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INTERNATIONAL CENTRE FOR THEORETICAL PHYSICS
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Research Workshop in Condensed Matter, Atomic and Molecular Physics (22 June - 11 September 1992)

Working Party on: "Energy Transfer in Interactions with Surfaces and Adsorbates" (31 August - 11 September 1992)

"Structures of Rh(110) Surface and their Phonon Spectra"

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

Structures of Rh(110) surface and their phonon spectra.

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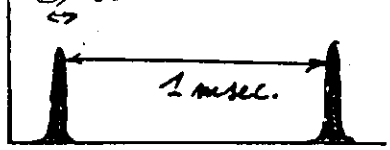
Rh (110) surface within the same T range presents different structures as a function of different temperature treatment and oxygen dosage!

Two clean (1x1), (1x2) and one oxygen induced structure (2x2), are reported

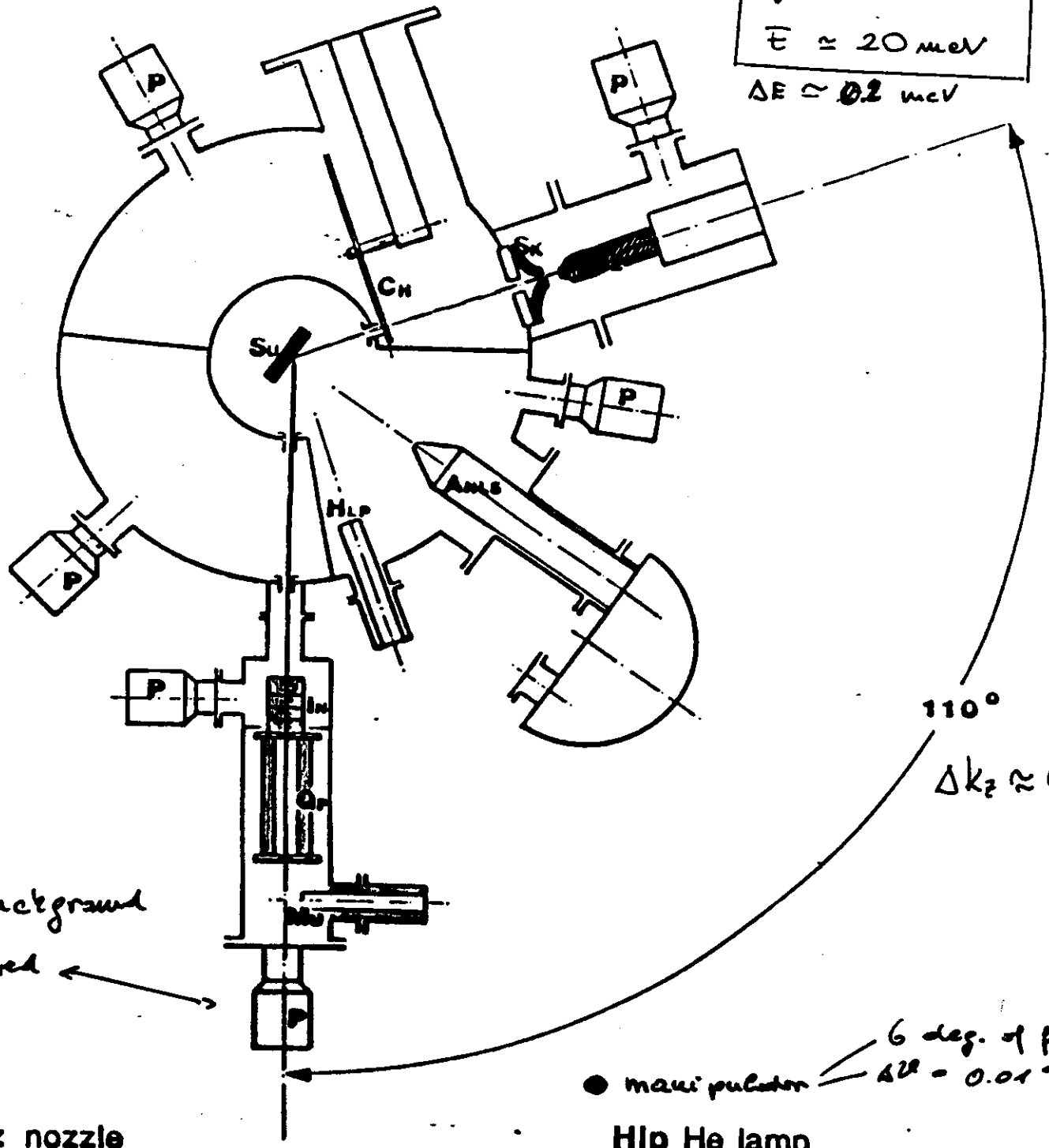


$v \simeq 1000$ m/sec

$\frac{\Delta v}{v} \simeq 1\%$

$E \simeq 20$ meV

$\Delta E \simeq 0.2$ meV



$\Delta k_z \approx$ Const.

le background

owered

6 deg. of freedom

● manipulator — $\Delta\theta = 0.01°$

- ● Nz nozzle
- ● Sk skimmer
  Ch chopper (360 Hz = ν)
- ● Su sample surface
  Anls electron energy analyzer

