



INTERNATIONAL ATOMIC ENERGY AGENCY
UNITED NATIONS EDUCATIONAL, SCIENTIFIC AND CULTURAL ORGANIZATION



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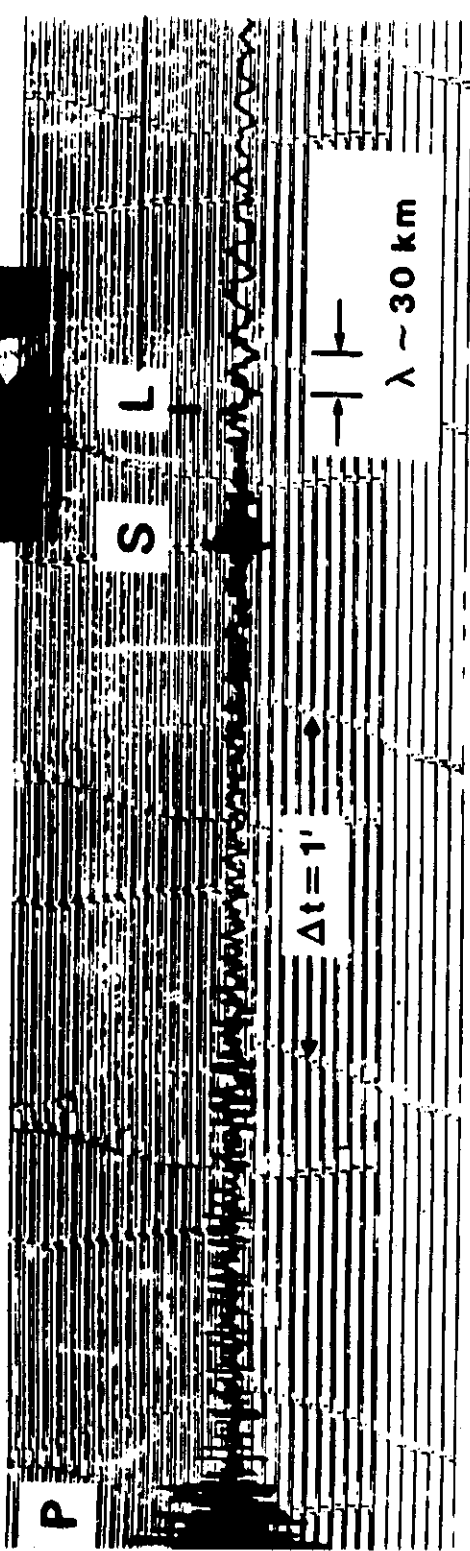
SMR/291 - 29

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 I)

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These are preliminary lecture notes, intended only for distribution to participants.



Terremoto nel centro Italia del 7 maggio 1984 (5.1 Richter)

registrato alla stazione sismografica al CCSEM di Erice

P = longitudinale di volume; S = trasversale di volume; L = di superficie

I-1

SURFACE PHONON

SPECTROSCOPY

BY Helium SCATTERING:

Interaction Diagram

J. F. Teennies & coworkers

MPI-SF
Göttingen

Milano
Univ.

GB, L. Miglio

Theory of surface phonons
& inelastic He scattering:

