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SPRING COLLEGE IN CONDENSED MATTER
ON
"THE INTERACTION OF ATOMS & MOLECULES WITH SOLID SURFACES"
(25 April - 17 June 1988)

SURFACE PHONONS AND THEIR SPECTROSCOPY BY He SCATTERING
(Part II)

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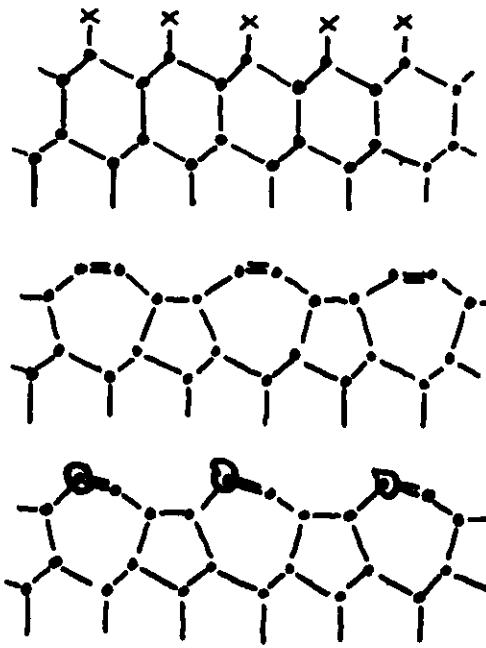
Surface Phonon Anomalies

expt.: substantial deviations of measured dispersion curves from predictions for ideal surfaces

theor.: microscopic mechanisms, forbidden or hindered in the bulk, are promoted at the surface by symmetry lowering

- surface relaxation & reconstruction — alkali halides *
  — Si, GaAs
- surface electronic states — graphite
  — GaSe
  — noble metals *
- change of electron-phonon interaction — refractory SC's *
  — CDW systems *