Hlp He lamp

- ● In Ionizer
- ● Qp Quadrupole mass filter
- ● Mu Multiplier
  P Turbo pumps

eam : $4 \cdot 10^8$ atoms per pulse ⎍ ; 5 μsec

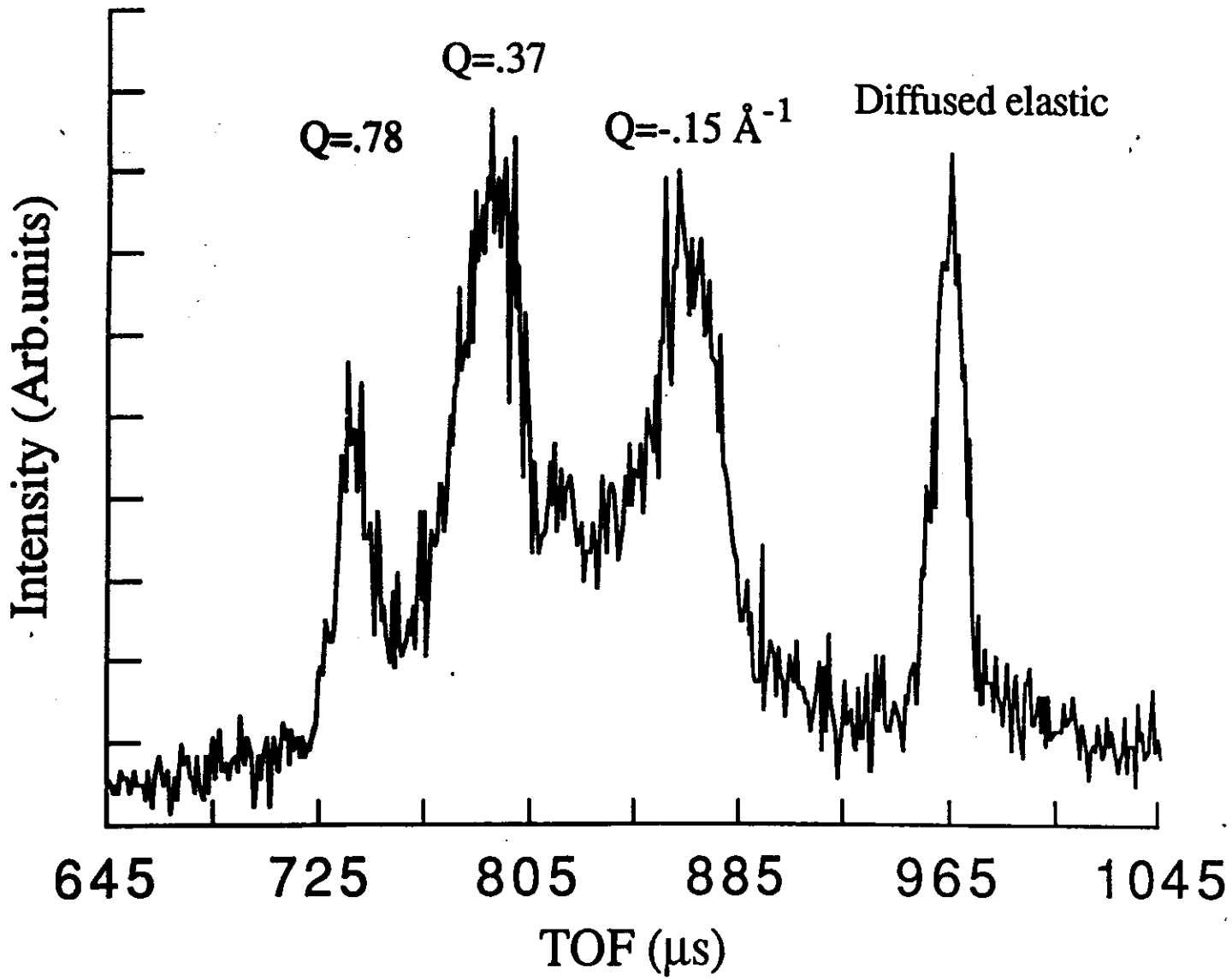
