Phonon Density of States Measured by Inelastic Nuclear Resonant Scattering

by Peng Gao

The measured data permit derivation of the phonon density of states derectly

- Tuning the energy of the incident x-rays with respect to the nuclear resonance
- The total yield of the delayed fluorescence photons.
- The incident photon flux

$$I(E) = I_0 \rho \sigma \frac{\eta_K \alpha_K}{1 + \alpha} \frac{\pi}{2} \Gamma S(E),$$

where I_0 is the incident photon flux, σ is the nuclear resonant cross section, η_K is the fluorescence yield, α, α_K are the total and partial internal conversion coefficients, respectively, and Γ is the nuclear level width. The effective area density of nuclei ρ also accounts for absorption within the material. $S(E)$ is the absorption probability per unit of energy. We will give it in terms of the quantum states $|\chi\rangle$ and the displacement operator $\hat{\mathbf{r}}$ of the nuclear motion

$$S(E) = \left\langle \frac{1}{dE} \sum_n |\langle \chi_n(E)| e^{-i\mathbf{k}\cdot\hat{\mathbf{r}}} |\chi_i\rangle|^2 \right\rangle_i .$$

$$A = \frac{1}{E_R} \int I_m(E) E \, dE - \frac{1}{E_R} \int R(E) E \, dE \int I_m(E) \, dE .$$

$$f = 1 - \frac{1}{A} \int I'_m(E) \, dE ,$$

$$S(E) = f\,\delta(0) + f \sum_{n=1}^{\infty} S_n(E) ,$$

$$S_1(E) = \frac{E_R \mathcal{D}(E)}{E(1 - e^{-\beta E})} ,$$

$$S_n(E) = \frac{1}{n} \int S_{n-1}(E - \epsilon) S_1(\epsilon) \, d\epsilon , \qquad n \geq 2 .$$

The experiment

- The experiments were performed at the undulator beamline NE#3 at the 6.5-GeV KEK-AR synchrotron radiation facility in Tsukuba, Japan

- The 14.4136-keV resonance of the Mössbauer isotope ^{57}Fe was employed because of its large resonance cross section, the tolerable electronic absorption in the materials used, and the convenient lifetime.

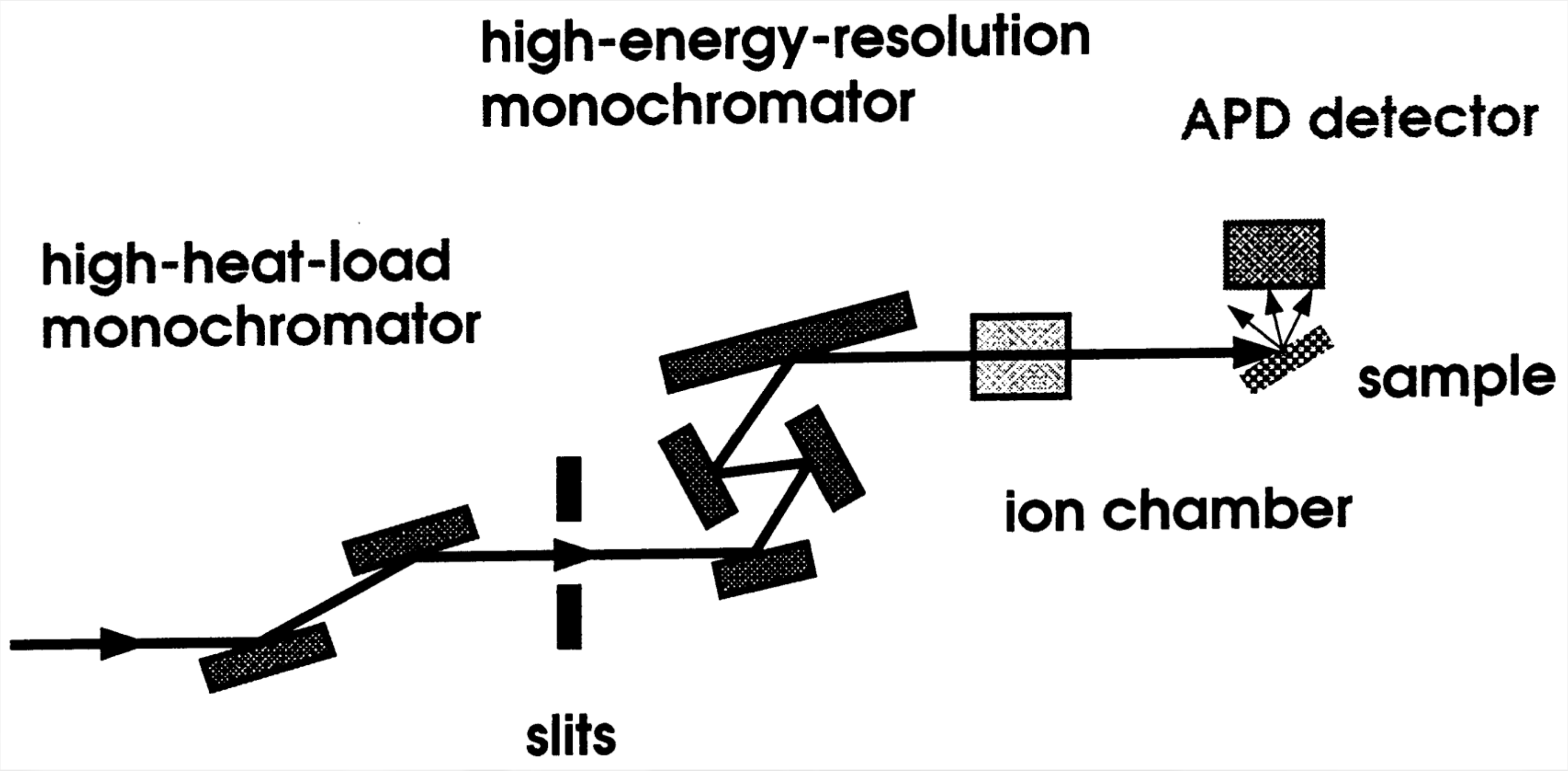
- A high-heat-load monochromator consists of two symmetric silicon (111) reflections in a nondispersive setting

