Measuring Velocity of Sound

with

Nuclear Resonant Inelastic X-ray Scattering

Michael Hu

HP-CAT
Carnegie Institution of Washington

PRB 67, 094304 (2003)

Measuring velocity of sound with nuclear resonant inelastic x-ray scattering

Michael Y. Hu,[1] Wolfgang Sturhahn,[2] Thomas S. Toellner,[2] Philip D. Mannheim,[3] Dennis E. Brown,[4] Jiyong Zhao,[2] and E. Ercan Alp[2]

[1]*HP-CAT and Carnegie Institution of Washington, Advanced Photon Source, Argonne, IL 60439*

[2]*Advanced Photon Source, Argonne National Laboratory, Argonne, IL 60439*

[3]*Department of Physics, University of Connecticut, Storrs, CT 06269*

[4]*Department of Physics, Northern Illinois University, DeKalb, IL 60115*

(Dated: Jan. 17, 2003)

Abstract

Nuclear resonant inelastic x-ray scattering is used to measure the projected partial phonon density of states of materials. A relationship is derived between the low-energy part of this frequency distribution function and the sound velocity of materials. Our derivation is valid for harmonic solids with Debye-like low-frequency dynamics. This method of sound velocity determination is applied to elemental, composite, and impurity samples which are representative of a wide variety of both crystalline and noncrystalline materials. Advantages and limitations of this method are elucidated.

PACS numbers: 61.10.Eq, 62.65.+k

Sound velocity

Measurements:

ultrasound

Brillouin scattering

acoustic phonon dispersion

* Debye DOS — NRIXS

Materials of interests:

geoscience, e.g. composition of earth core

thin films, multilayers, nano particles

Debye sound velocity and partial DOS

What NRIXS measures:

$$\mathcal{D}(E,\hat{\mathrm{k}}) = \frac{1}{\tilde{N}} \sum_{\nu=1}^{\tilde{N}} \frac{1}{N} \sum_{l=1}^{3N} |\hat{\mathrm{k}} \cdot \mathrm{e}_l^{\nu}|^2 \, \delta(E - E_l)$$

The phonon DOS:

$$\nu(E) = \frac{1}{3N} \sum_{l}^{3N} \delta(E - E_l)$$

If we deinfe a projection and selection function,

$$\mathcal{D}(E,\hat{\mathrm{k}}) = \chi(E,\hat{\mathrm{k}}) \, \nu(E)$$

For harmonic solids with Debye-like "low-frequency" dynamics, in the low energy region,

$$\chi(\hat{\mathrm{k}}) = \frac{\tilde{m}}{m} \left(\frac{v_D}{v_{\hat{\mathrm{k}}}} \right)^3$$

For an isotropic or a polycrystalline sample,

$$\chi = \frac{\tilde{m}}{m}$$

and

$$\boxed{\mathcal{D}(E) = \left(\frac{\tilde{m}}{m} \right) \frac{E^2}{2\pi^2 \hbar^3 n v_D^3}}$$

where,

$$\frac{1}{v_D^3} = \frac{1}{3} \sum_{s=1}^{3} \int \frac{d\Omega_q}{4\pi} \frac{1}{c_{\hat{\mathrm{q}}s}^3}$$

Projected Debye sound velocity

$$\frac{1}{v_{\hat{k}}^3} = \sum_{s=1}^{3} \int \frac{d\Omega_q}{4\pi} \frac{(\hat{k} \cdot \hat{p}_{\hat{q}s})^2}{c_{\hat{q}s}^3}$$

Then, the low-energy portion of the measured projected partial DOS has the following form,

$$\mathcal{D}(E, \hat{k}) = \left(\frac{\tilde{m}}{m}\right) \frac{E^2}{2\pi^2 \hbar^3 n v_{\hat{k}}^3}$$

where $\tilde{m}$ is the mass of the nuclear resonant isotope, m the average atomic mass of all atoms in the sample, and n is the number density of atoms.