Ω ; $8 \cdot 10^{-6}$ sr

face spot : 0.7 mm

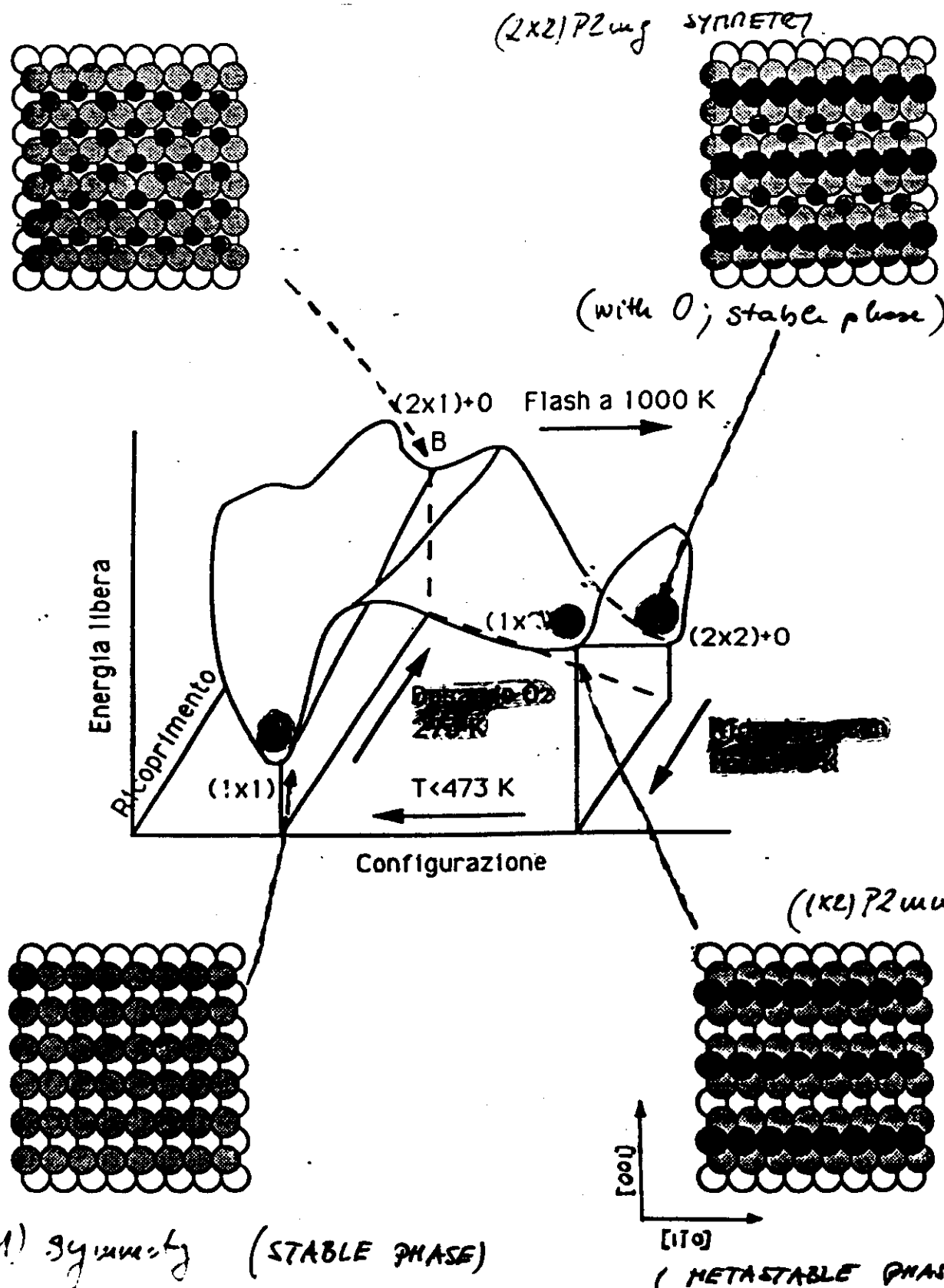
$E_{He} = 18.62$ meV

$\Delta E \approx 0.2$ meV

Rh(110)(1x1) [001]
Angle of incidence = 61°
Sampling time ~ 20 min.