- alkali halides
- covalent semiconductors
- layered crystals

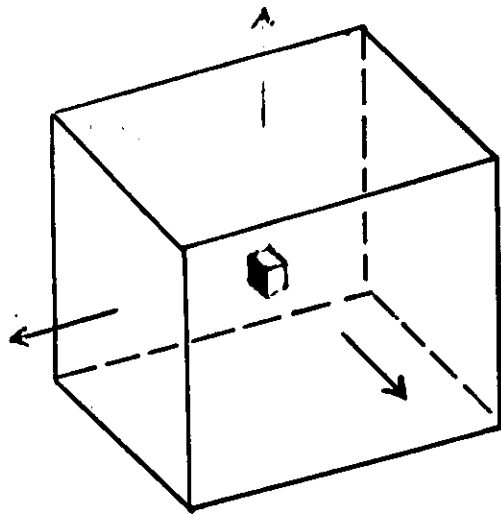
Theory of surface
phonon anomalies

- noble metals
- refractory super-
conductors
- CDW systems

MPI-FKF
Stuttgart

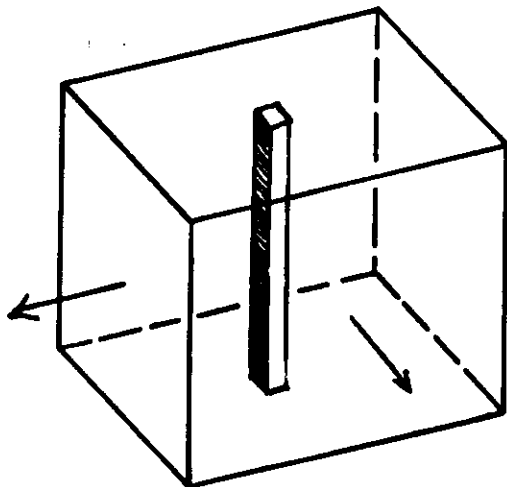
(H. Bilz), W. Kress

I-3



$$\underline{k} = (k_x, k_y, k_z)$$

$$\omega_j(\underline{k})$$

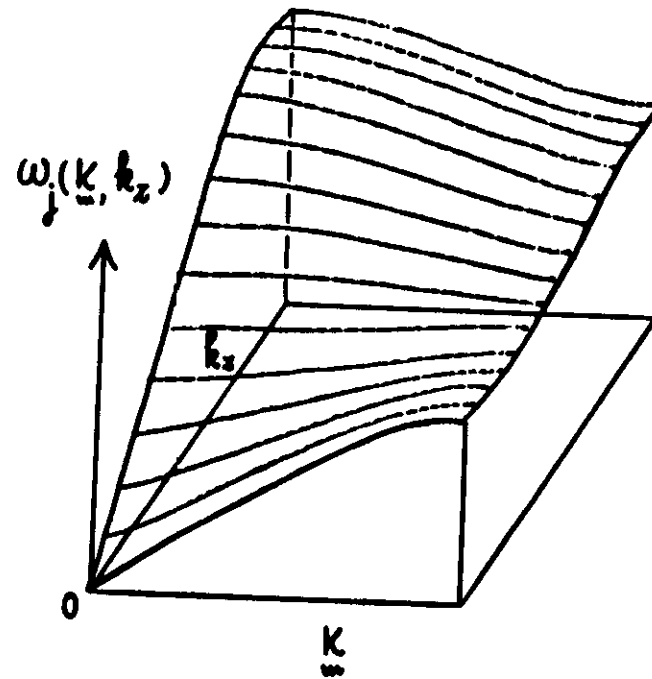


$$\underline{K} = (k_x, k_y)$$

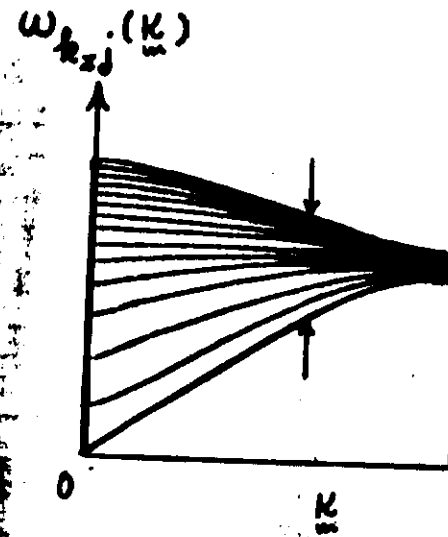
$$\omega_s(\underline{K})$$

$$s = (k_z, j)$$

Phonon dispersion in 3D
(e.g., $j = TA_1$)



xy-dispersion from
in-plane force constants

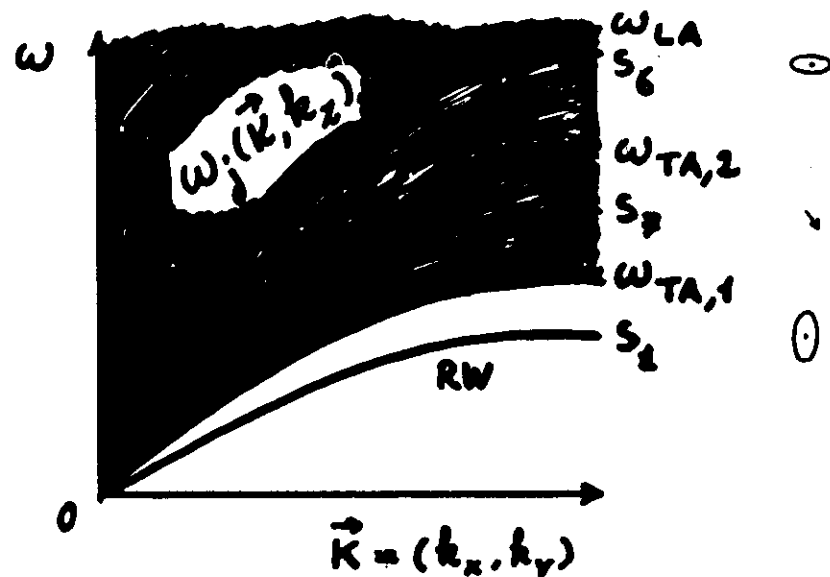
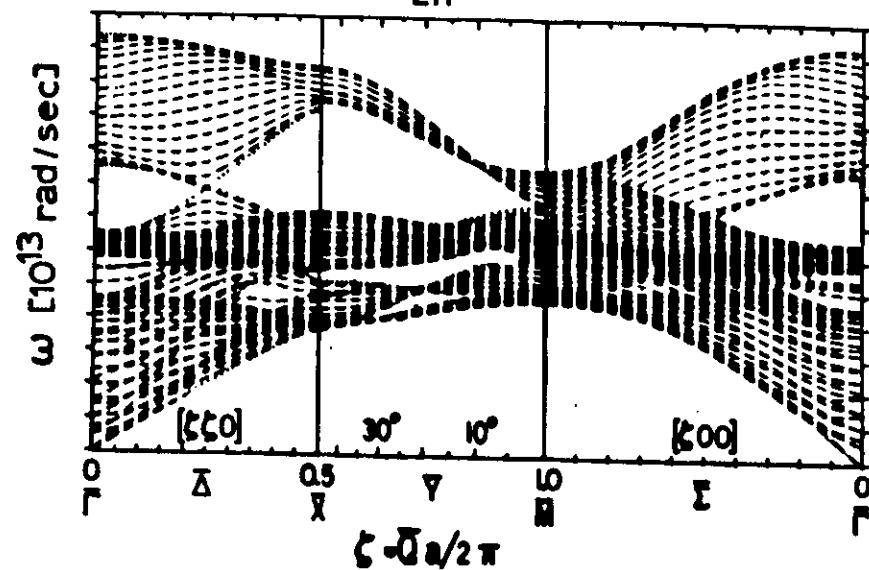


