“Phonons”

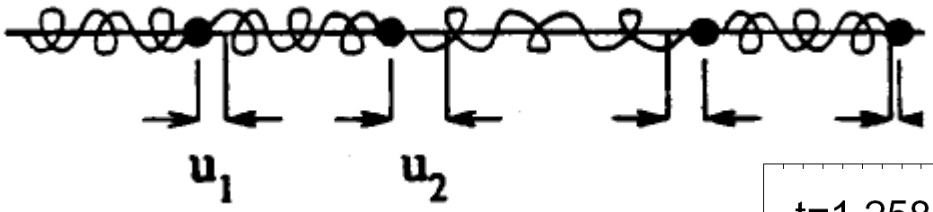
Vibrational normal modes

–Evolution from molecule to solid
–Heat conduction
–What are vibrations like in glasses?

P. B. Allen, visiting Applied Physics at Columbia
On leave from SUNY Stony Brook

Euken
Einstein
Debye
Born
Peierls
Frenkel
Brockhouse

PBA and J. Kelner
Am. J. Phys. 66, 497 (1998)

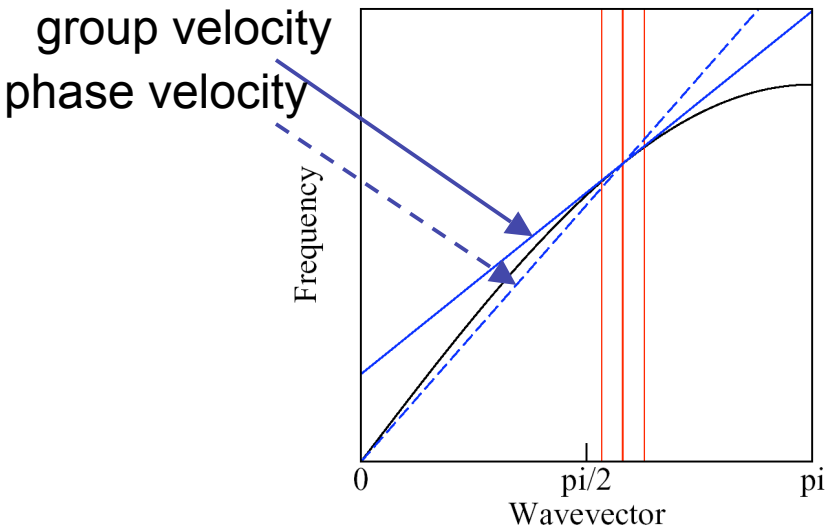


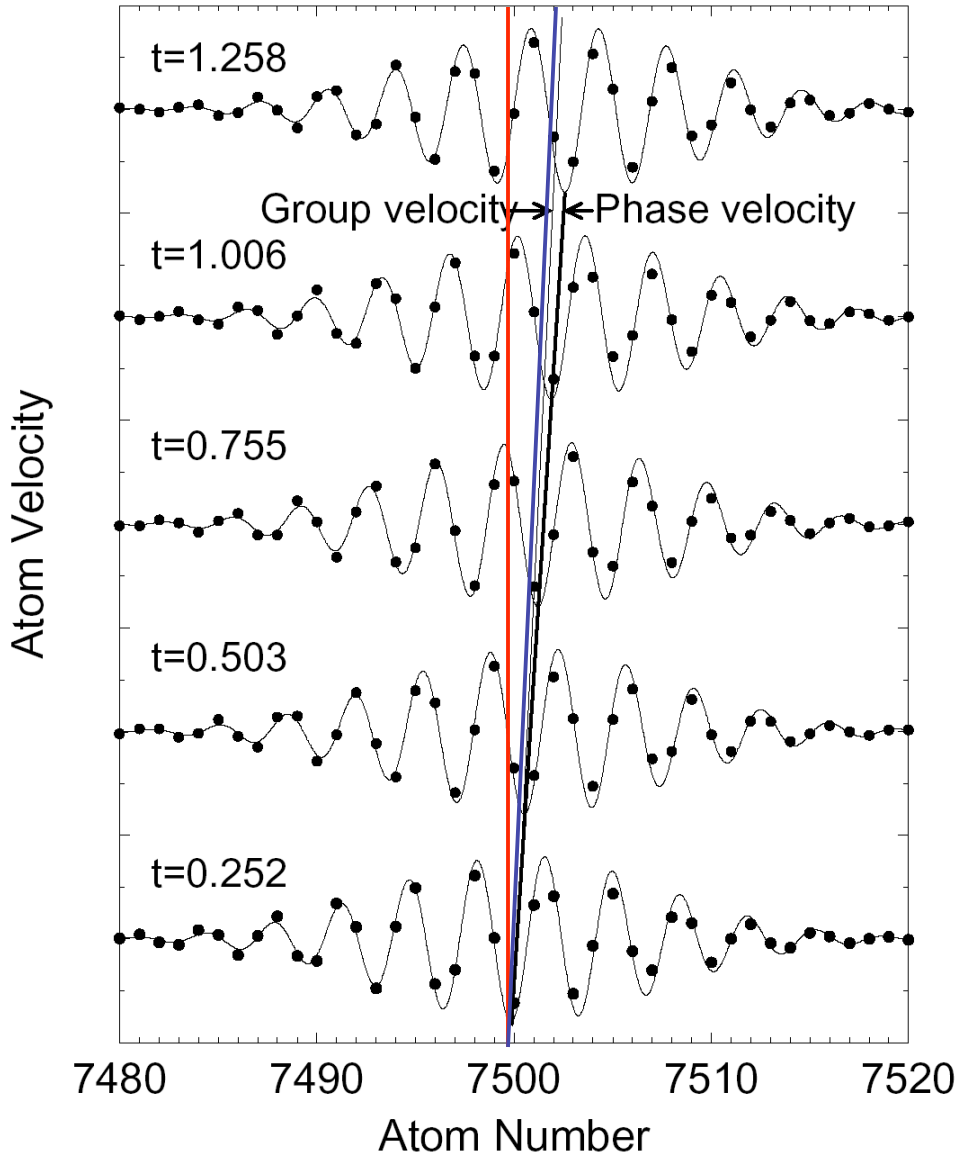
$$V = \frac{1}{2}\sum_{n=1} k_n(u_n - u_{n+1})^2$$