Caveats

Harmonic lattice approximation

Debye behaviour up to not too low energies

1 THz, **4** meV

Not too soft materials

$f_{LM} > 0.1$

The low-energy region of NRIXS DOS

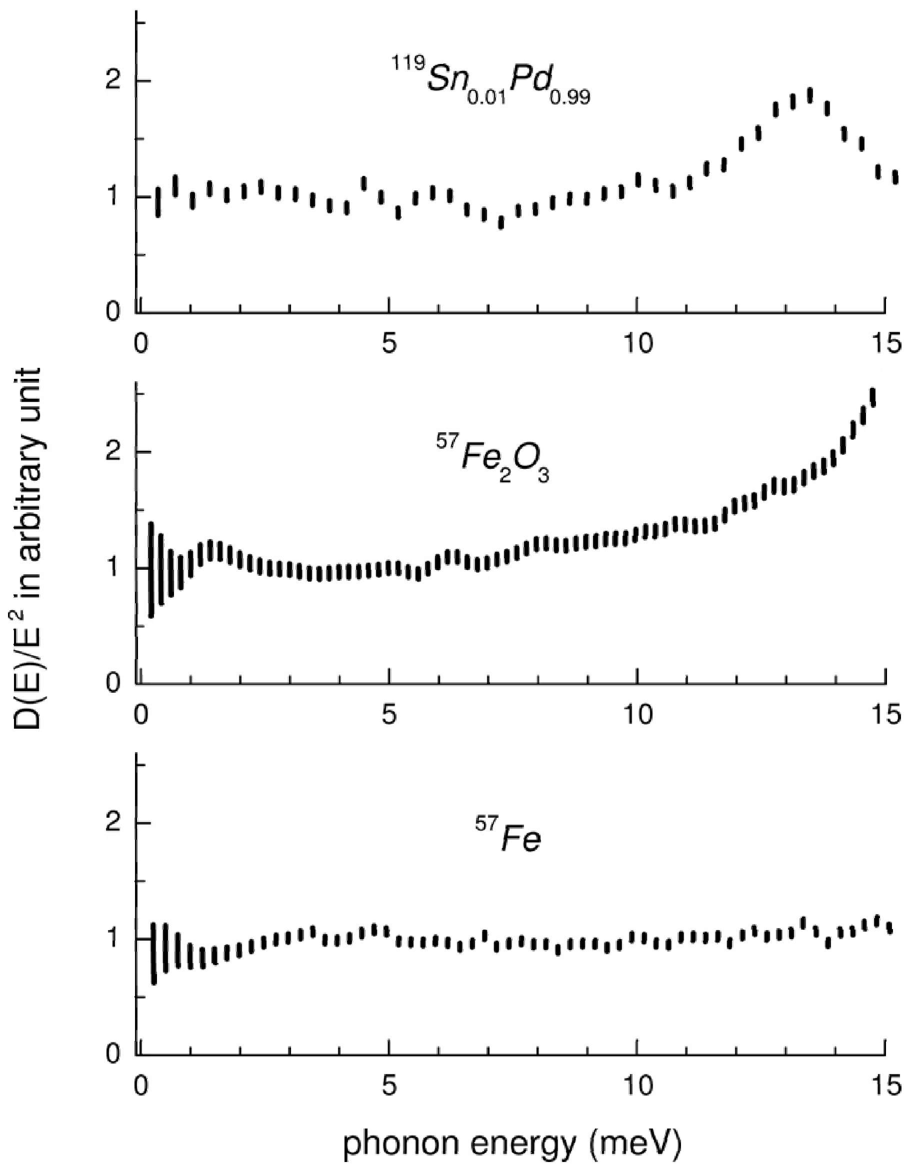

FIG. 1: The measured PDOS divided by energy squared. The size of symbols indicates the statistical error bar derived from signal counts. These samples were measured with resolutions of 0.85 meV for $^{119}Sn_{0.01}\mathrm{Pd}_{0.99}$, 0.6 meV for $^{57}Fe_2\mathrm{O}_3$, and 1 meV for bcc iron.

Comparison of sound velocities

	velocity of sound (m/s)	$\tilde{m}/m$
Palladium	2193±35[a]	1.12
	2104[b]	
	2372[c]	
Hematite	4279±84[a]	1.76
	4653[d]	
Iron	3488±48[a]	1.00
	3412[b]	
	3707[c]	

[a]Our results from NRIXS.
[b]The lower limits from ref. 1.
[c]The upper limits from ref. 1.
[d]Calculated with bulk and shear moduli from ref. 2.

[1] G. Simmons and H. Wang, *Single Crystal Elastic Constants and Calculated Aggregate Properties* (The M.I.T. Press, Cambrige, Massachusetts, 1971).

[2] R. C. Liebermann and E. Schreiber, J. Geophys. Res. **73**, 6585 (1968).

Examples

Phonon Density of States of Iron up to 153 Gpa

H. K. Mao, J. Xu, V. V. Struzhkin, J. Shu, R. J. Hemley, W. Sturhahn, M. Y. Hu, E. E. Alp, L. Vocadlo, D. Alf, G. D. Price, M. J. Gillan, M. Schwoerer-Bhning, D. Husermann, P. Eng, G. Shen, H. Giefers, R. Lbbers, G. Wortmann

Science, 292, 914 (2001).

Sound velocities of iron-nickel and iron-silicon alloys at high pressures

Jung-Fu Lin, Viktor V. Struzhkin, Wolfgang Sturhahn, Eugene Huang, Jiyong Zhao, Michael Y. Hu, Ercan E. Alp, Ho-kwang Mao, Nabil Boctor, and Russell J. Hemley

GEOPHYSICAL RESEARCH LETTERS, 30, 2112 (2003).

How many resonant nuclei are needed ?

$$\sigma(E) = \frac{\pi}{2}\,\sigma_0\Gamma\,S(E)$$

$$\overline{\sigma} \sim \frac{\pi}{2}\,\sigma_0\Gamma\,\overline{S'(E)} \sim \sigma_0\Gamma\,\frac{\pi}{2}\,\frac{1-f}{2\Theta_{\rm D}}$$

$$\overline{\sigma} \sim 10^{-1}\sigma_{\rm Thomson} \sim 10^{-25} cm^2$$

If we let the count rate $\eta\, I_0\, \overline{\sigma}\, n\, d \sim 1$, and assume

$$I_0 \sim 10^8\, ph/sec$$

$$d \sim 10\, \mu m$$

$$\eta \sim 0.1$$

then

$$n \sim 10^{21}\, nuclei/cm^3$$