z-dispersion from
interplanar force constants

↓
bandwidth of
surface-projected
bulk phonon bands

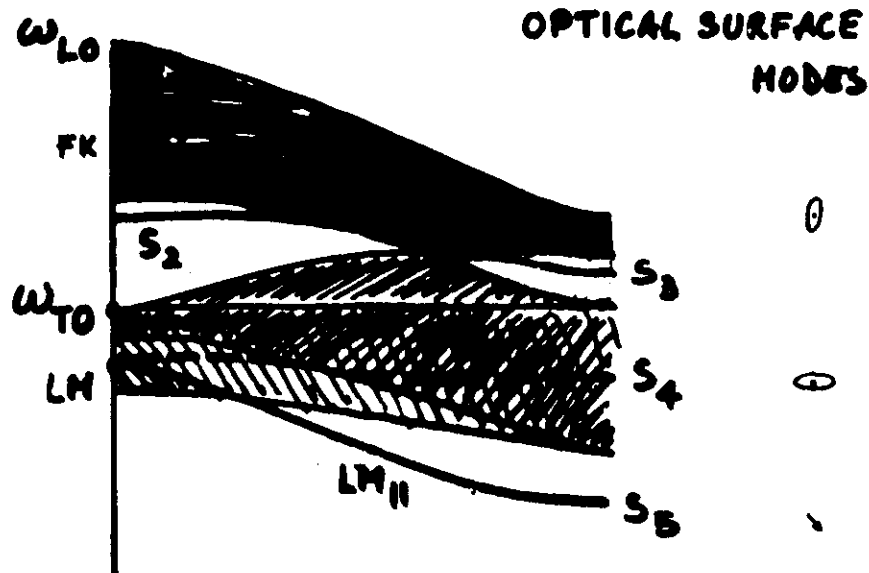
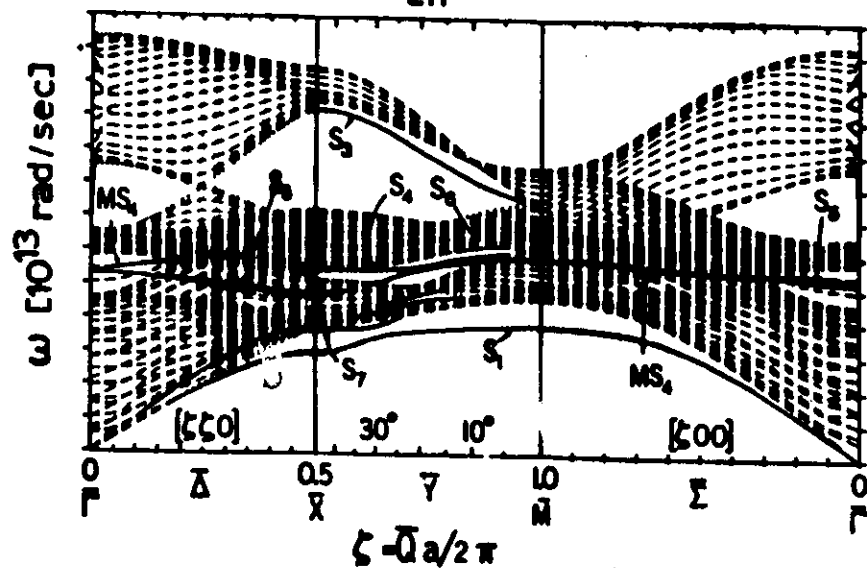
SLAB-ADAPTED BULK

LiF

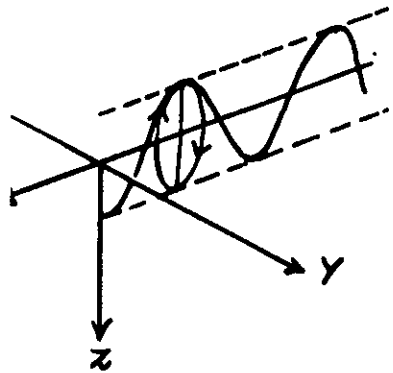


15-LAYER SLAB

LiF



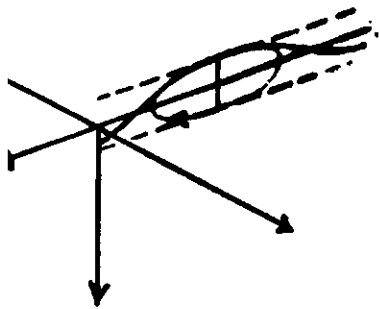
Polarization of surface modes



sagittal $\textcircled{\perp}$
(quasi-transverse)

S_1 (Rayleigh wave)

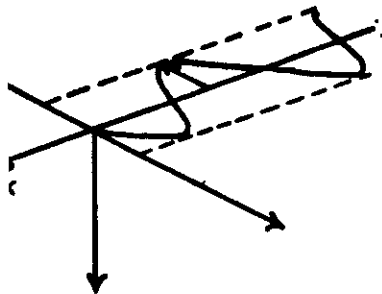
S_2 (S_3) (optical)



sagittal $\textcircled{\perp}$
(quasi-longitudinal)

S_4 (Lucas mode, opt.)

S_6 (acoustic)

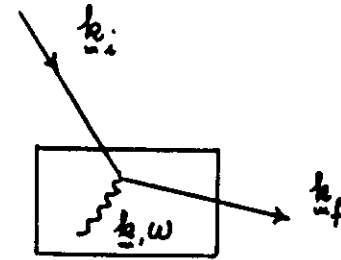


shear horizontal $\textcircled{\parallel}$
(transverse)

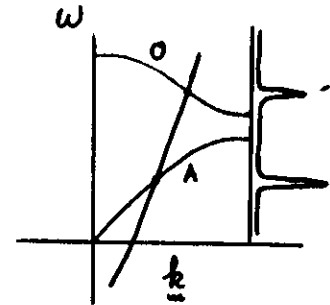
S_5 (Lucas mode, opt.)