$$M_n \frac{d^2 u_n}{dt^2} = -\frac{\partial V}{\partial u_n}$$

$$u_n(t) = |A_Q| \cos(Qna \pm \omega_Q t + \phi_Q)$$

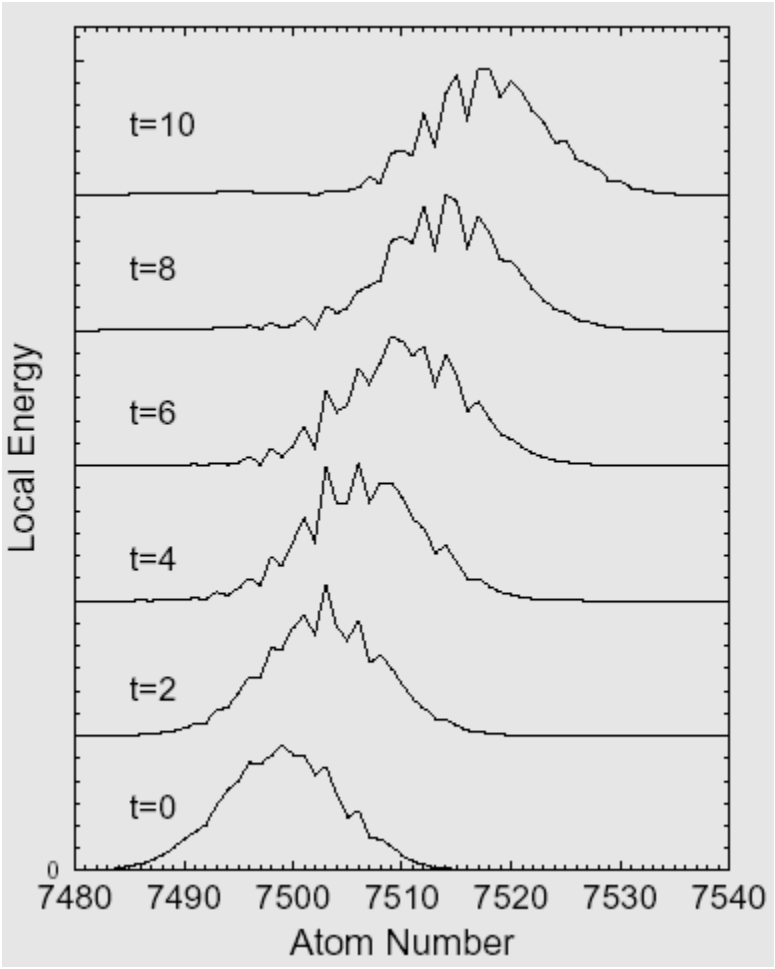
$$\omega_Q = 2\sqrt{k/M}\,\sin(Qa/2)$$

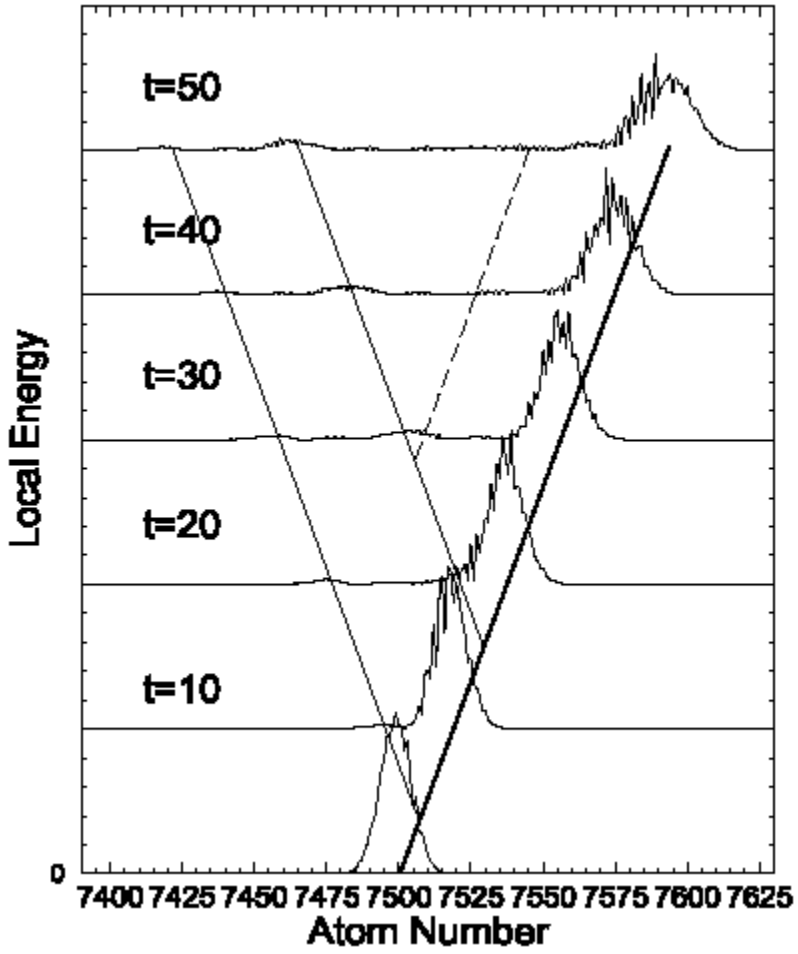




Energy transport, weakly disordered 1d chain

0.93 < K < 1.07 uniform random deviations

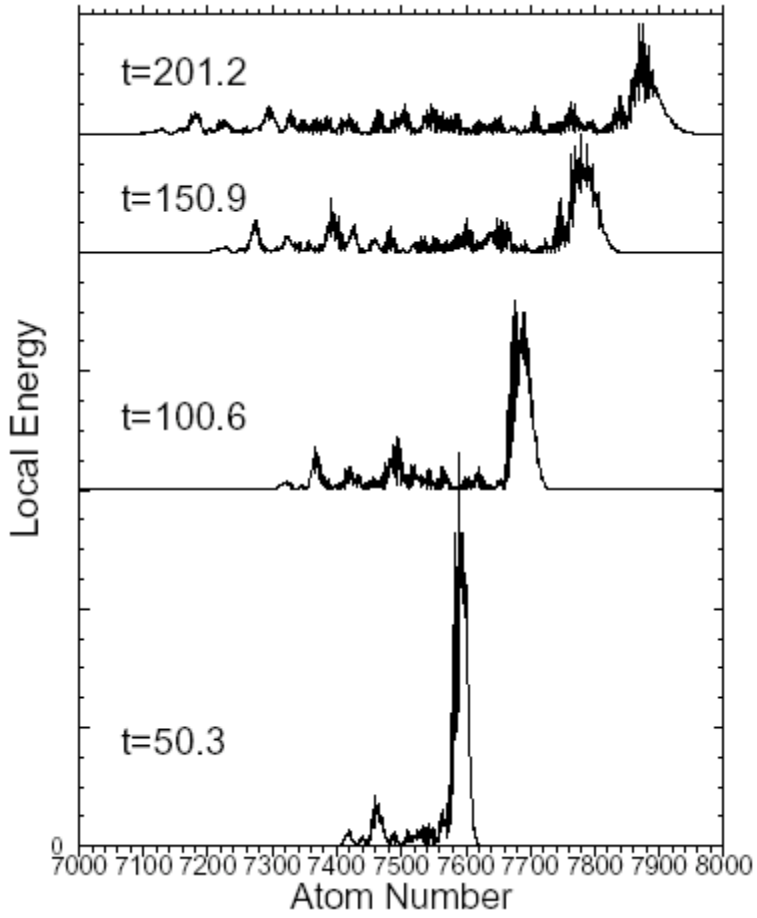