Silicon surface reconstruction

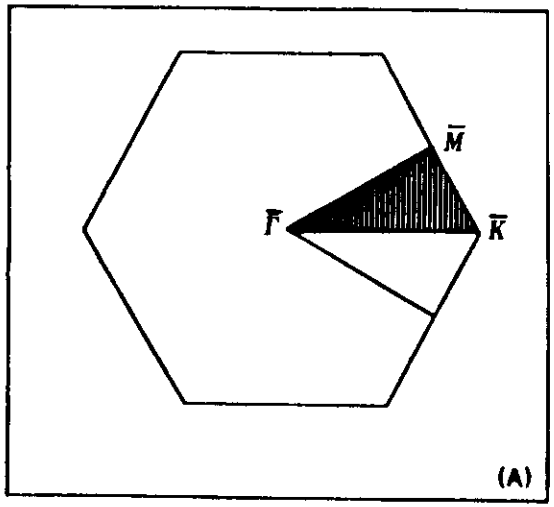


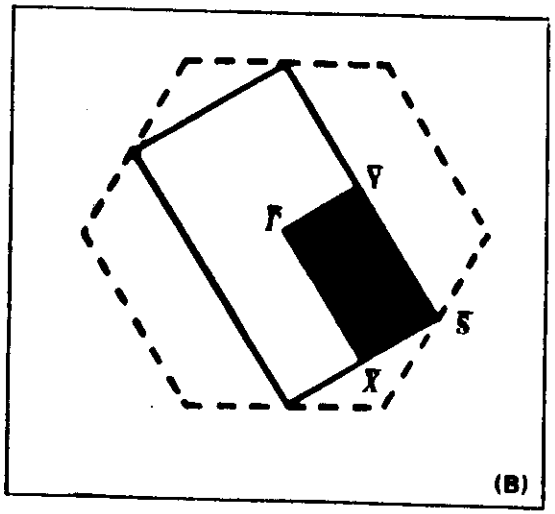
Si(111) 1×1 : H

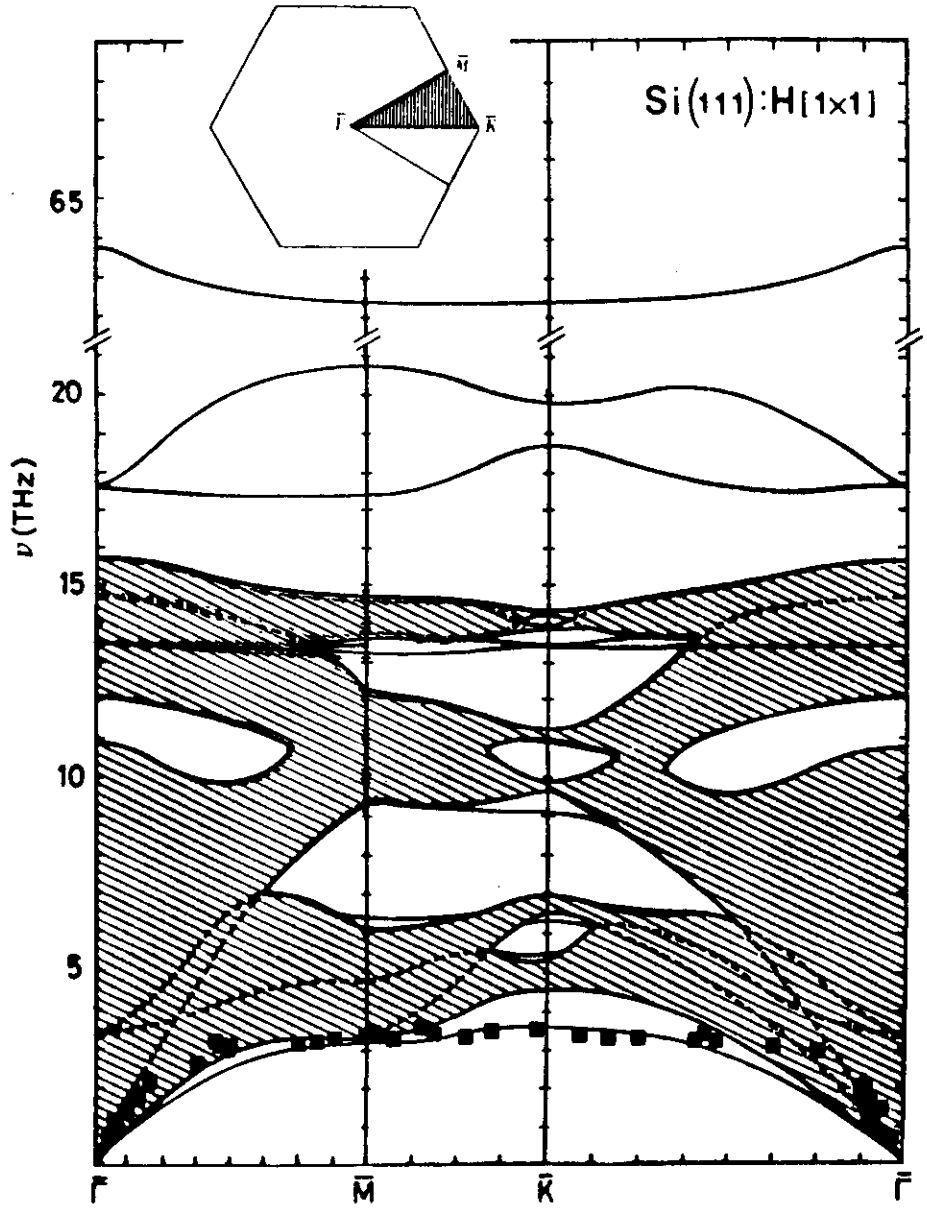
Si(111) 2×1

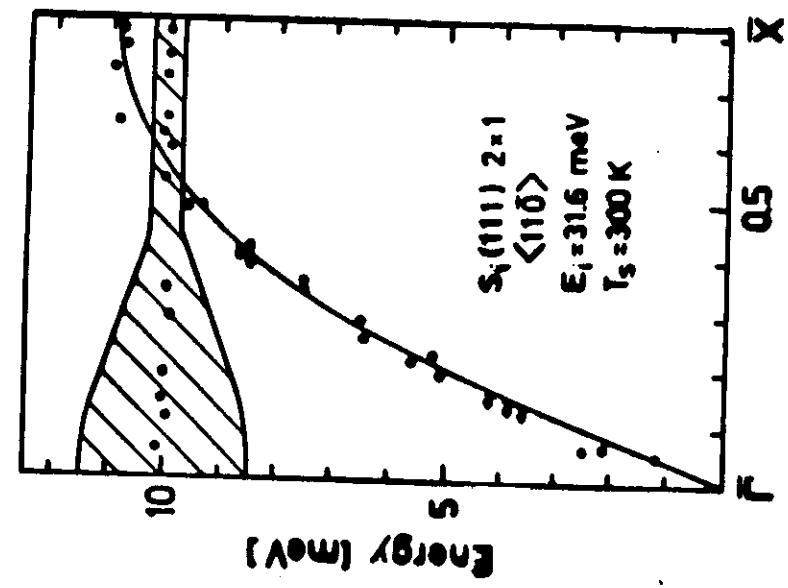
— interface

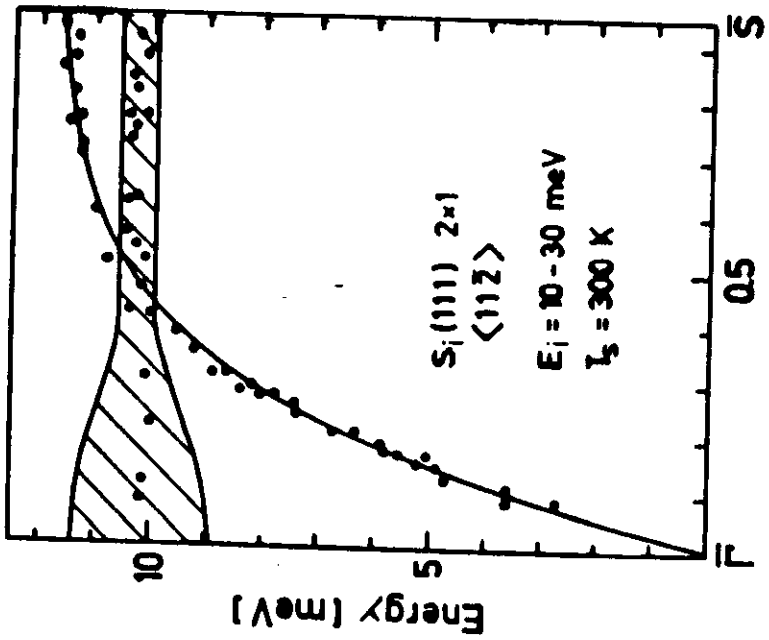
← buckling


$\bar{M}$
$\bar{\Gamma}$
$\bar{K}$
(A)


$\bar{\Gamma}$
$\bar{Y}$
$\bar{S}$
$\bar{X}$
(B)

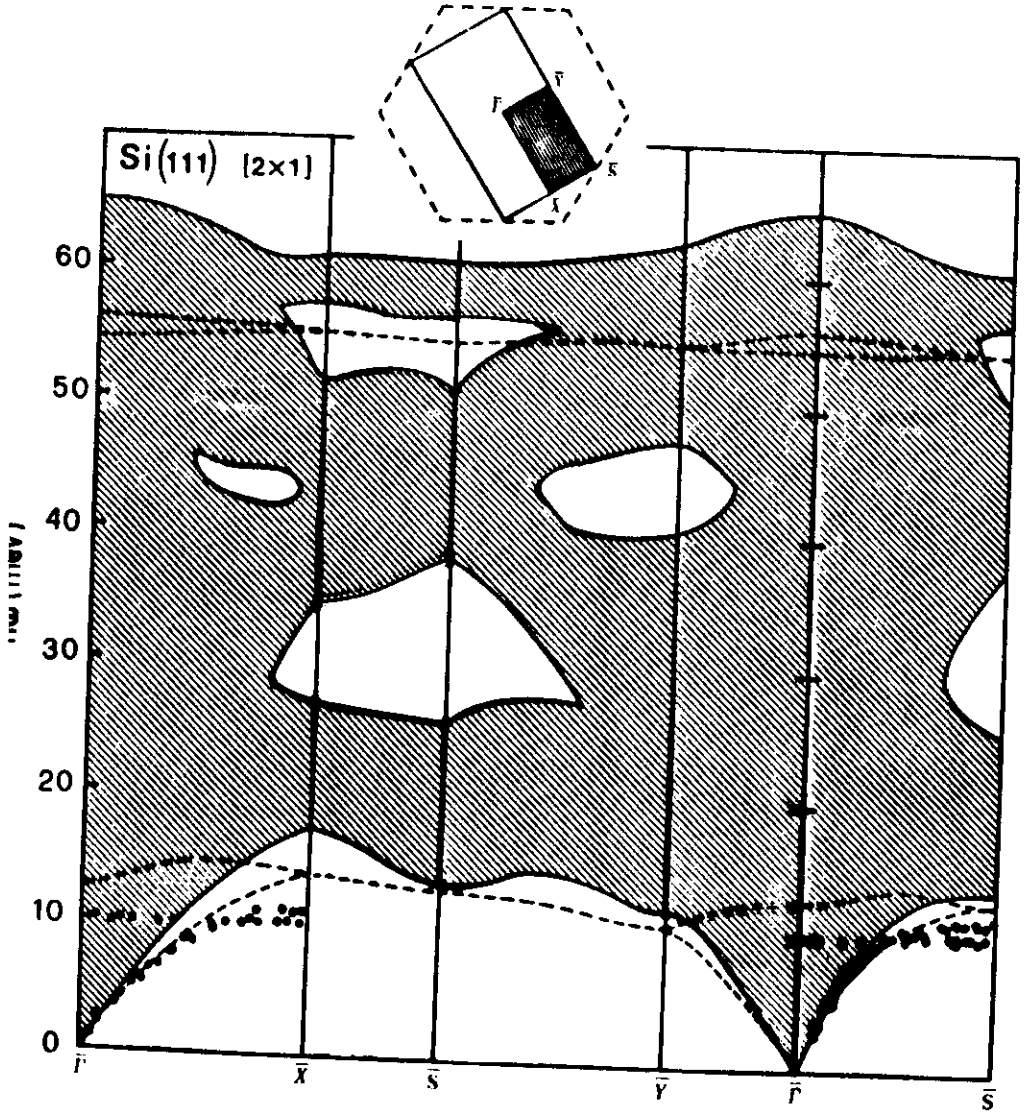

Si(111):H[1x1]
65
20
15
10
5
ν (THz)
$\bar{\Gamma}$
$\bar{M}$
$\bar{K}$
$\bar{\Gamma}$