S_7 (acoustic)

Neutron scattering

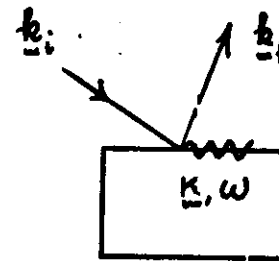


$$\underline{k}_f = \underline{k}_i + \underline{k} + \underline{g}$$

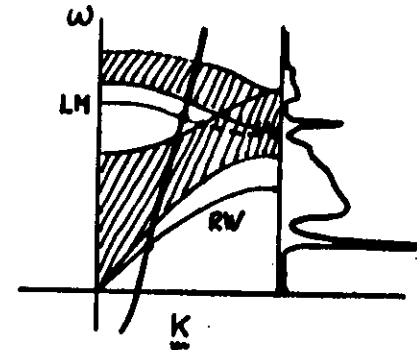


$$(2m/\hbar)\omega = -\underline{k}_i^2 + (\underline{k}_i + \underline{k} + \underline{g})^2$$

Atom scattering



$$\underline{K}_f = \underline{K}_i + \underline{K} + \underline{G}$$

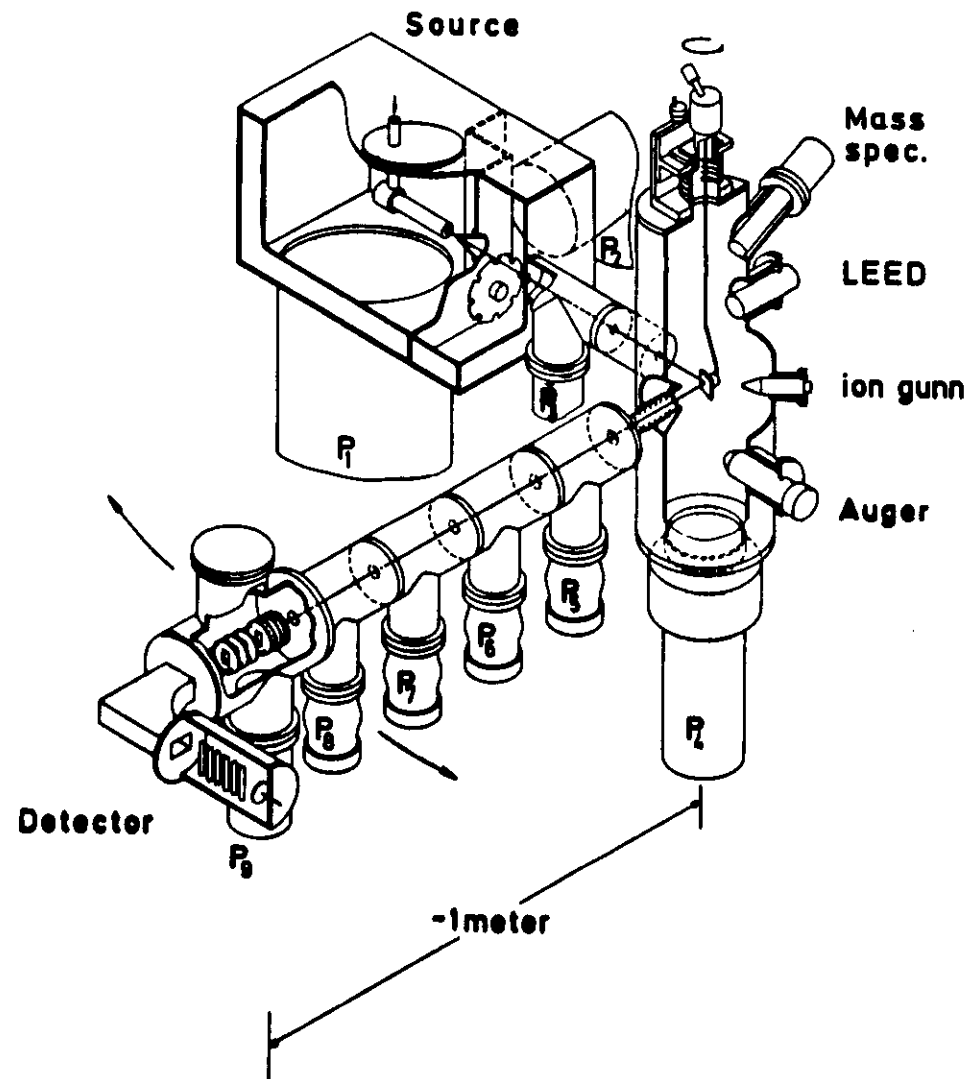


$$(2m/\hbar)\omega = -\underline{k}_i^2 + \frac{(\underline{K}_i + \underline{K} + \underline{G})^2}{\sin^2 \theta_f}$$

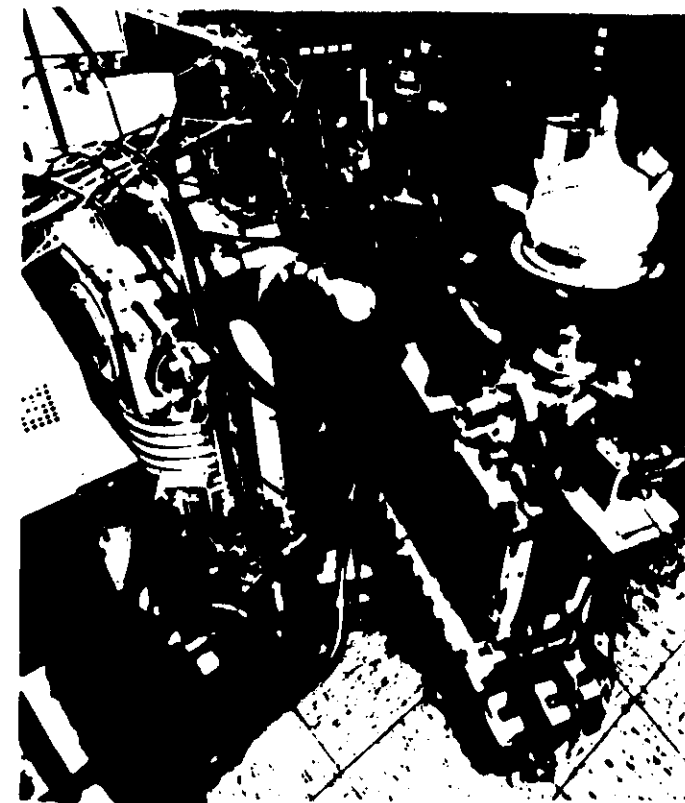
Theory:

1. Spectral densities of surface vibrations
→ Green functions
2. From TOF spectra to surf. phon densities
→ scattering theory