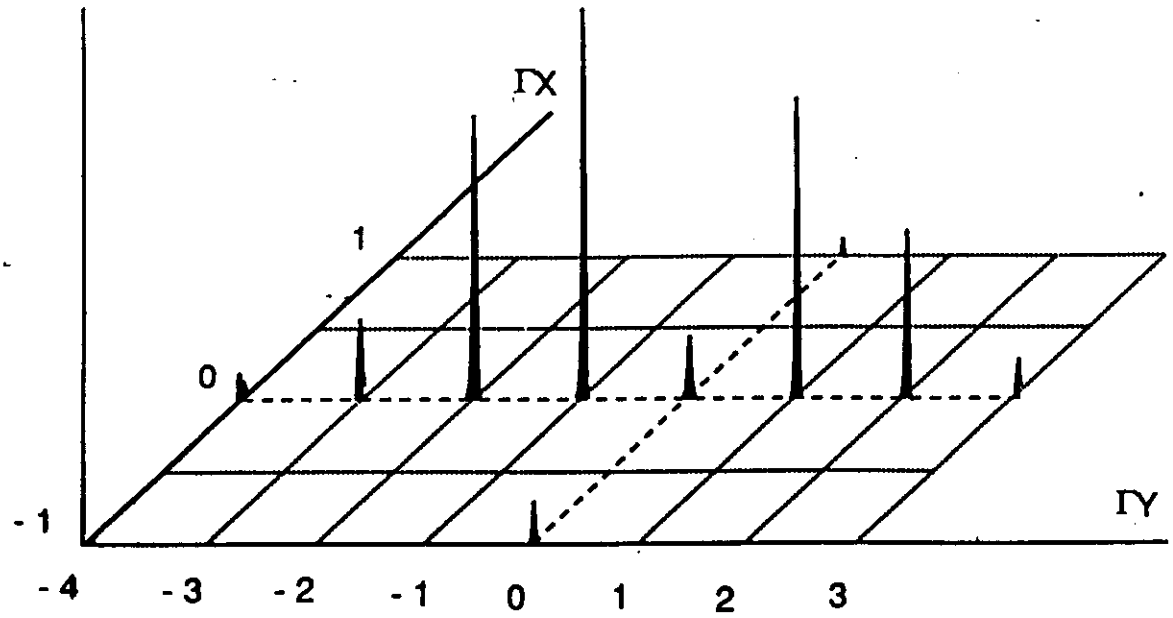
HALF MONOLAYER



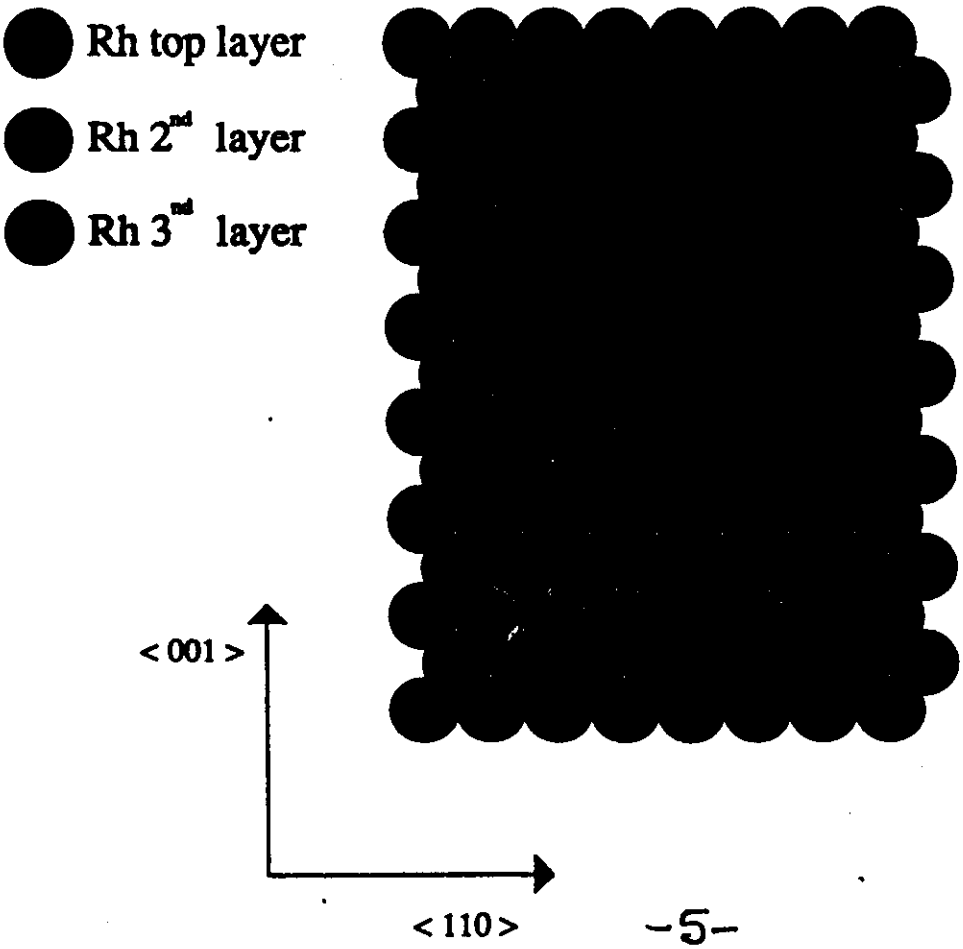
(1x1) symmetry (STABLE PHASE)