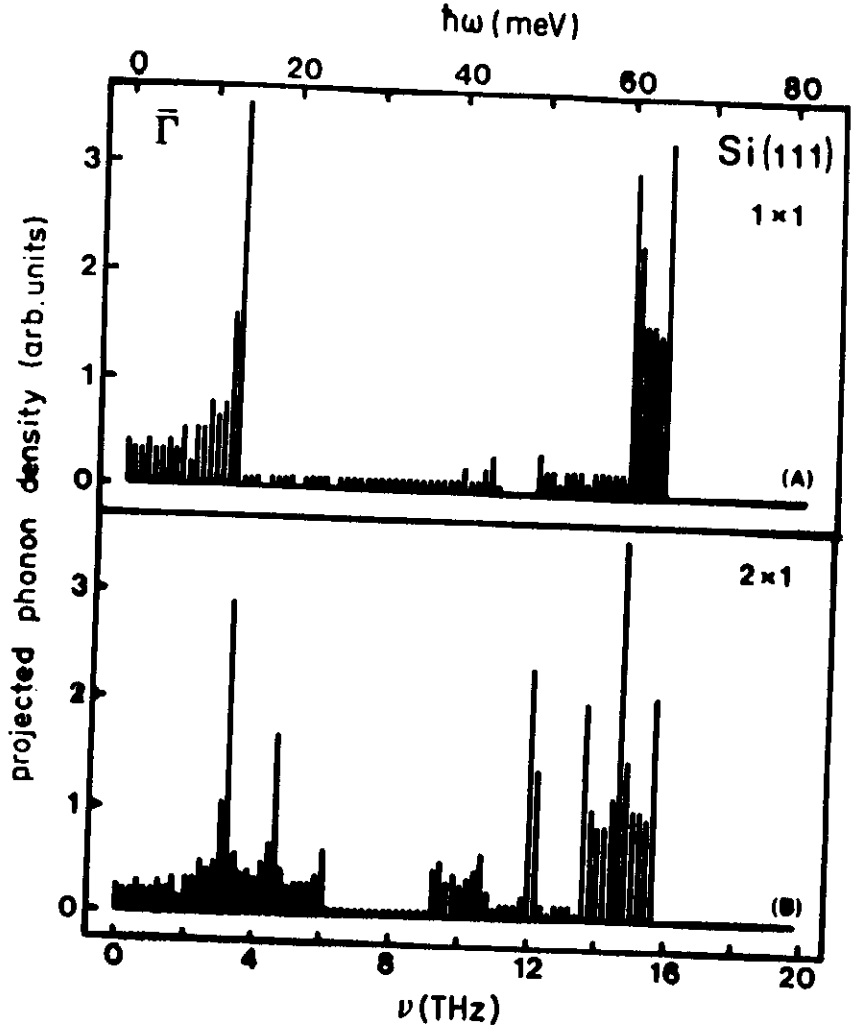


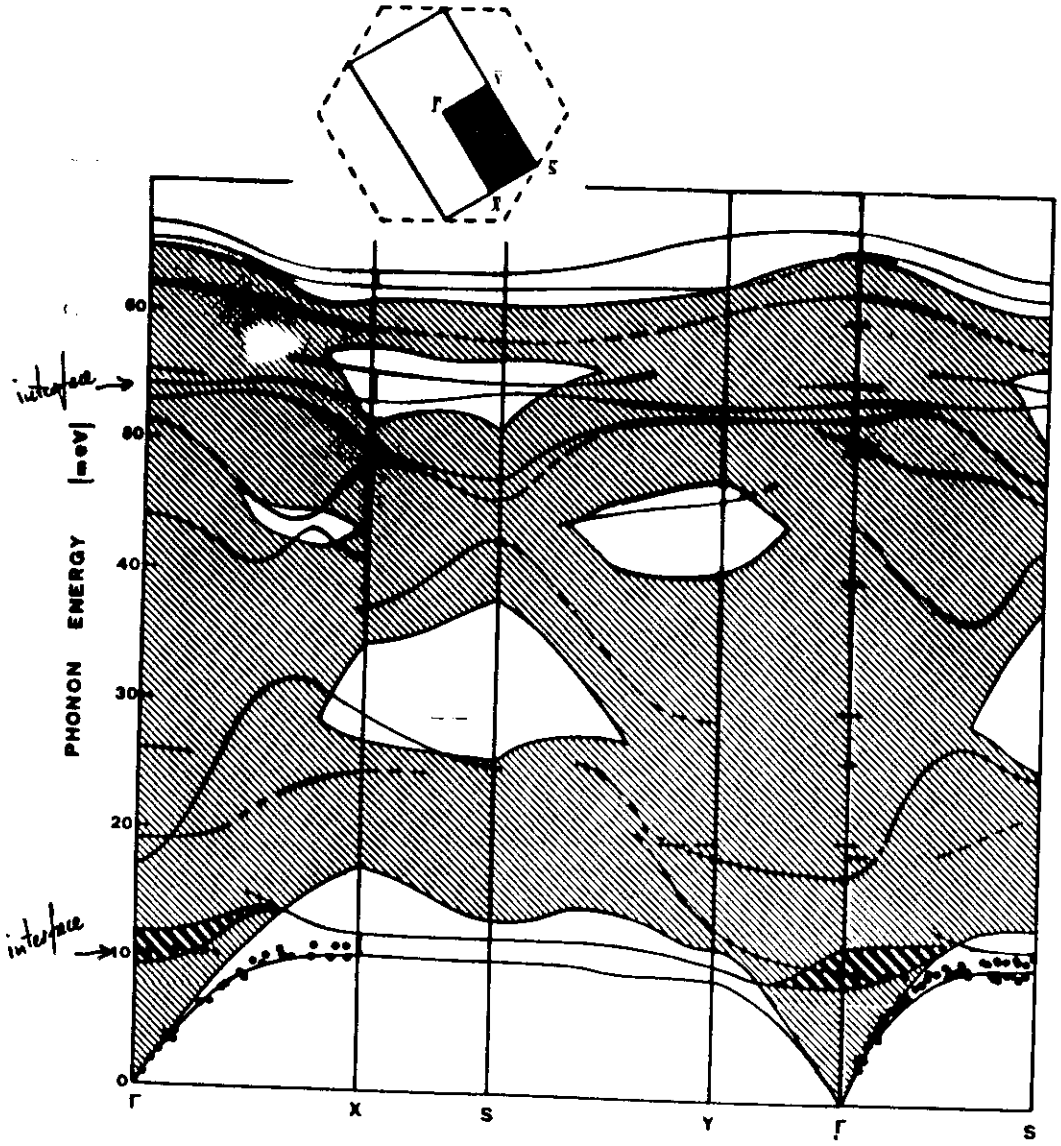


Leap reconstruction

- Folding effects
  (aspects of ideal surface dynamics)
- Gaps at folding points
  (depend on local geometry)
  buckling → gaps
- "Interface" dynamics
  (perturbed ideal-surface dynamics)
  → isotropy (e.g., modes at 55 meV and 10 meV)
- "Surface" dynamics
  (surface localized modes)
  → anisotropy

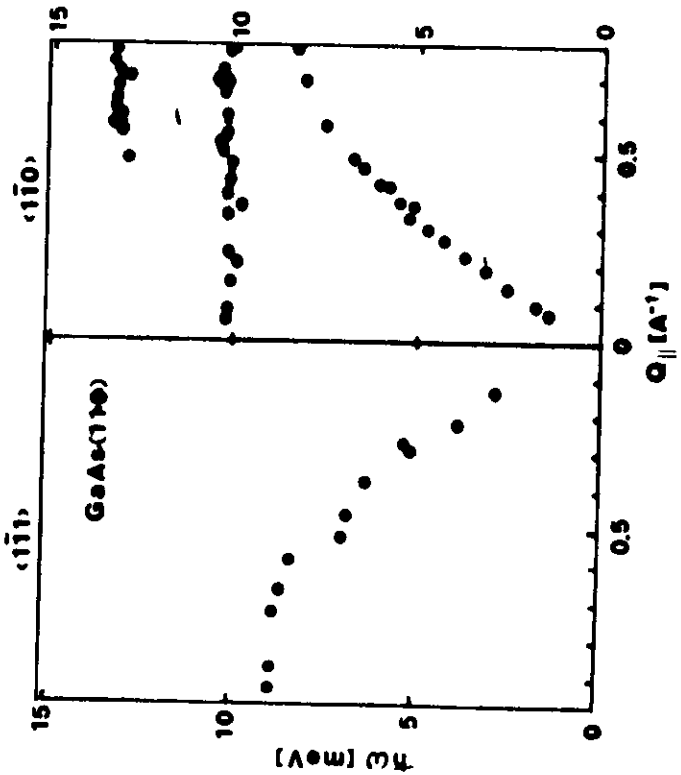

Si(111) [2×1]
60
50
40
30
20
10
0
$\bar{\Gamma}$
$\bar{X}$
$\bar{S}$
$\bar{Y}$
$\bar{\Gamma}$
$\bar{S}$


ħω (meV)
0
20
40
60
80
$\bar{\Gamma}$
Si(111)
1×1
(A)
2×1
(B)
projected phonon density (arb.units)
0
1
2
3
0
4
8
12
16
20
ν(THz)