I-9



source



camera
di scattering

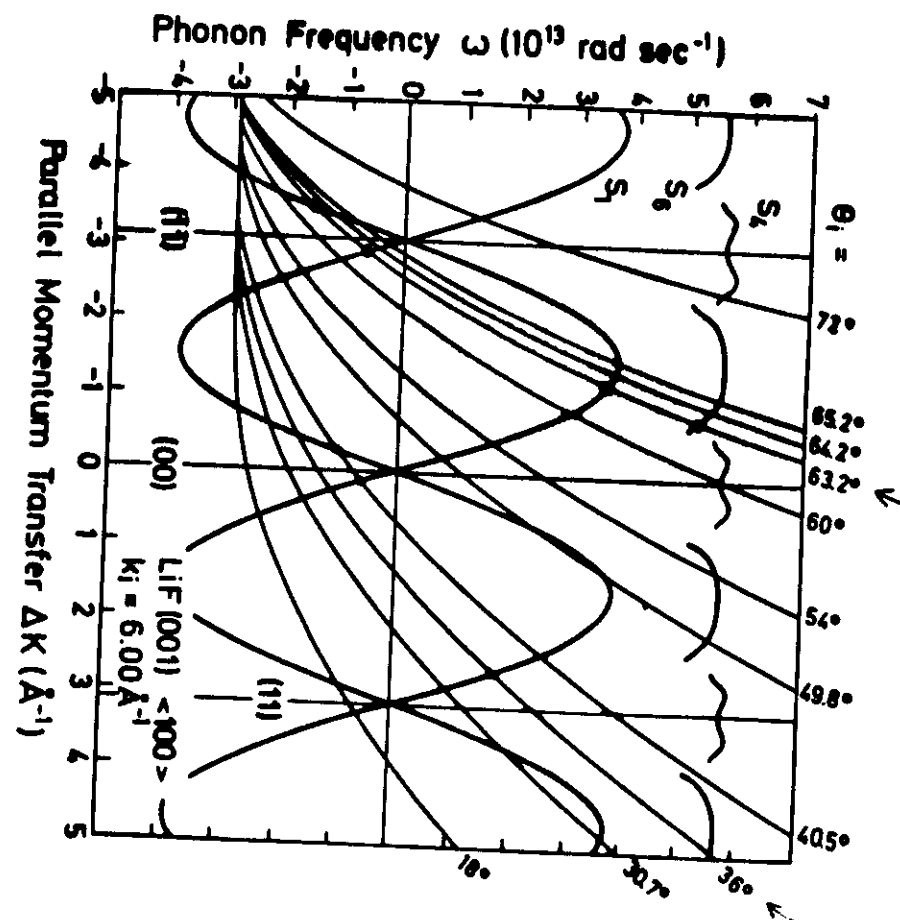
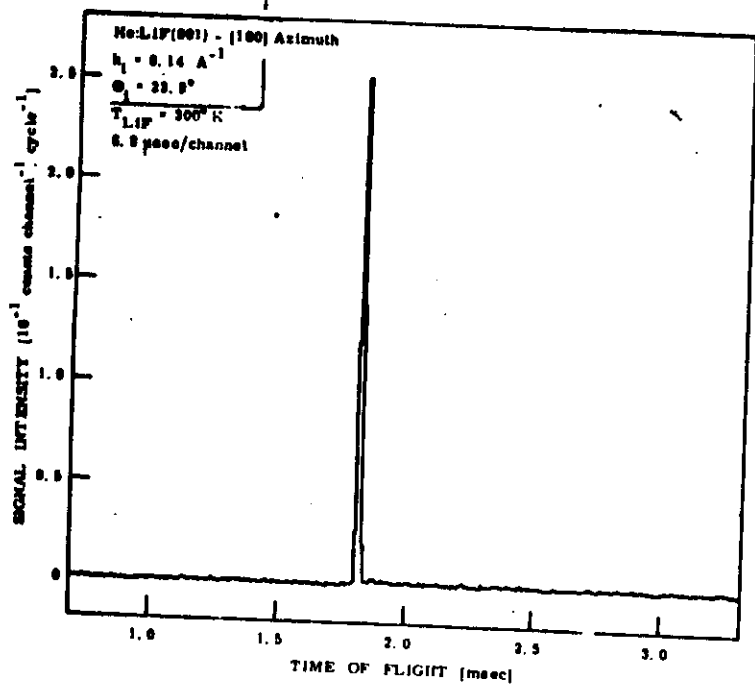
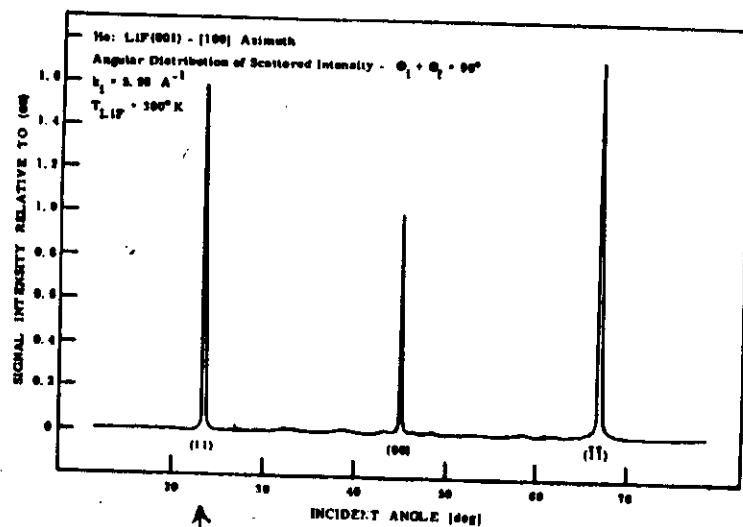
camera di
ionizzazione