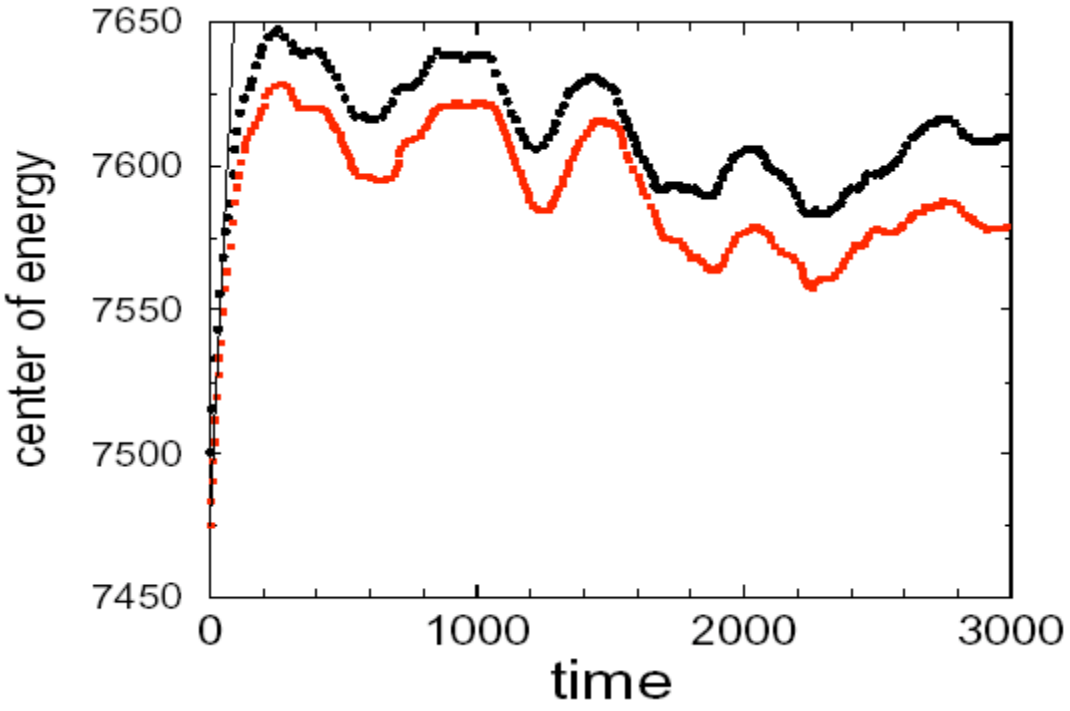


Ballistic motion of wavepacket for 0 < t < 100

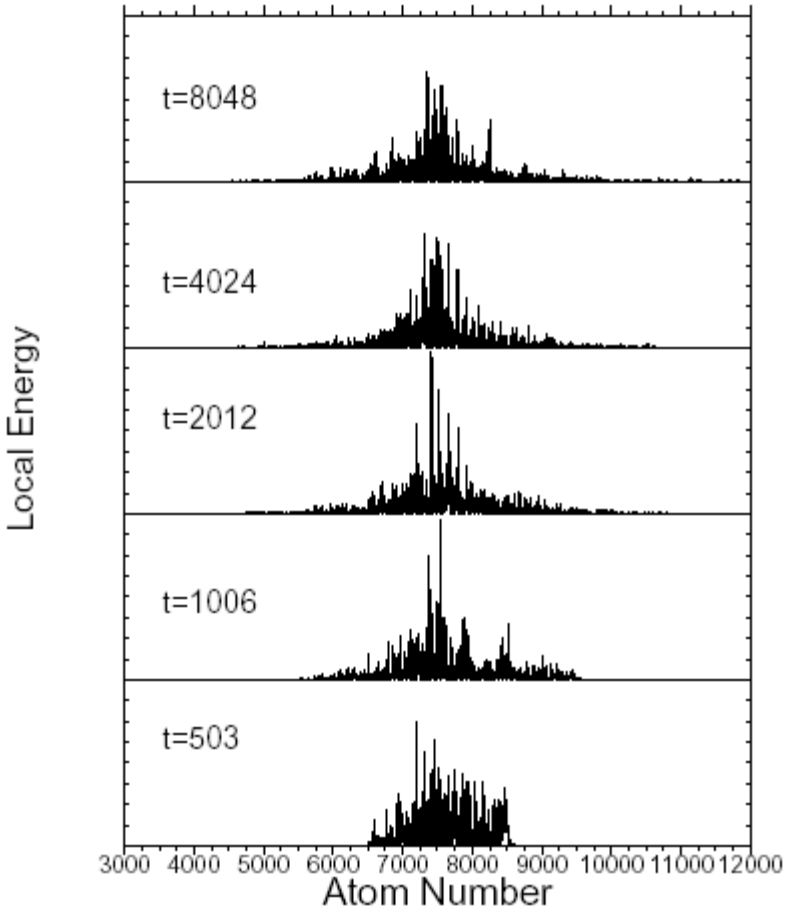
Center of energy stops systematic motion by t=200

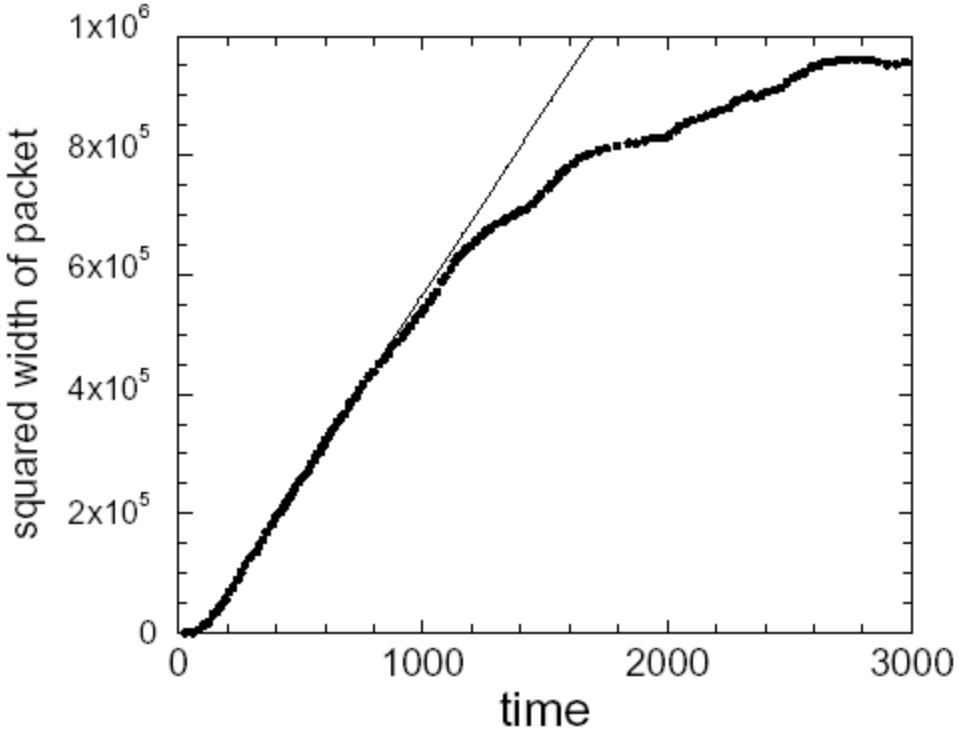
Non-Chaotic Evolution





Diffusive motion, 100 < t < 1000
Localization, t > 2000 (no further energy transport)