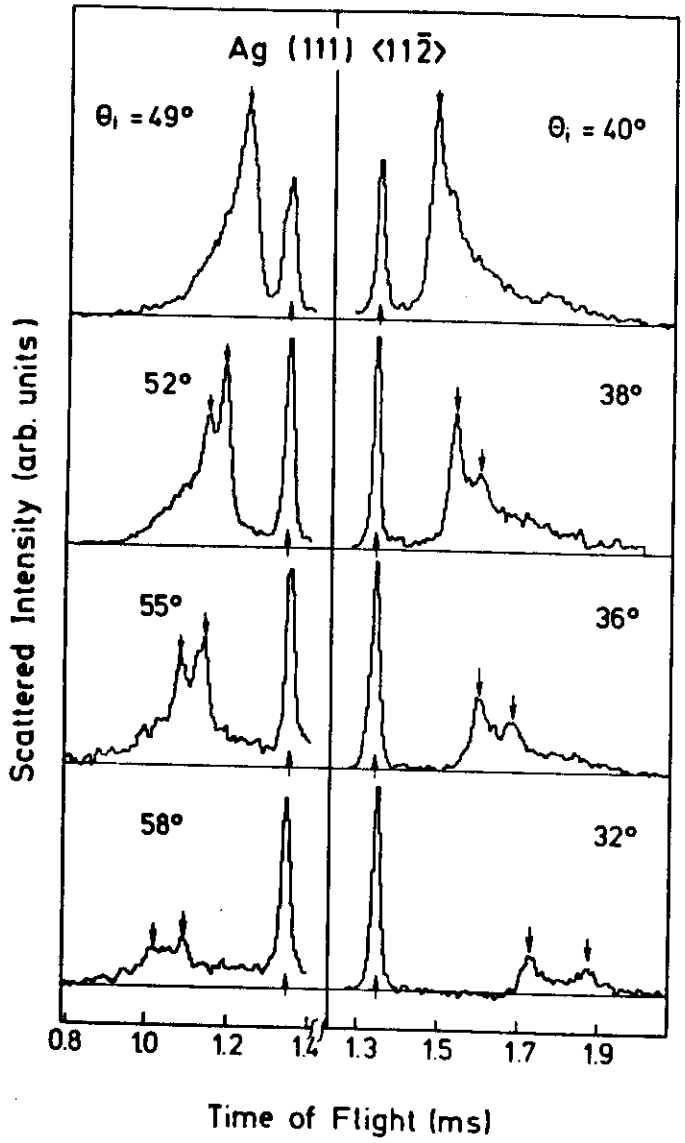


$(1\bar{1}0)$: E_i = 20 to 30 meV
$(11\bar{1})$: E_i = 30 meV
T_s = 300 K

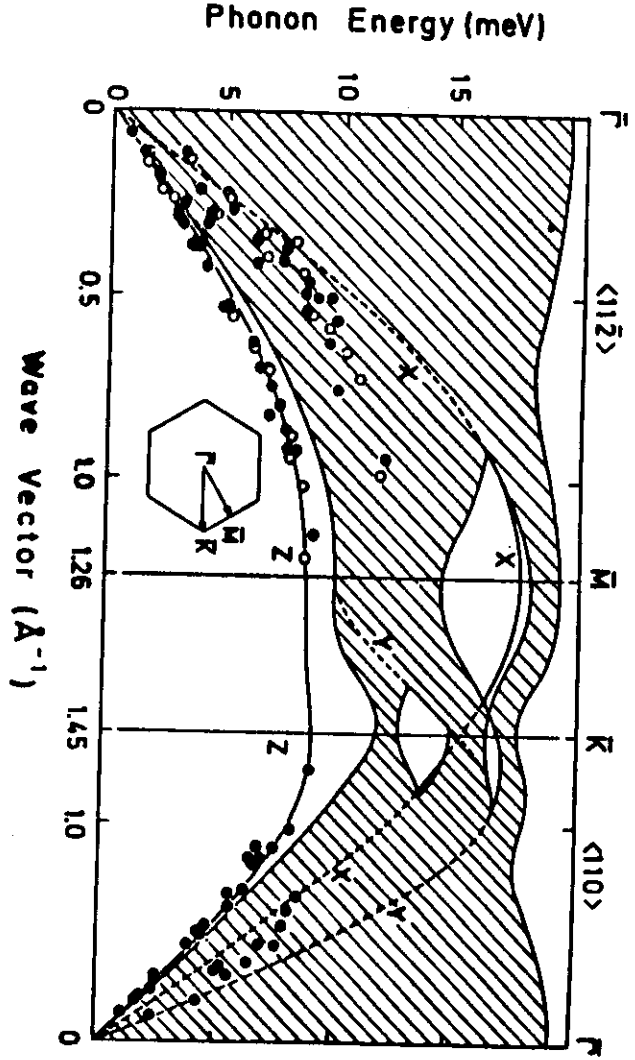
from J.P. Toennies, Ch. Wöll and U. Harten (to be published and private communication)



from Harten, Toennies & Wöll



Ag (111)



Theory: Armand
Expt.: Toennies, Harte et al.

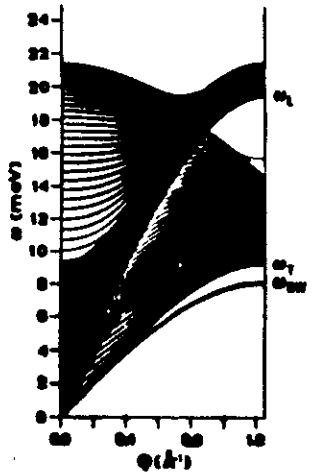


FIG. 3. Surface phonons for Ag(111) relative to the point $\bar{P}'$ of Fig. 1. ω_{SV}, SW dispersion curve. ω_T and ω_L, dispersion curves for bulk transverse and longitudinal thresholds.

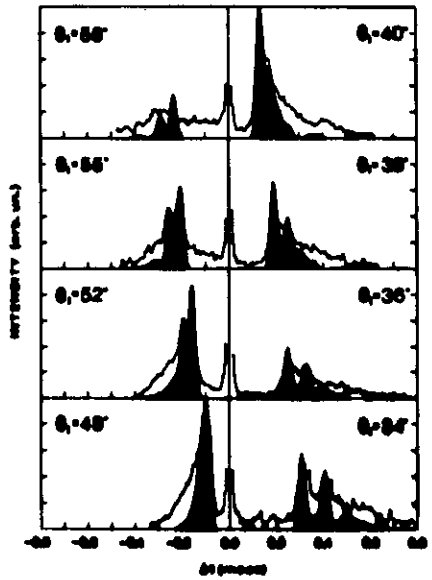
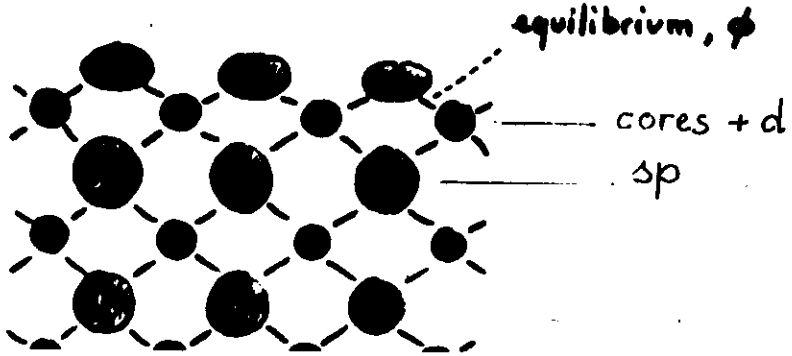
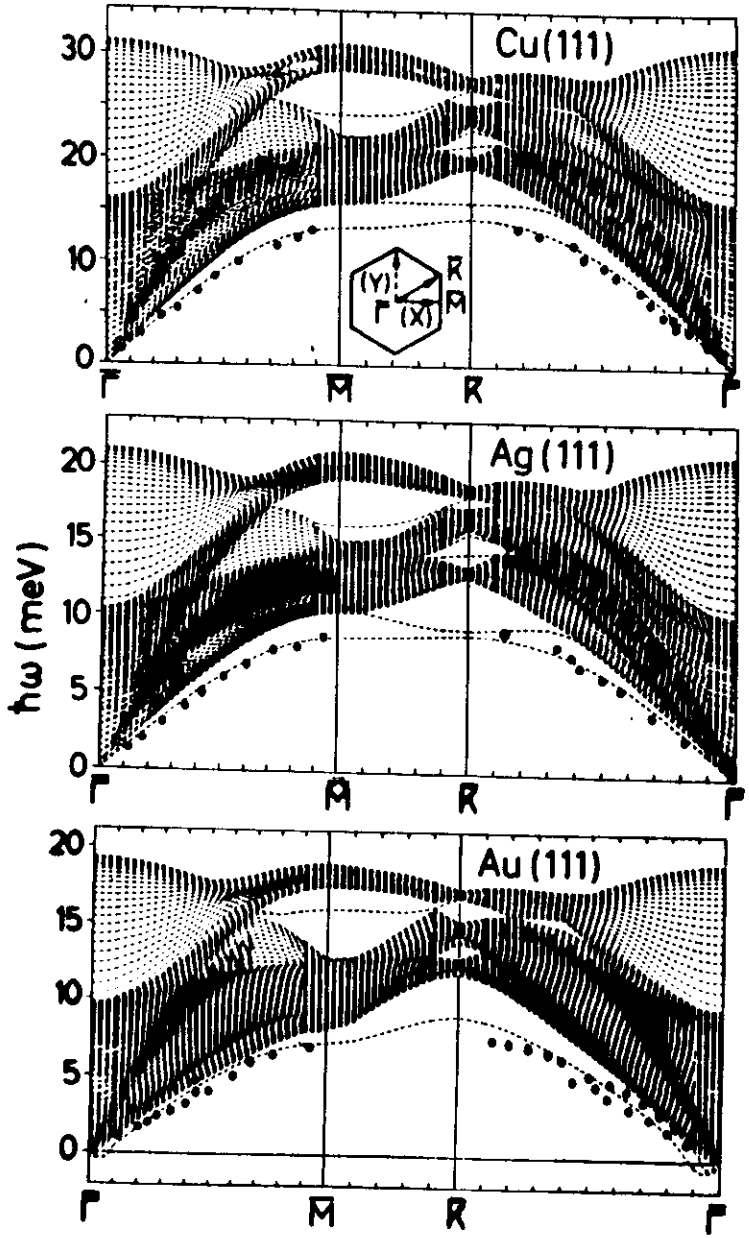