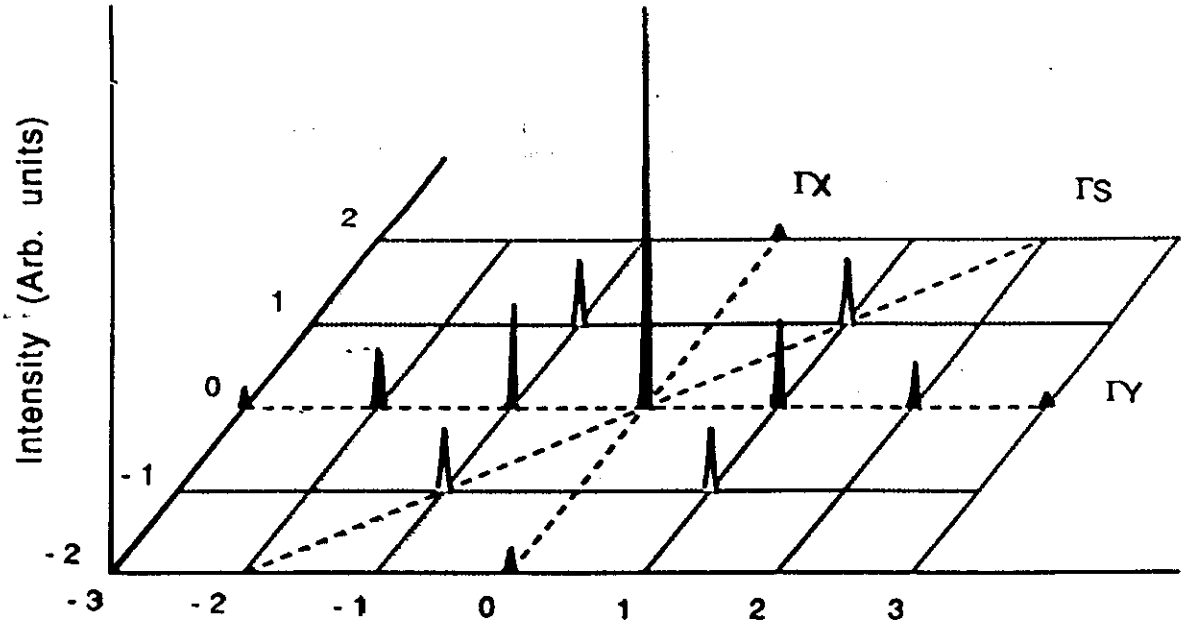
(METASTABLE PHASE)

All three symmetry structures exist at 370 K (according to the previous temperature/(O,H) treatment !