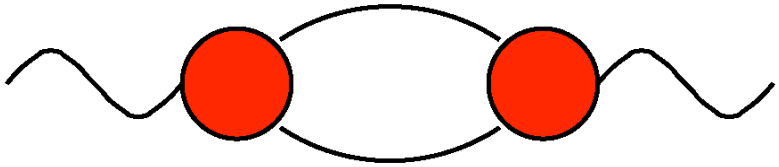
Phonon dispersion in tungsten metal

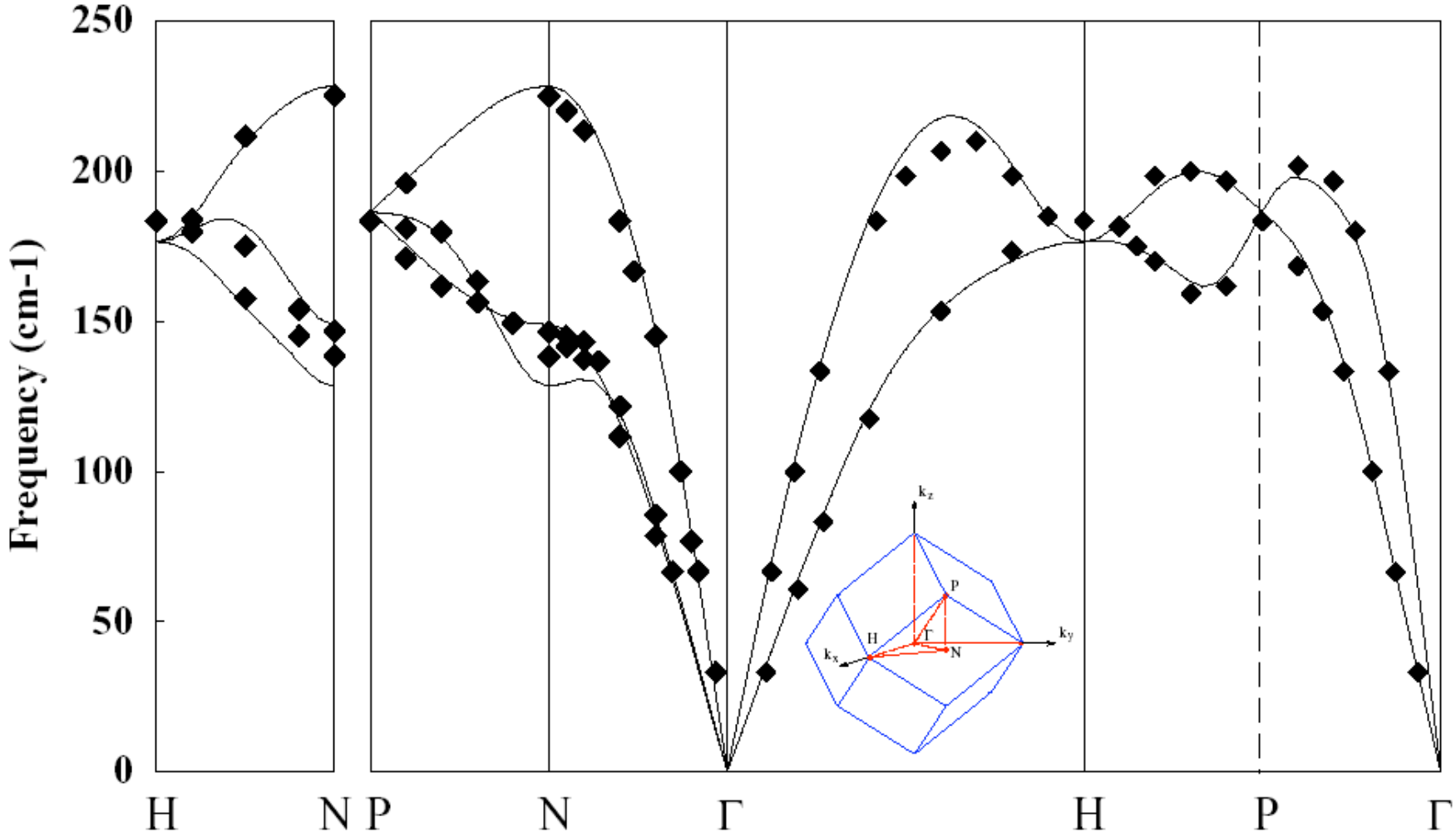
"first principles" calculation

Density-functional theory

C. Bungaro, thesis, SISSA, 1995

(with Baroni and Gironcoli)





Heat Conduction by Phonons

$$j_Q \equiv -\kappa \nabla T$$

Experiments: Euken
Theories: Einstein, Debye

R. Peierls, thesis, Zurich, 1929

"Phonon gas model"

$$j_Q = \sum_k v_k(\hbar\omega_k) N_k(\vec{r})$$

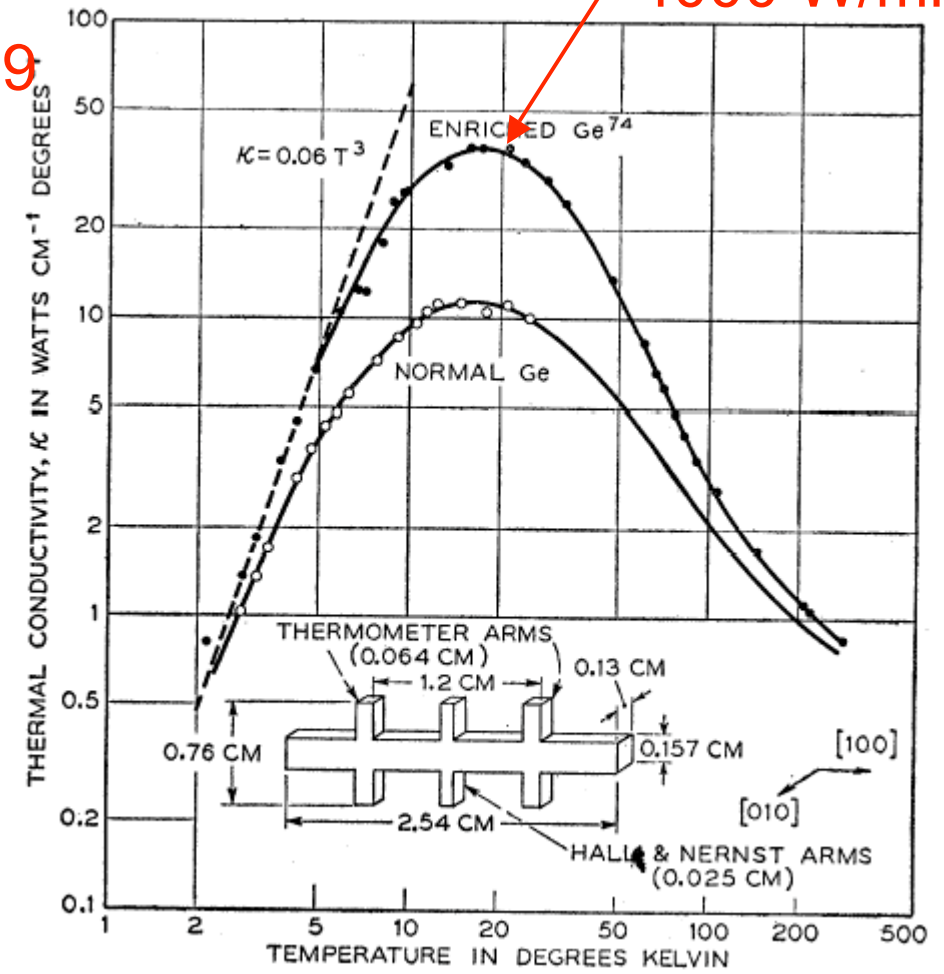
$$N_k(\vec{r}) = n_k[T(\vec{r} - \vec{v}_k\tau)]$$