FIG. 4. TOF spectra for He/Ag(111) for $E_i = 17.8$ meV. The histograms are the experimental data of Ref. 5. The calculated curves refer to the point $\bar{P}'$ of Fig. 1 and are normalized to the SW experimental peaks.

V. Bortolani, A. Franchini, F. Nizzoli, and G. Santoro
PHYSICAL REVIEW LETTERS 6 February 1984





VOLUME 55, NUMBER 21 PHYSICAL REVIEW LETTERS 18 NOVEMBER 1985

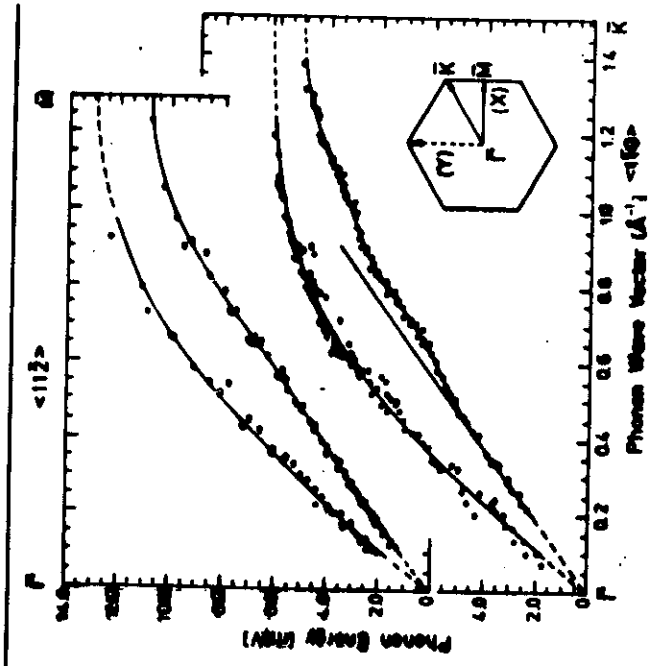
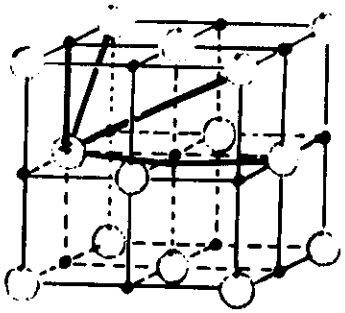
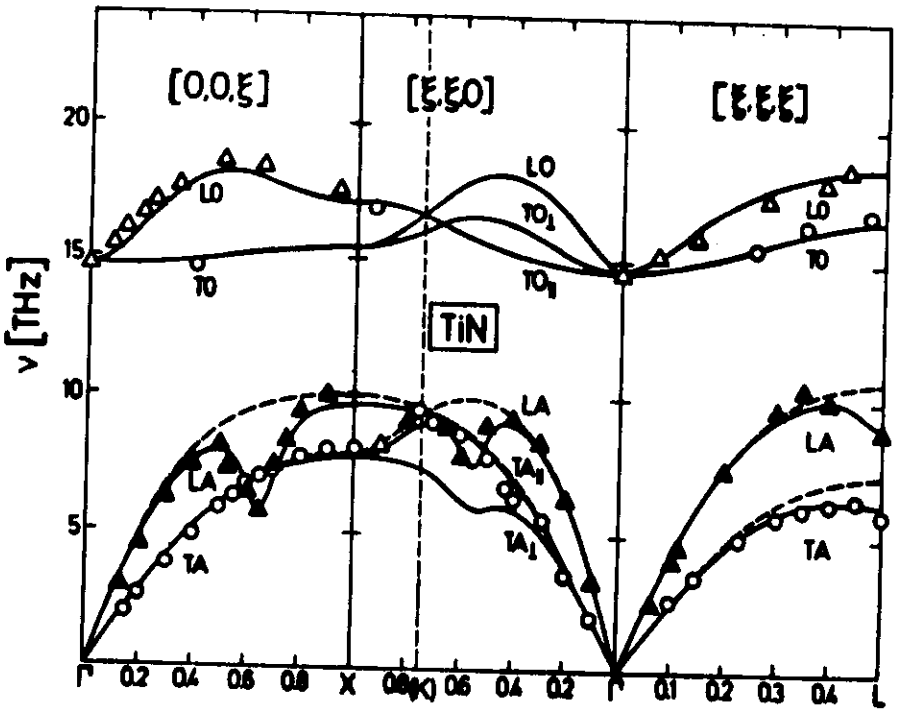


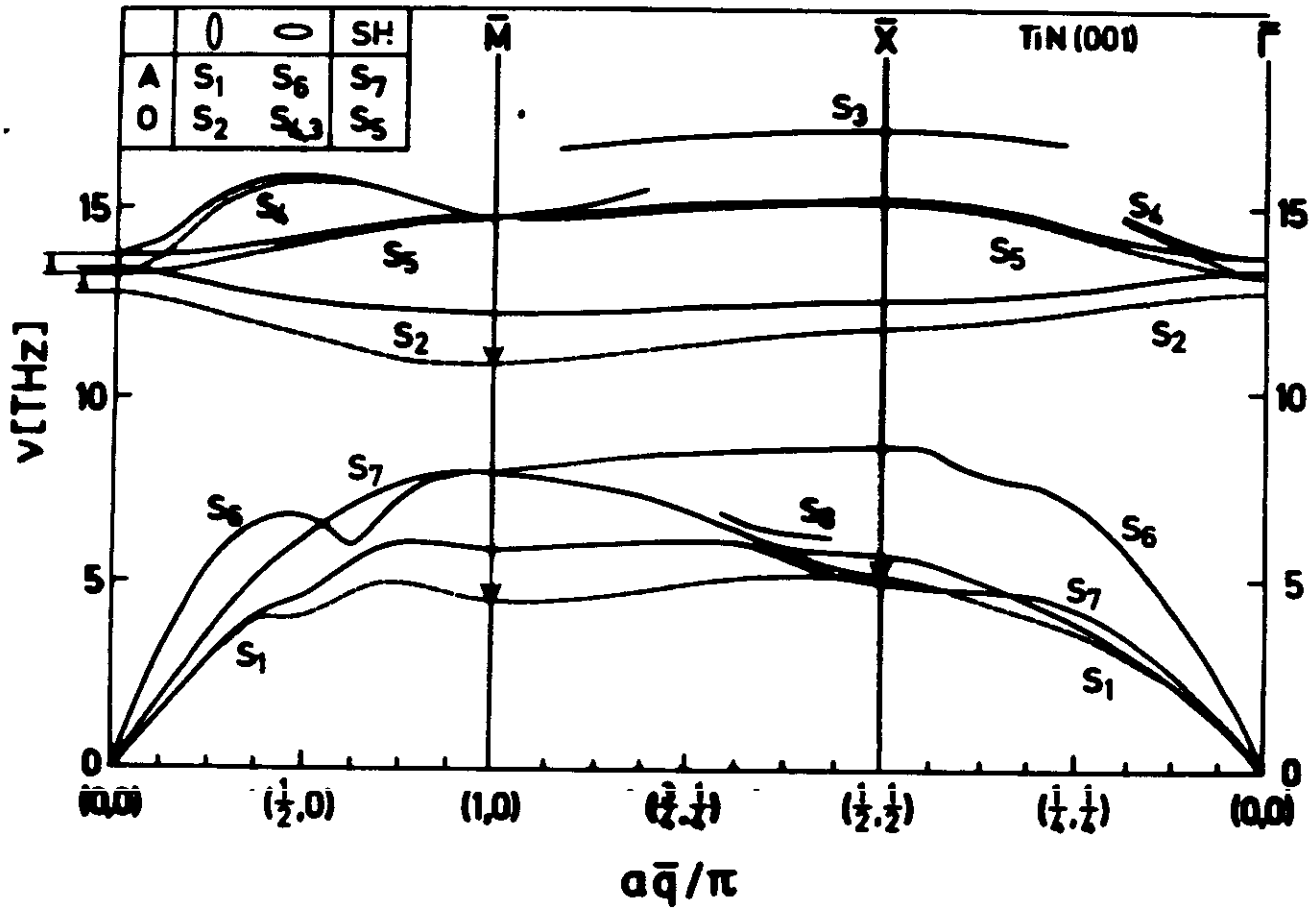
FIG. 2. Measured surface-phonon dispersion curves for Pt(111). The upper two curves are for the $\bar{\Gamma}$-$\bar{M}$ ($\langle 11\bar{2}\rangle$) direction and the bottom two curves for the $\bar{\Gamma}$-$\bar{K}$ ($\langle 1\bar{1}0\rangle$) direction. The beam energies in both experiments were at fixed values between 10 and 32 meV. The target temperature in the $(11\bar{2})$ measurements was 400 K, and in the $(1\bar{1}0)$ measurements 160 K. The curves show the best-fit Fourier expansions. The solid line in the lowest set of data corresponds to a group velocity of 11.1 MeV Å.





