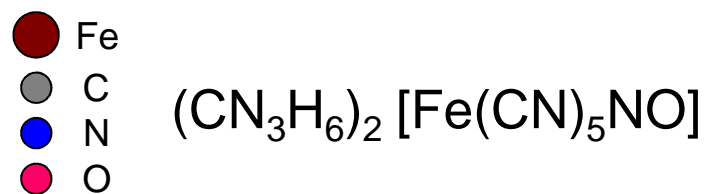
This cannot be missed



To apply Born-von-Karman fit to DOS

Atomic structure of guanidium nitroprusside:

H. Paulsen *et al*, JACS 2002.



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