$$\kappa \approx \frac{1}{3} C(T)\bar{v}\ell(T)$$

Isotopic and Other Types of Thermal Resistance in Germanium*

T. H. Geballe and G. W. Hull
Bell Telephone Laboratories, Murray Hill, New Jersey

4000 W/mK



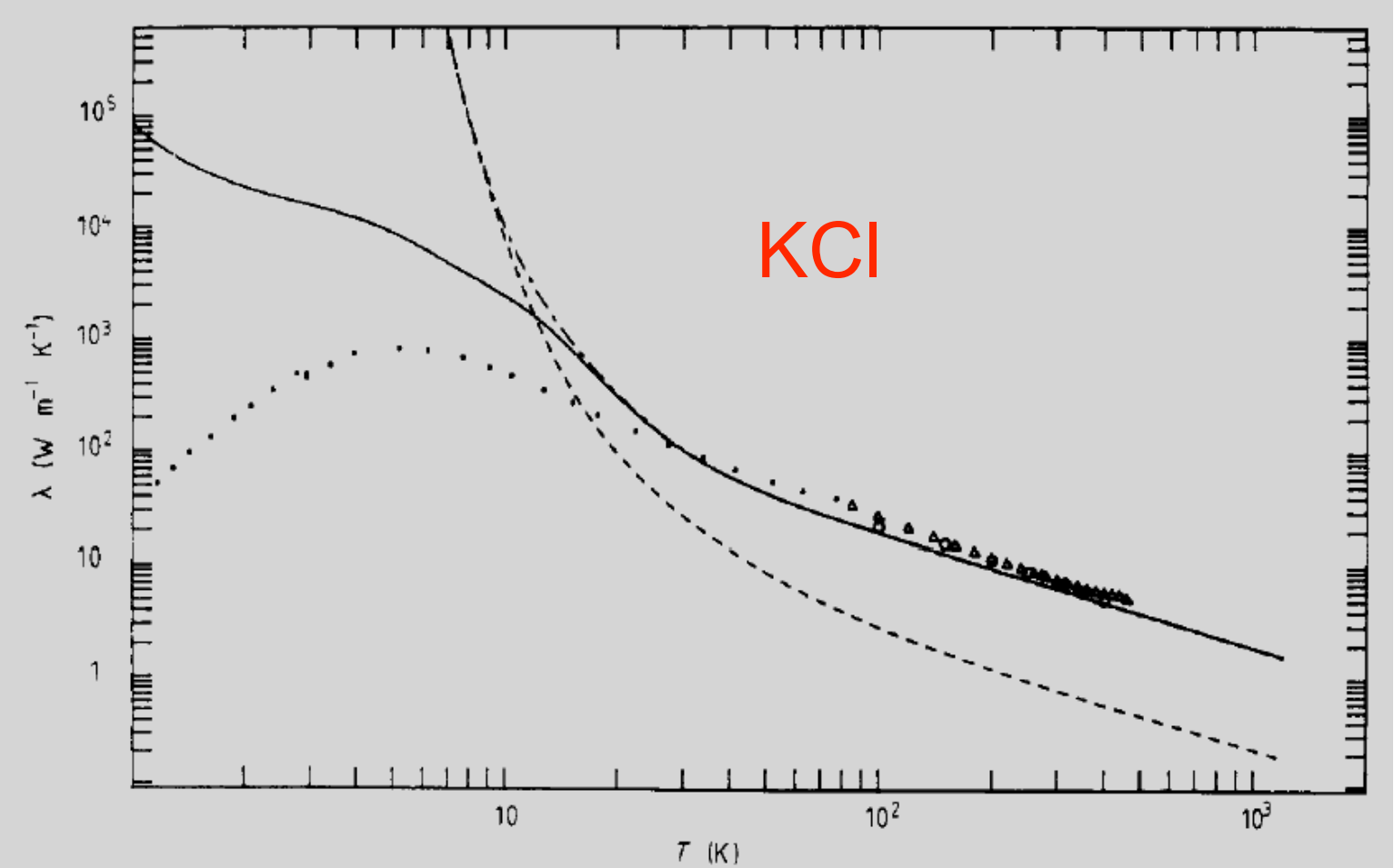
J. Phys. C: Solid State Phys. **20** (1987) 1047–1061.

Calculation of the thermal conductivity of alkali halide crystals

Sune Pettersson

Department of Theoretical Physics, University of Umeå

Thesis supervised by Arne Claesson

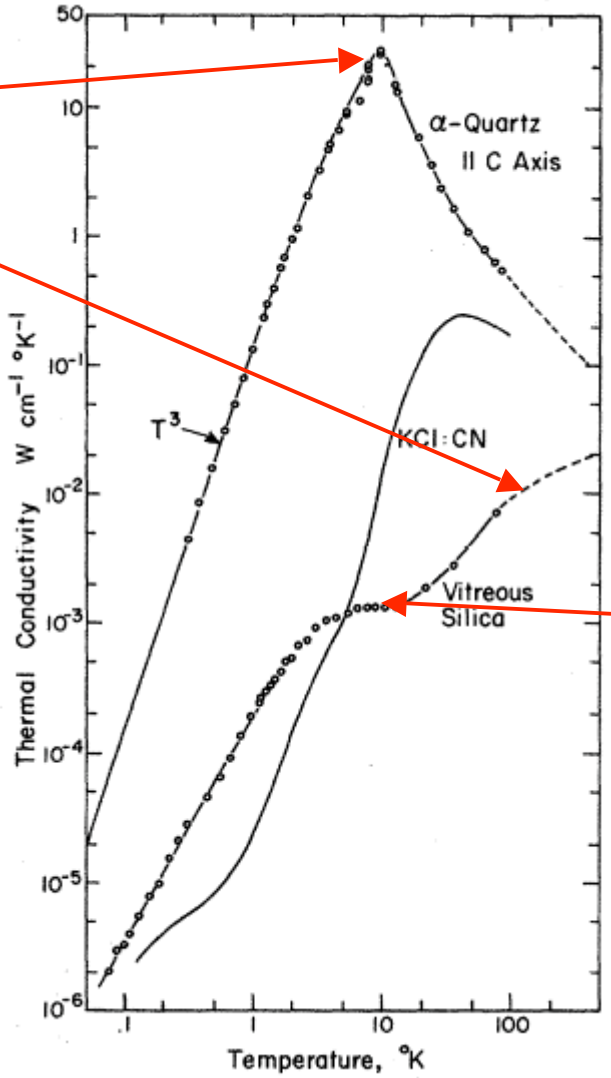


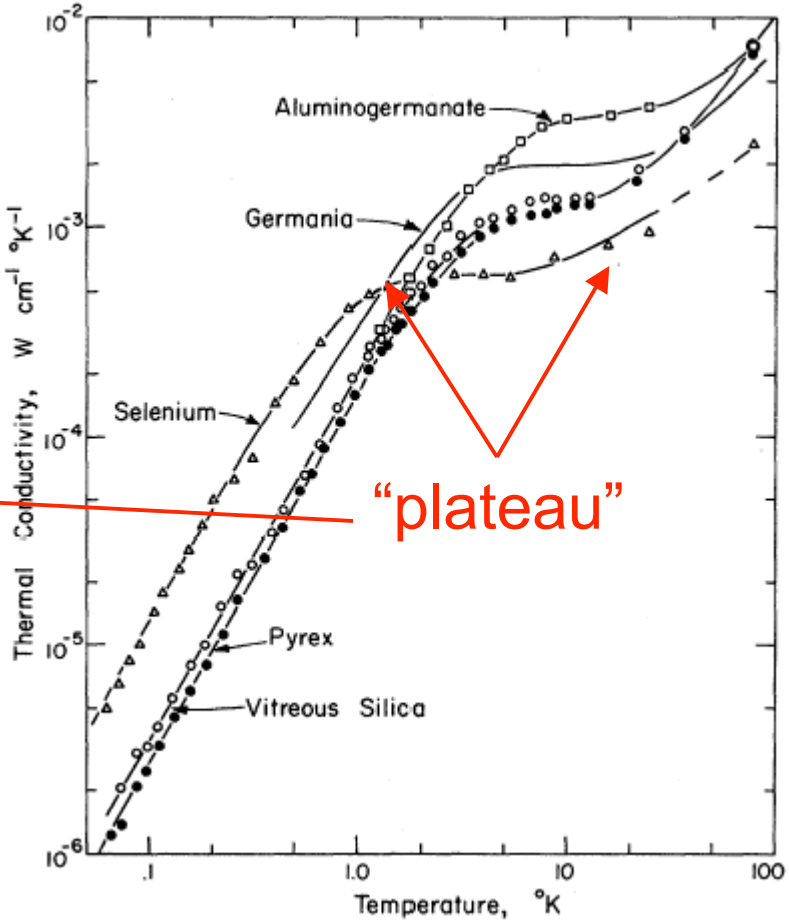
Thermal Conductivity and Specific Heat of Noncrystalline Solids*