Cluster model (Miura, Kress & Bilz, 1984)

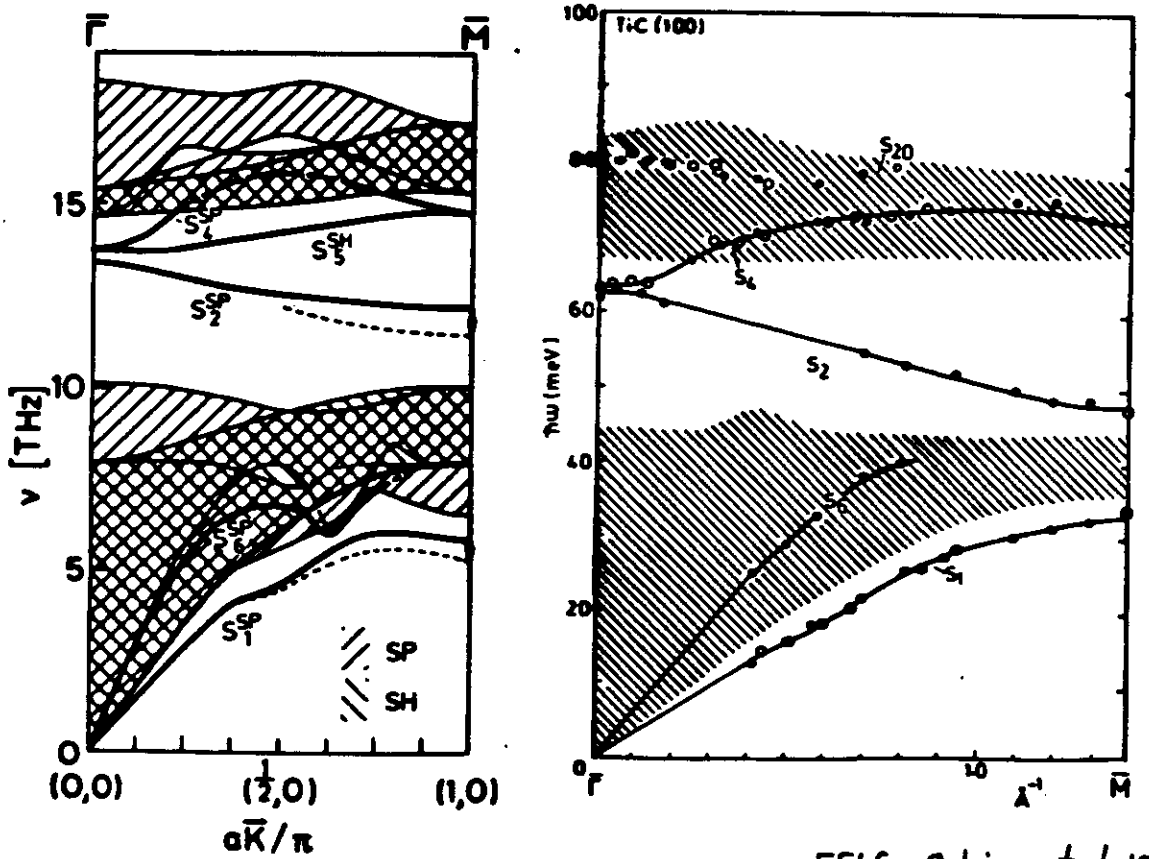
emphasizes role of excitations of pd states near Fermi surfaces induced by vibrations



91-II

G.B, Bilz, Kress & Miura (PRL 1984)

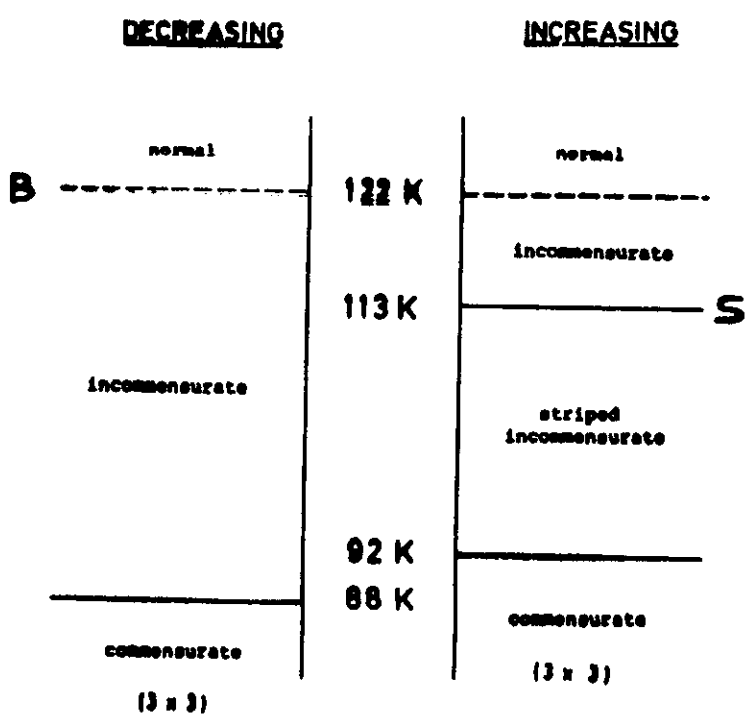
Anomalies in the Surface-Phonon Dispersion of TiN (001)