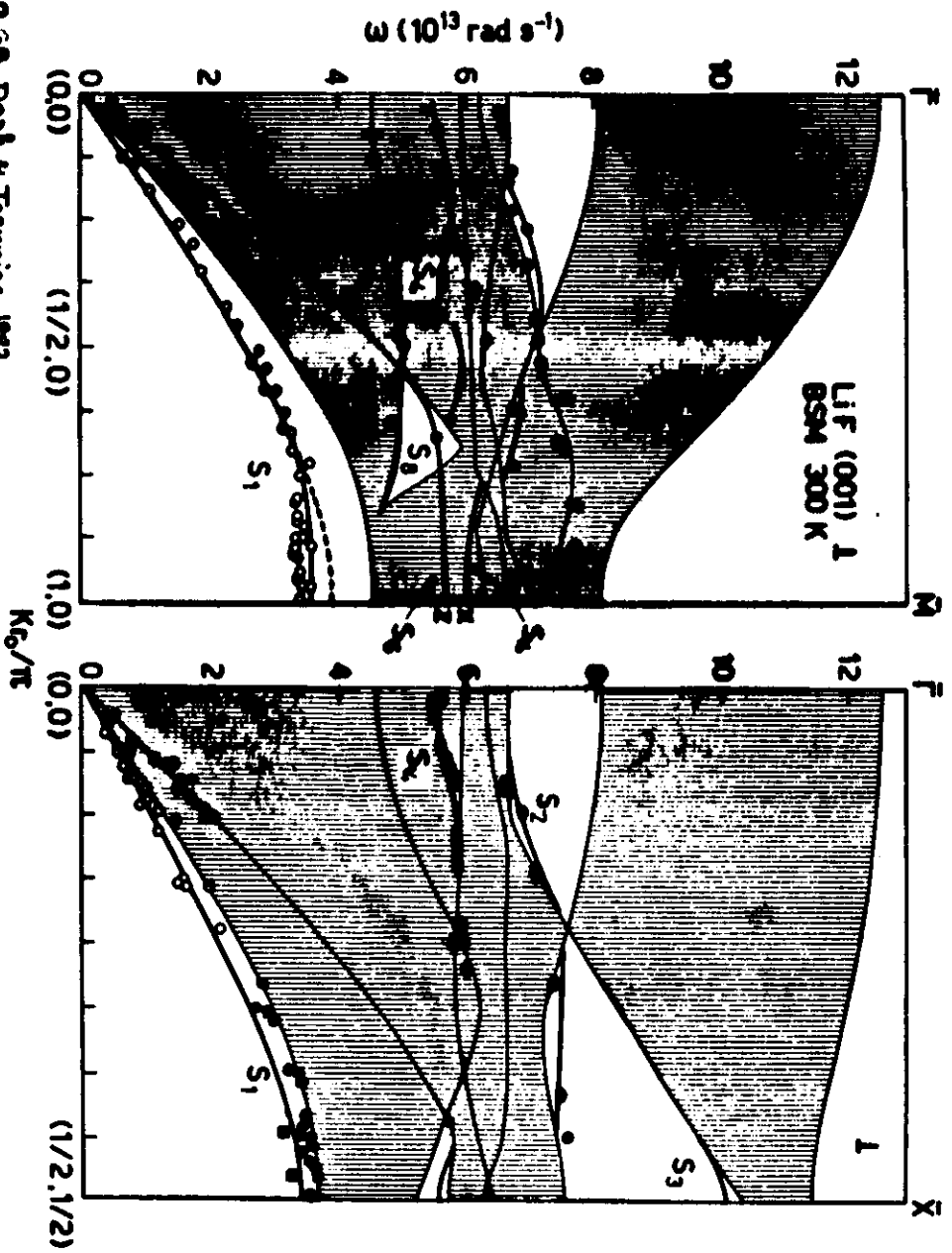
spettrometro
di massa

8 stadi di
pompaggio

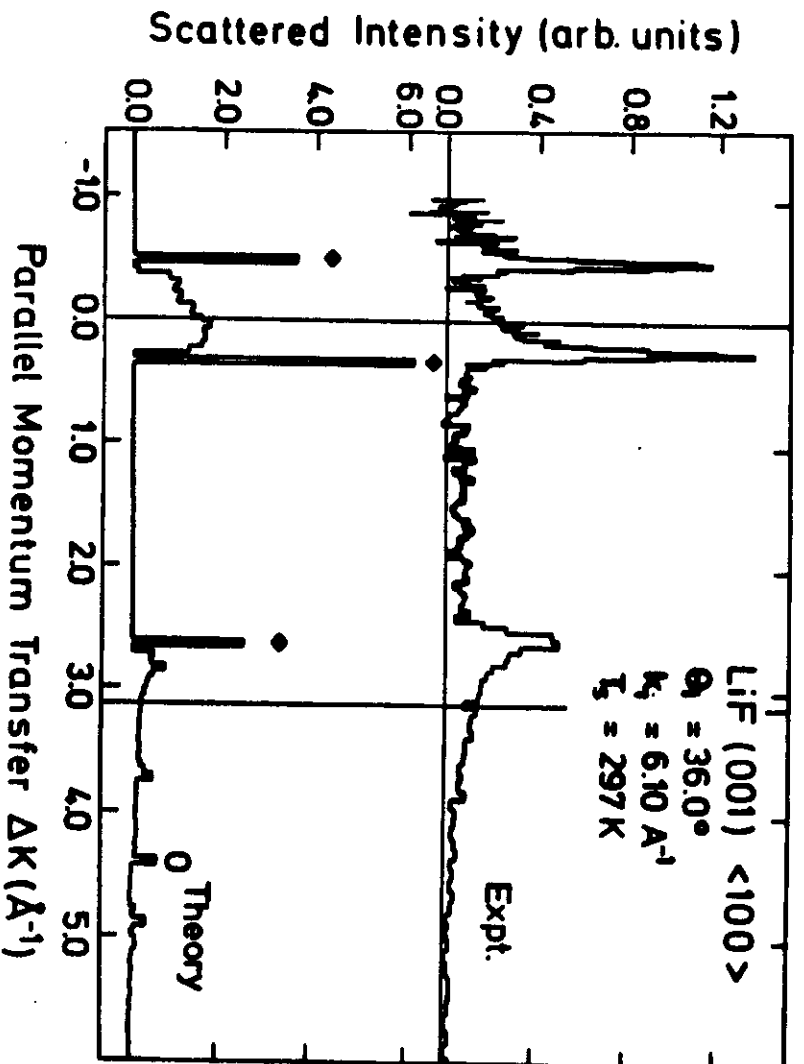
MPI-SF Göttingen





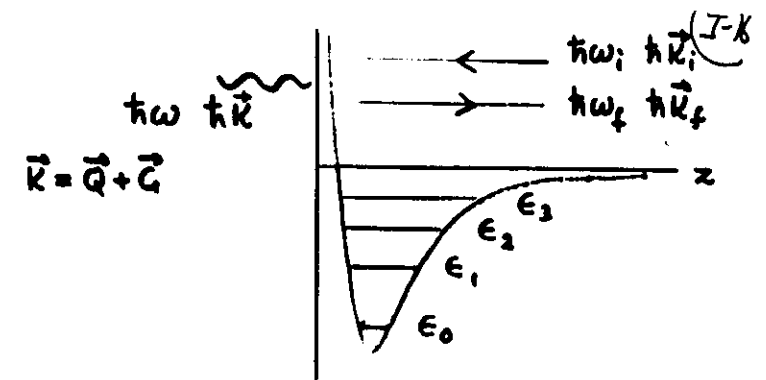
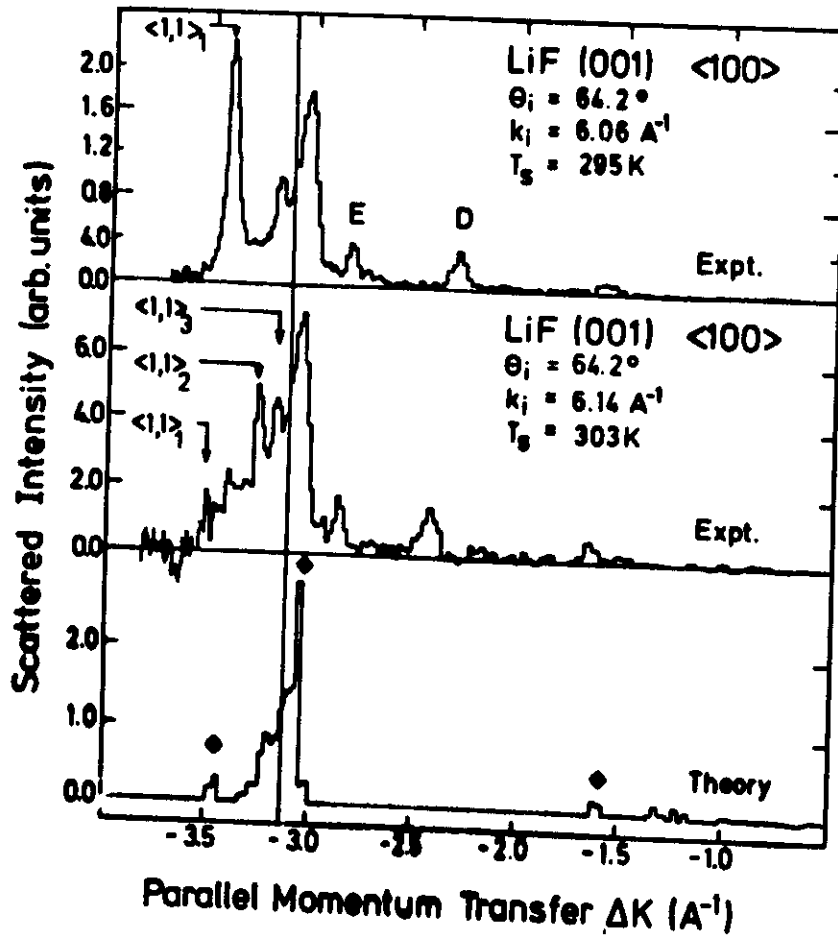


○ S.B. Doak & Toennies, 1983.
● R. Tatarak et al. 1987.

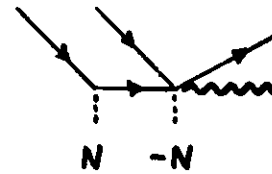


Resonance enhancement

(Evans, Celli, Benedek, Brundage, Dole & Tien, Phys. Rev. Letters 1983)

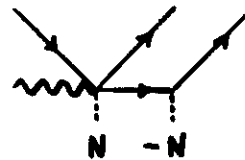


Elastic resonance



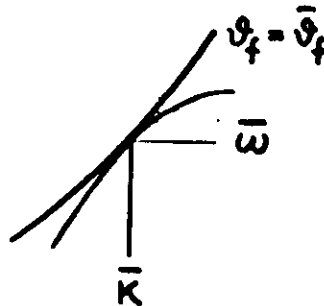
$$\omega_i = \frac{\hbar}{2m} (\vec{k}_i + \vec{N})^2 - \frac{1}{\hbar} |\epsilon_n|$$

Phonon-assisted resonance (CFT, PRL 1976)