R. C. Zeller† and R. O. Pohl
Laboratory of Atomic and Solid State Physics, Cornell University, Ithaca, New York 14850

3000 W/mK

1 W/mK



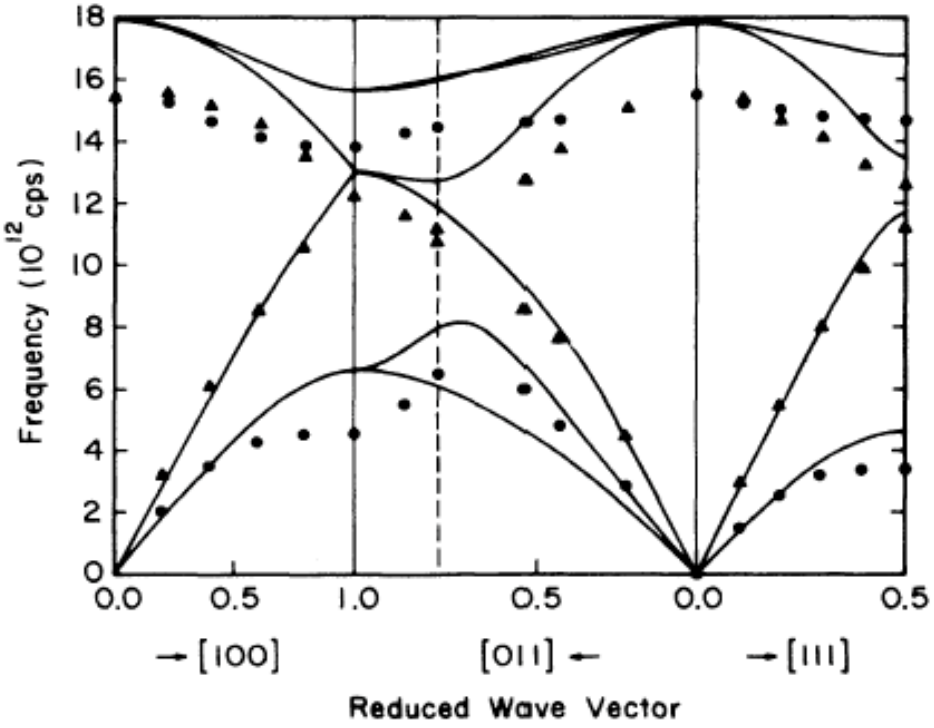


"plateau"

"Phase diagram of silicon by molecular dynamics"

J. Q. Broughton and X. P. Li

Phys. Rev. B 35, 9120-9127 (1987)

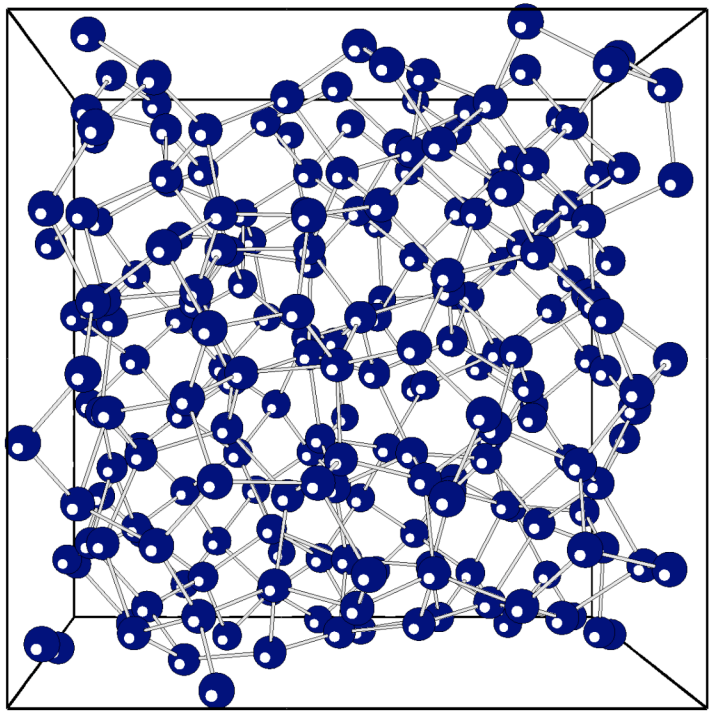


interatomic forces

[16]F. H. Stillinger and T. A. Weber, Phys. Rev. B **31**, 5262 (1985).

amorphous silicon

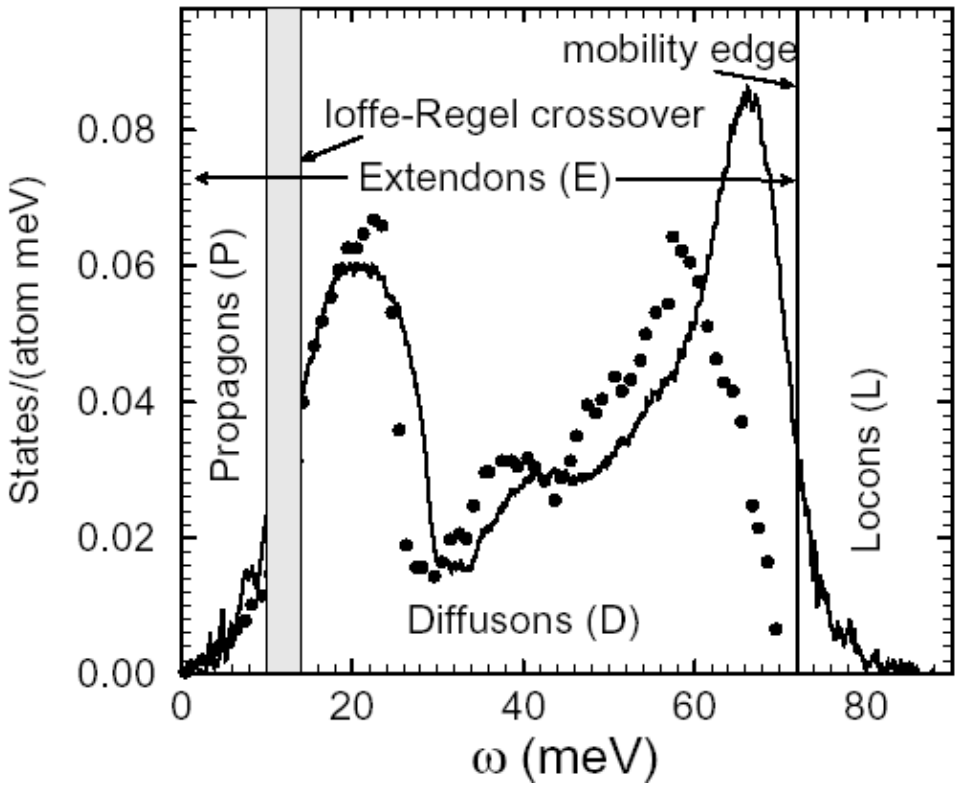
PBA, J. L. Feldman, J. Fabian



atom coordinates

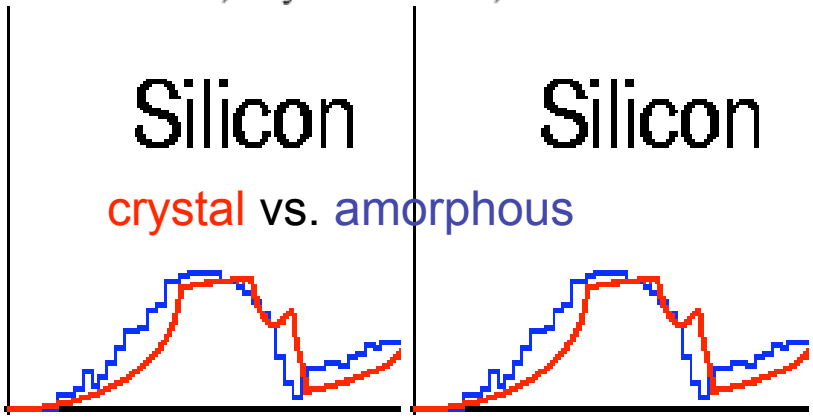
[15]F. Wooten, K. Winer, and D. Weaire, Phys. Rev. Lett. **54**, 1392 (1985).