EELS : Oshima et al 1986

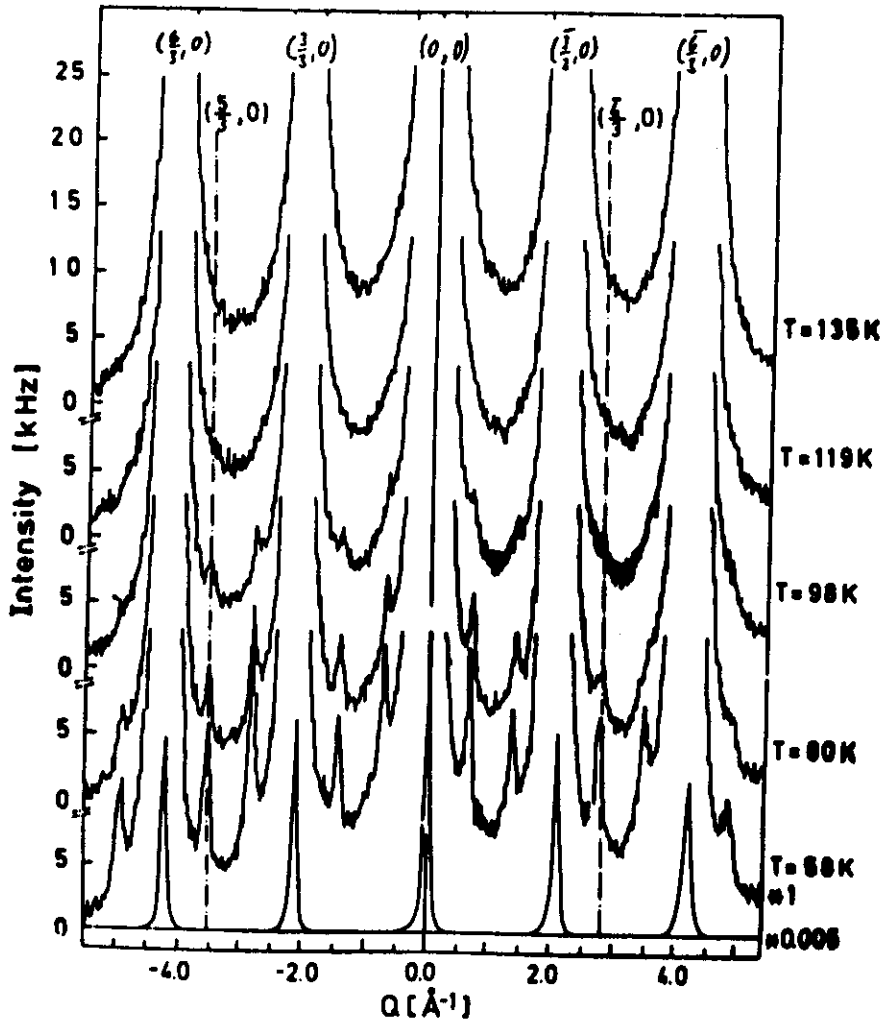
I-II

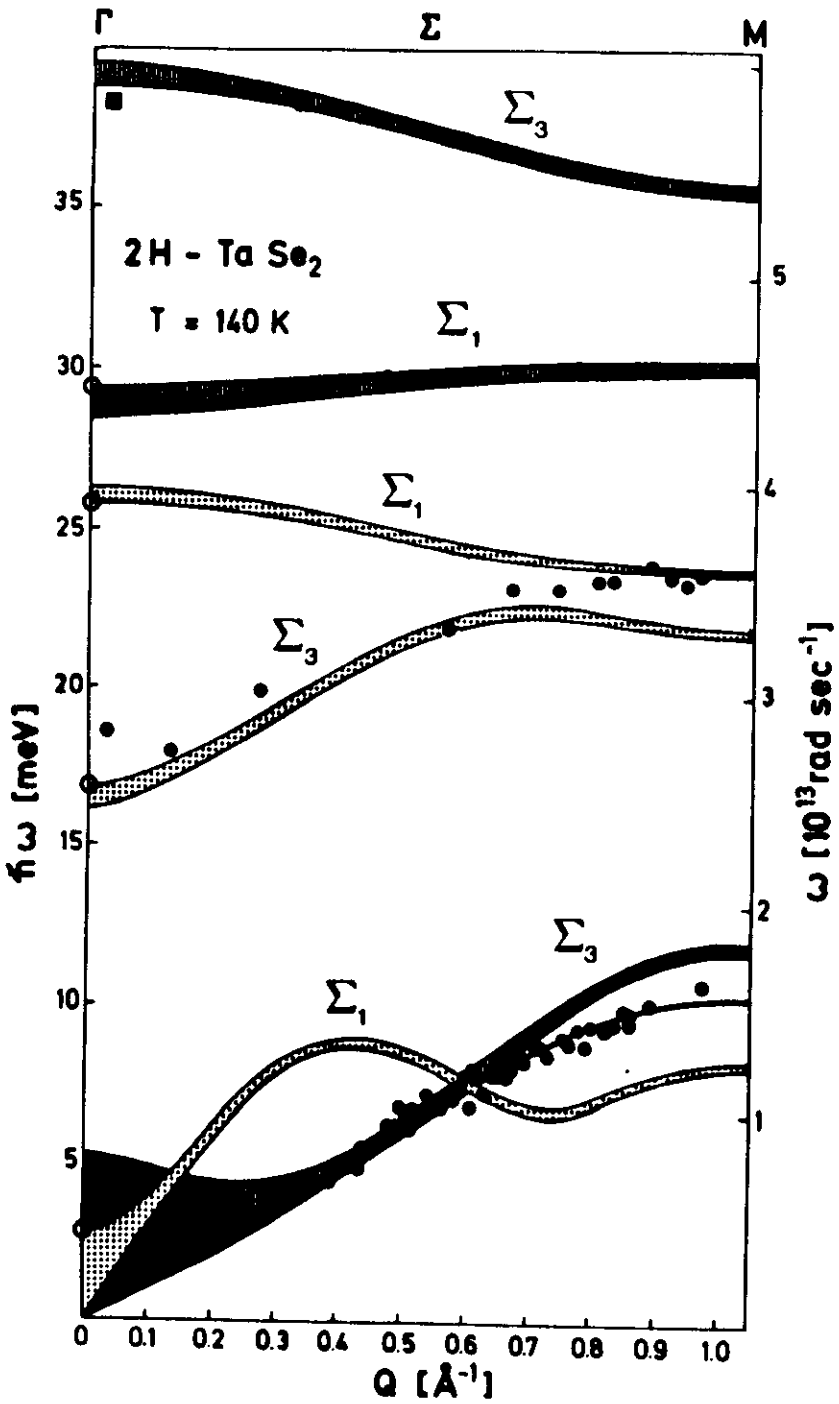
2H - $TaSe_2$



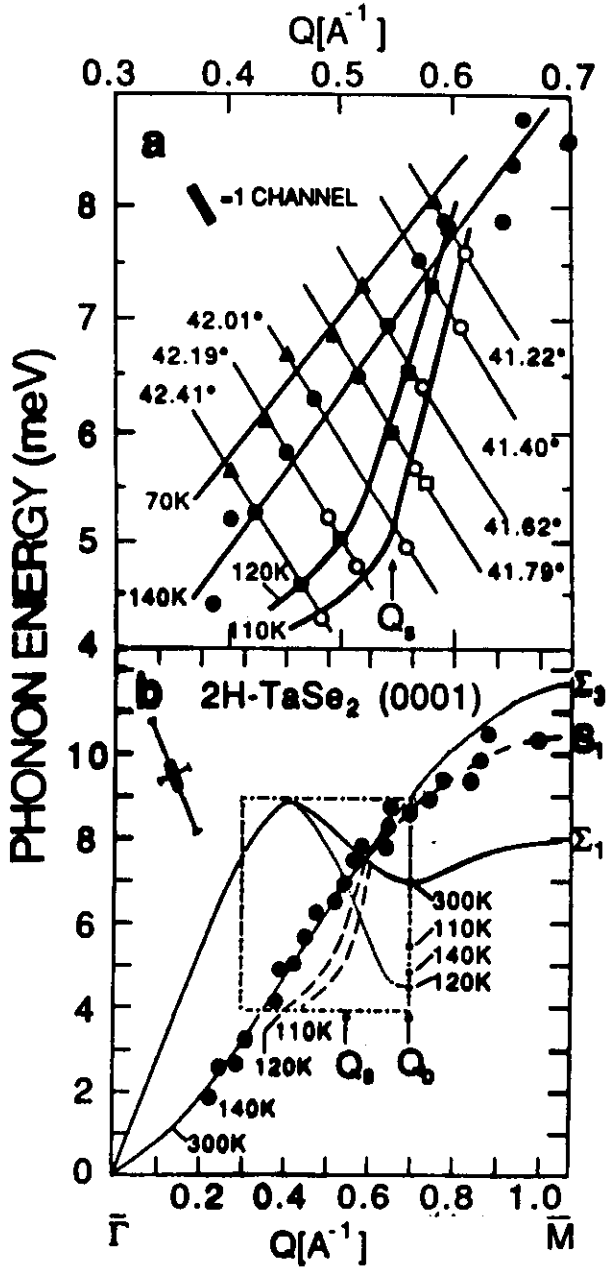
2H - $TaSe_2$ (001) <100>

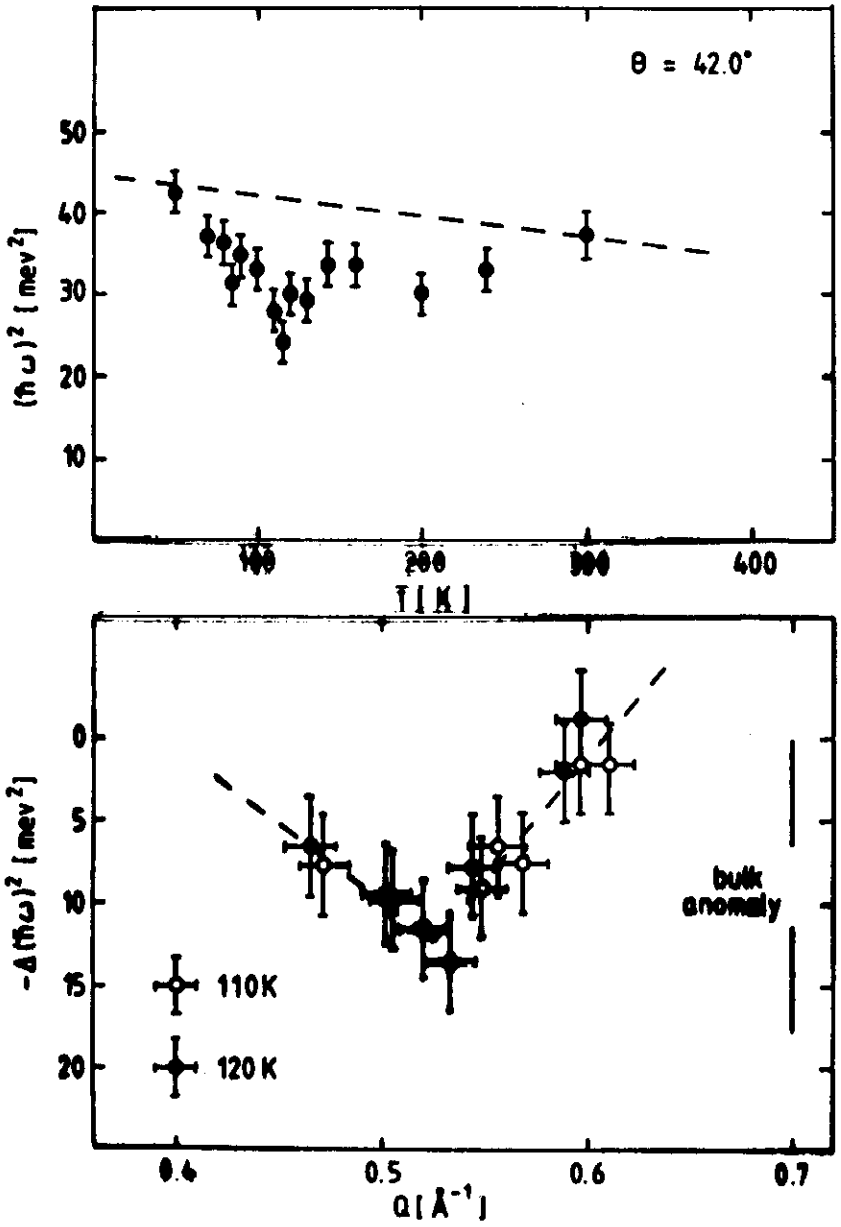
k_i = 11.7 Å^{-1}
E_i = 71.5 meV





Benedek, Brusdeylins, Miglio, Shofonick and Toennies (Phys. Rev. Letters




θ = 42.0°
$(\hbar\omega)^2$ [mev^2]
50
40
30
20
10
100
200
300
400