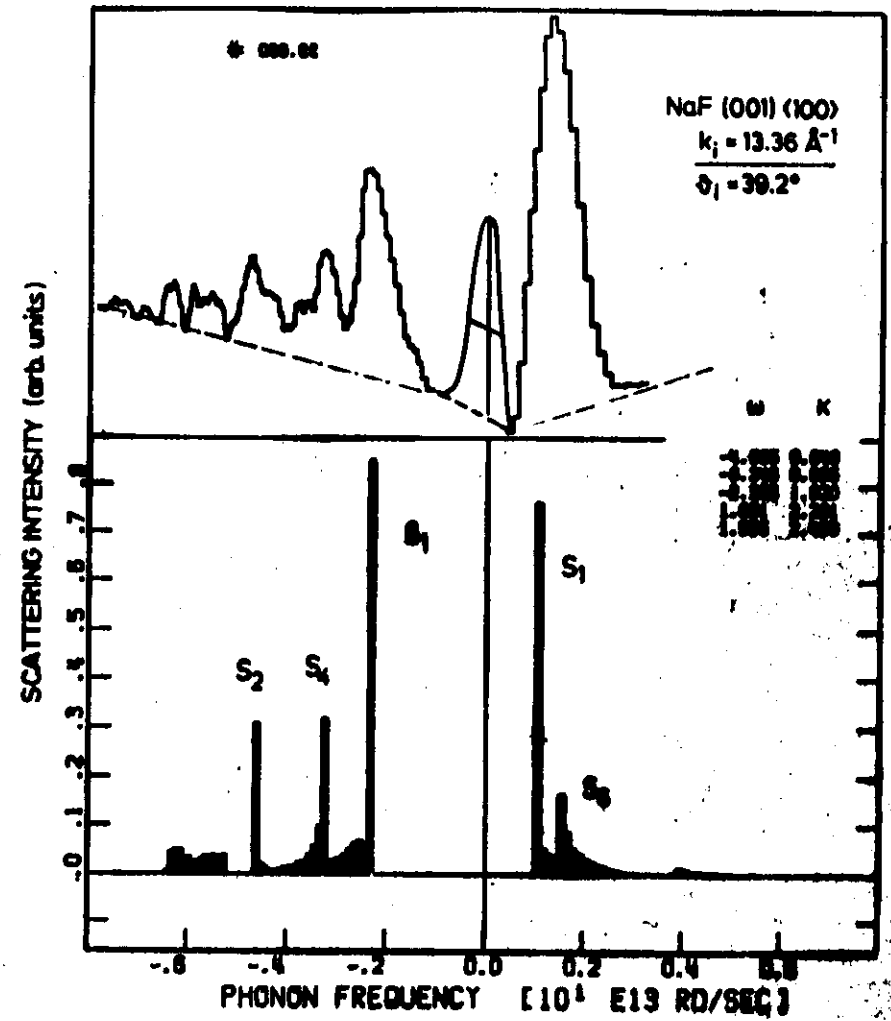
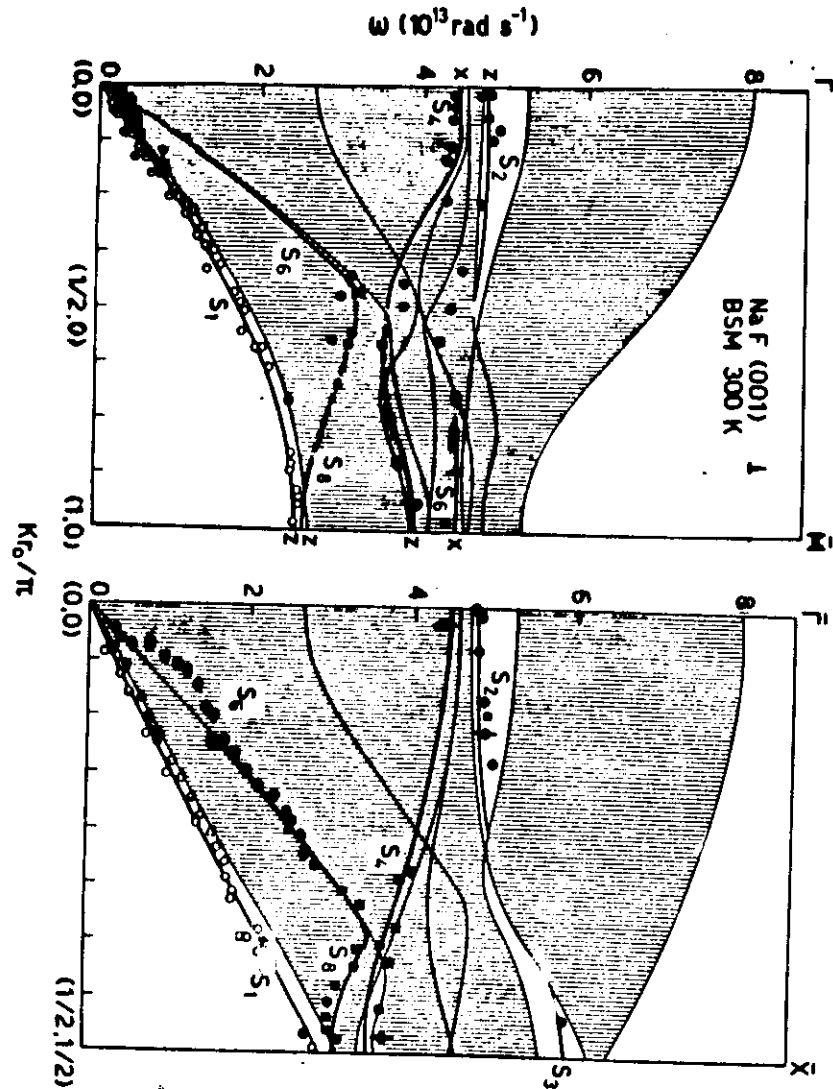


$$\omega_i + \omega = \frac{\hbar}{2m} (\vec{k}_i + \vec{k} + \vec{N})^2 - \frac{1}{\hbar} |\epsilon_n|$$

Kinematical focussing (G.B., PRL 1975)



$$\frac{dR}{d\vartheta_f d\varphi_f} = \frac{\bar{v}_R A(\vec{k}) \sin^{\frac{1}{2}} 2\vartheta_f}{[2\omega_f (\bar{w}_R - \bar{w}) (\bar{\vartheta}_f - \vartheta_f)]^{1/2}}$$



... which may experiment

show something unexpected!

microscopic mechanisms

that are forbidden or hindered in the bulk

are promoted at the surface

by the symmetry lowering

e.g., important (enhanced)

manifestations

of electron-phonon interaction

→ anomalies in surface

phonon dispersion → Next lecture

From technical applications

to fundamental aspects of

solid state theory