vibrational densitv of states

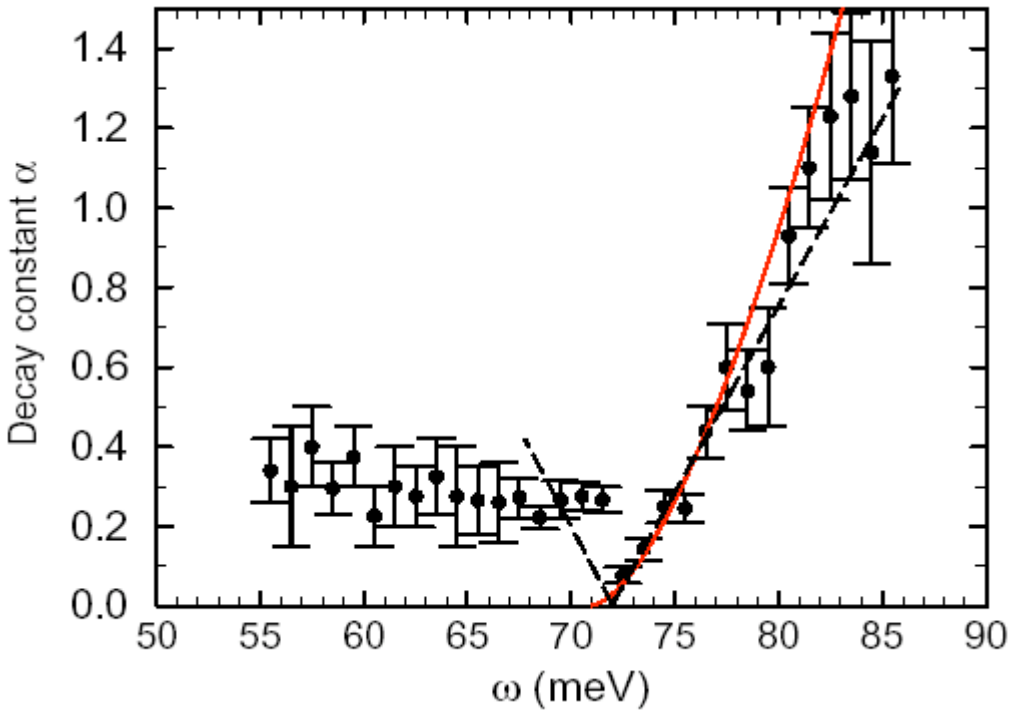


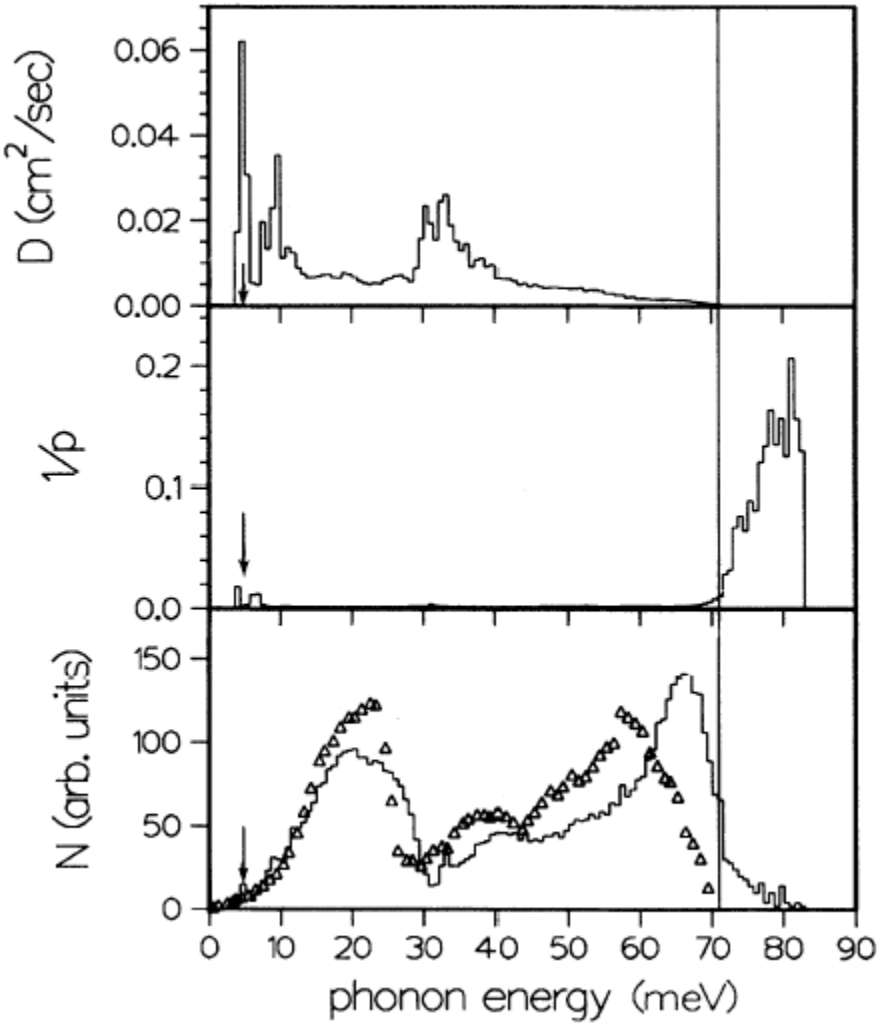
Neutron Scattering data

[20]W. A. Kamitakahara, C. M. Soukoulis, H. R. Shanks, U. Buchenau, and G. S. Grest, Phys. Rev. B **36**, 6539 (1987).