T [K]
$-\Delta(\hbar\omega)^2$ [mev^2]
0
5
10
15
20
110K
120K
bulk anomaly
0.4
0.5
0.6
0.7
Q [Å^{-1}]

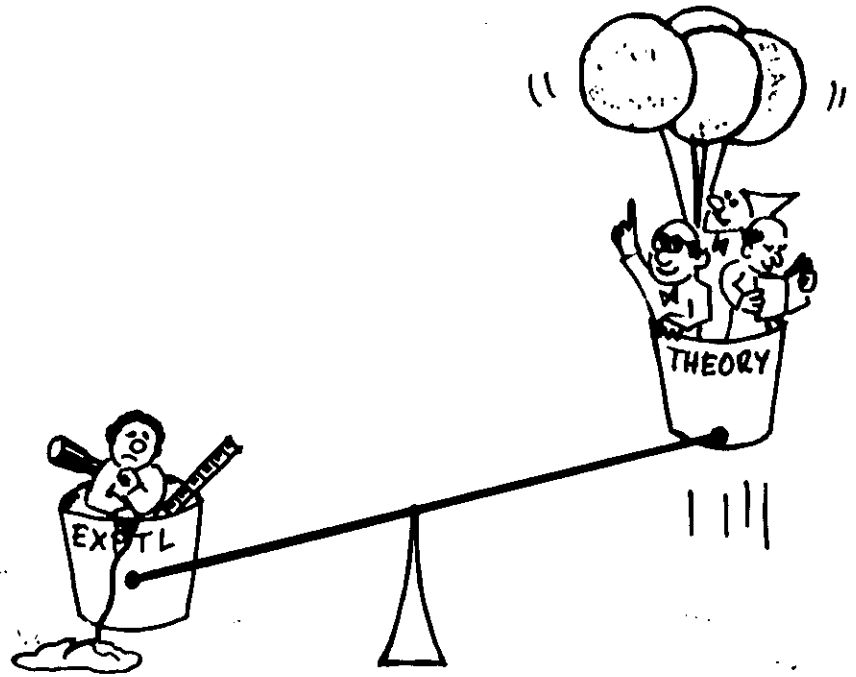
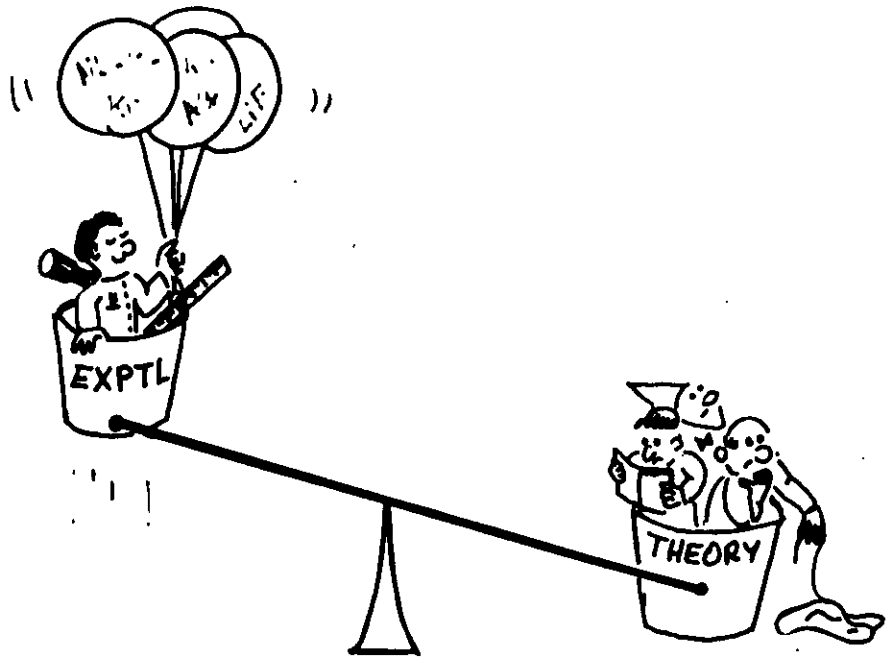

EXPTL
THEORY

fig 3



like neutron spectroscopy

stimulated investigation

on microscopic models,

surface phonon spectroscopy

will trigger new developments

in microscopic ab-initio theories

e.g. : C. Calandra and coworkers
(Na, K)