- A high-resolution, nested monochromator uses asymmetric silicon (422) and symmetric silicon(1064) reflections.

- The photon flux on the sample was monitored with an ion chamber for proper normalization of the data.

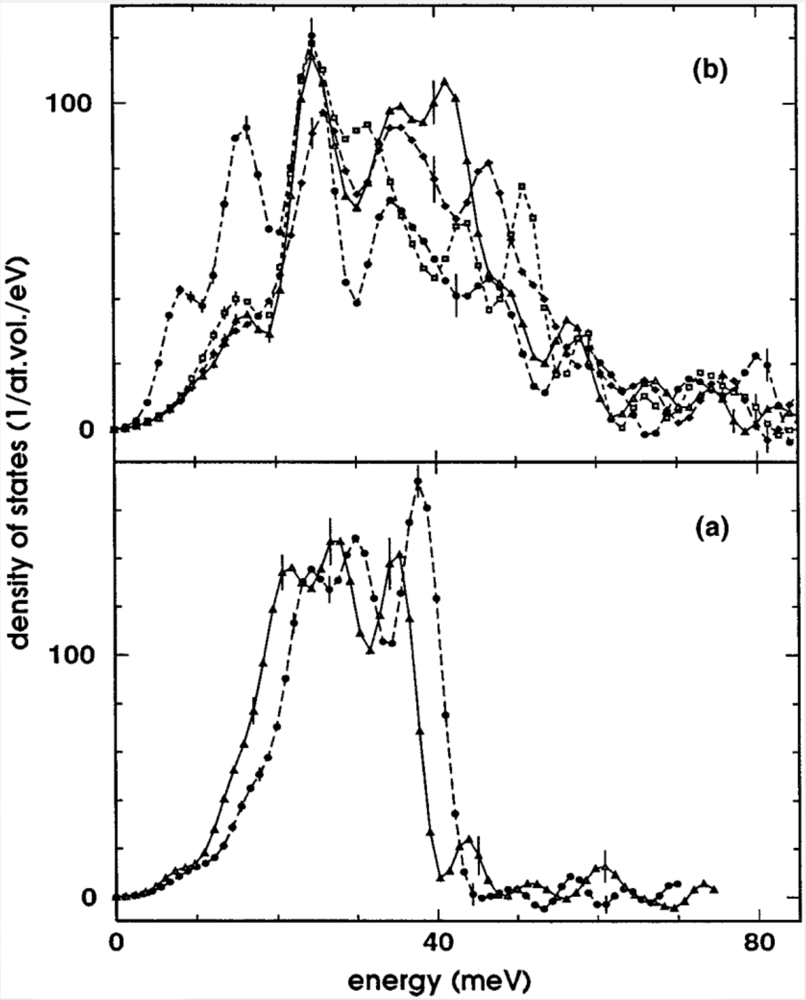
- An avalanche photodiode (APD) with an active area of 2 cm^2 was used to detect the emitted fluorescence radiation.

Set-up diagram



The result

- The phonon DOS of different materials are shown.(a) a-iron (circles, dashed line) and stainless steel (triangles,solid line). (b) SrFeOx with x= 3(triangles, solid line), x=2.86 (diamonds, dashed line), x= 2.74 (rectangles, dotted line), and x=2.5 (circles, dashed-dotted line).



Conclusion

- The information that can be derived from such measurements can be used to support existing or develop new models for the interatomic forces and for the coupling of phonons to other quasiparticles. Thus, for example, vibrational entropies and other thermodynamical properties of order-disorder alloys can be studied and temperature-dependent phonon spectra can provide data about the phonon interaction. In addition, materials with noncrystalline structure, such as glasses and liquids, can easily be investigated on the basis of a trend analysis.

Reference

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THANK YOU