$$\frac{1}{p_i} = \sum_l \left[\sum_\alpha \epsilon_i(l,\alpha)^2 \right]^2$$





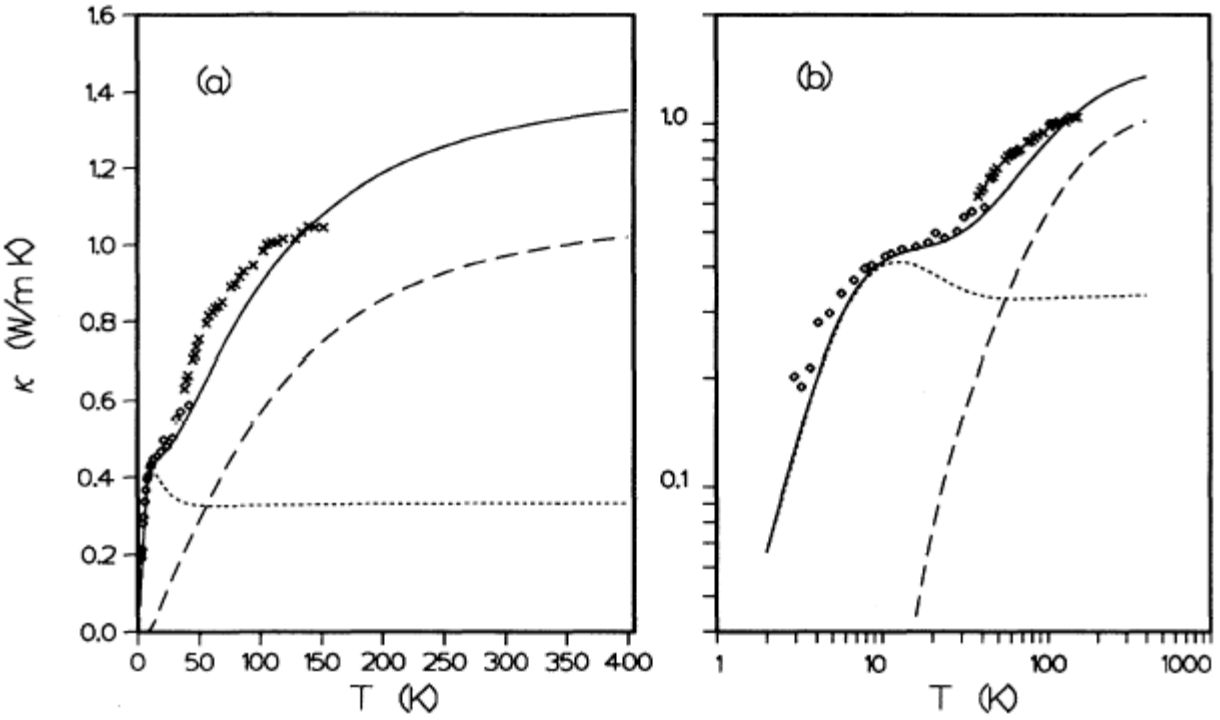
Phonon gas model: $\mathbf{J} = \frac{1}{V} \sum_i \mathbf{v}_i \hbar\omega_i \delta N_i$,

does not apply! Group velocity v_i is undefined!

Lattice analog of Kubo-Greenwood formula (Allen and Feldman, 1987)

$$\kappa = \frac{1}{V} \sum_i C_i(T) D_i$$

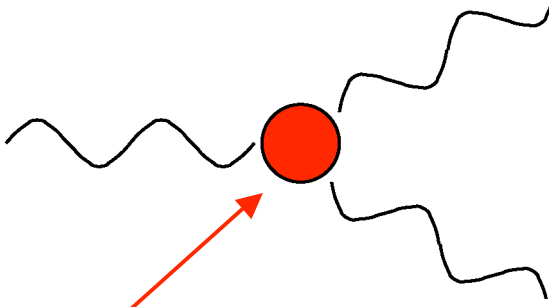
$$D_i = \frac{\pi V^2}{3\hbar^2 \omega_i^2} \sum_j^{\neq i} |S_{ij}|^2 \delta(\omega_i - \omega_j)$$



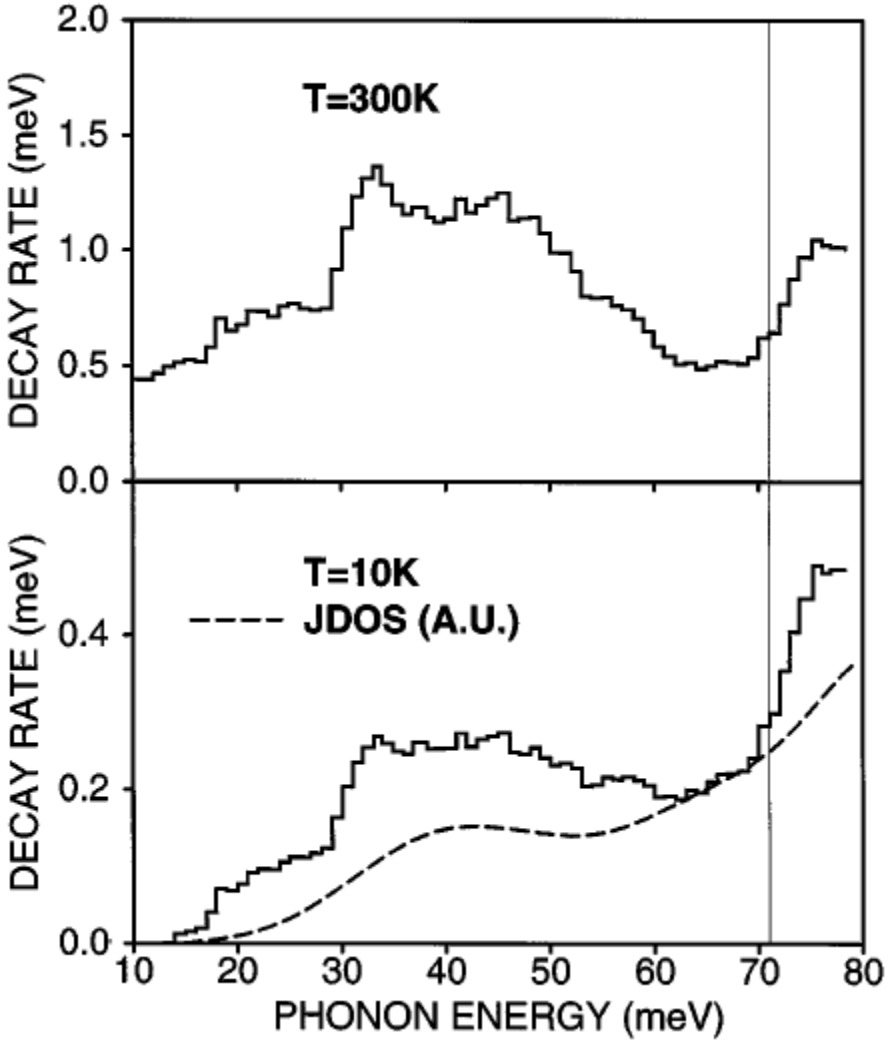
"Anharmonic Decay of Vibrational States in Amorphous Silicon"

Jaroslav Fabian and Philip B. Allen

Phys. Rev. Lett. 77, 3839 (1996)



$$V(j,k,l) = \sum_{a,b,c}\sum_{\alpha\beta\gamma} \frac{\partial^3 V}{\partial u_{a\alpha}\partial u_{b\beta}\partial u_{c\gamma}} \frac{e^j_{a\alpha}}{\sqrt{m_a}} \frac{e^k_{b\beta}}{\sqrt{m_b}} \frac{e^l_{c\gamma}}{\sqrt{m_c}}$$



$$2\Gamma(j) = \frac{\hbar^2\pi}{4\omega(j)} \sum_{k,l} \frac{|V(j,k,l)|^2}{\omega(k)\omega(l)} \times \left(\frac{1}{2}[1+n(k)+n(l)]\delta[\omega(j)-\omega(k)-\omega(l)] + [n(k)-n(l)]\delta[\omega(j)+\omega(k)-\omega(l)] \right). \quad (1)$$

Observation of Giant Kohn Anomaly in the One-Dimensional Conductor $K_2Pt(CN)_4Br_{0.3}\cdot 3H_2O$

B. Renker, H. Rietschel, L. Pintschovius, W. Gläser,
P. Brüesch, D. Kuse, and M. J. Rice

Phys. Rev. Lett. 30, 1144 (1973)

Peierls-Overhauser Insulator, or "band Jahn-Teller system"

partly-filled electron energy band

"Peierls gap"