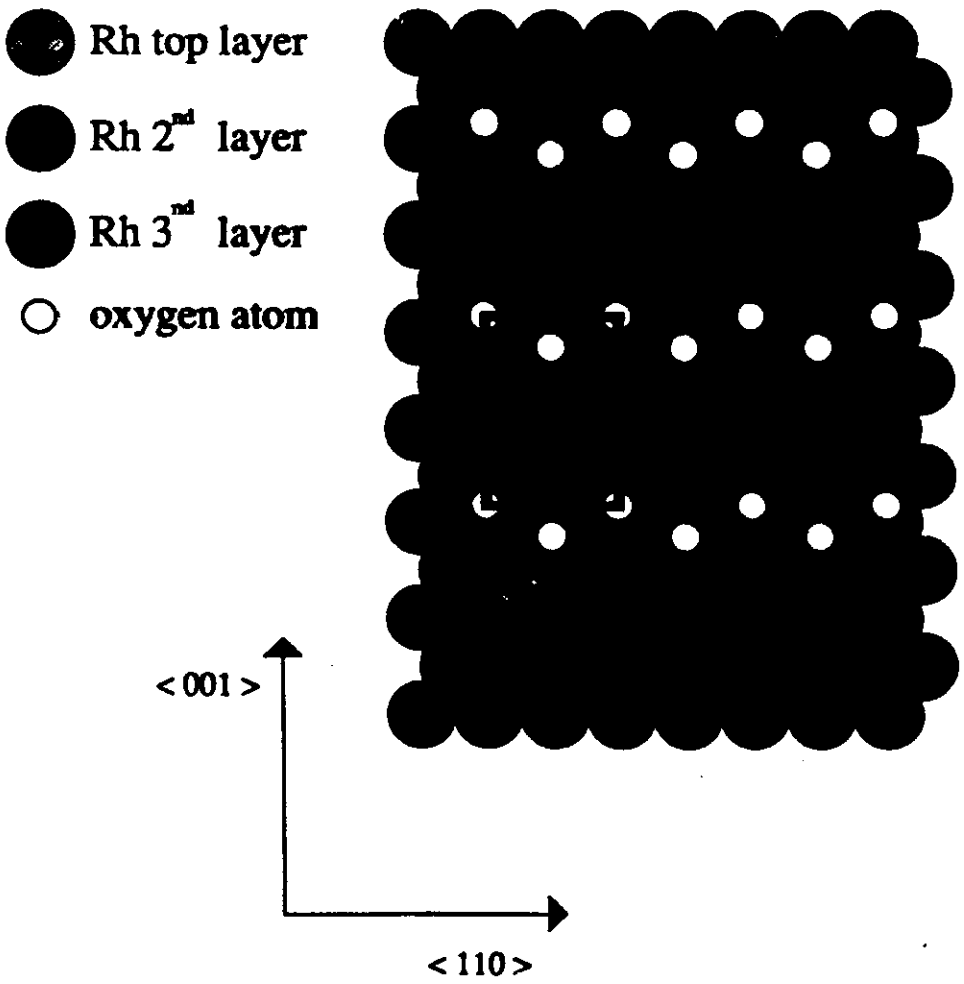


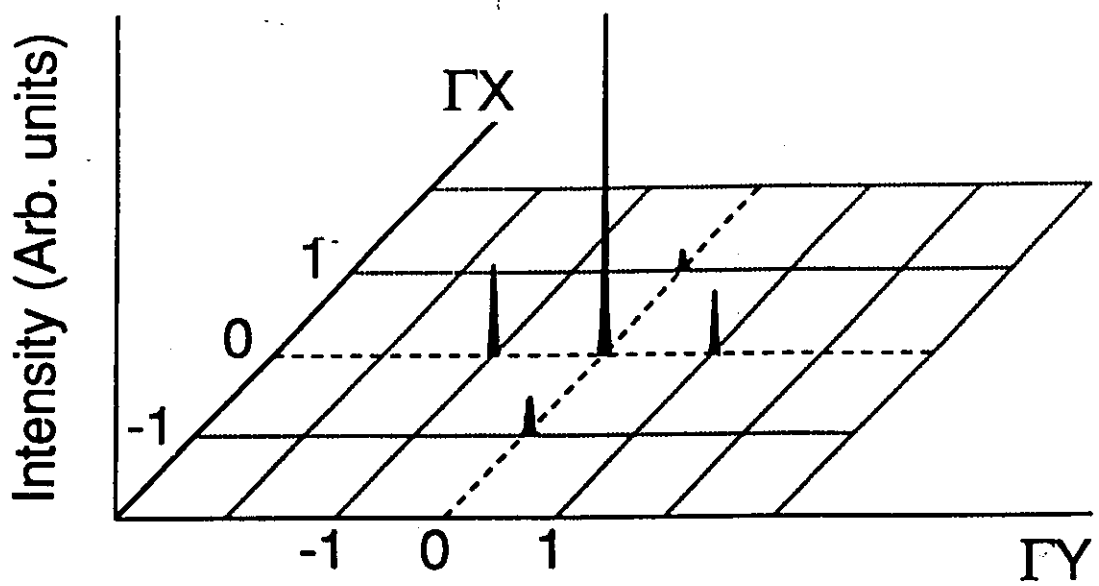
[redacted] Diffraction pattern, T=470K
He beam energy = 18.62 meV
(0,-4) x 10
(0,±3) x 5
(±1,0) x 100
Unit mesh on ΓY = 0.72 Å^{-1}, on ΓX = 1.2 Å^{-1}



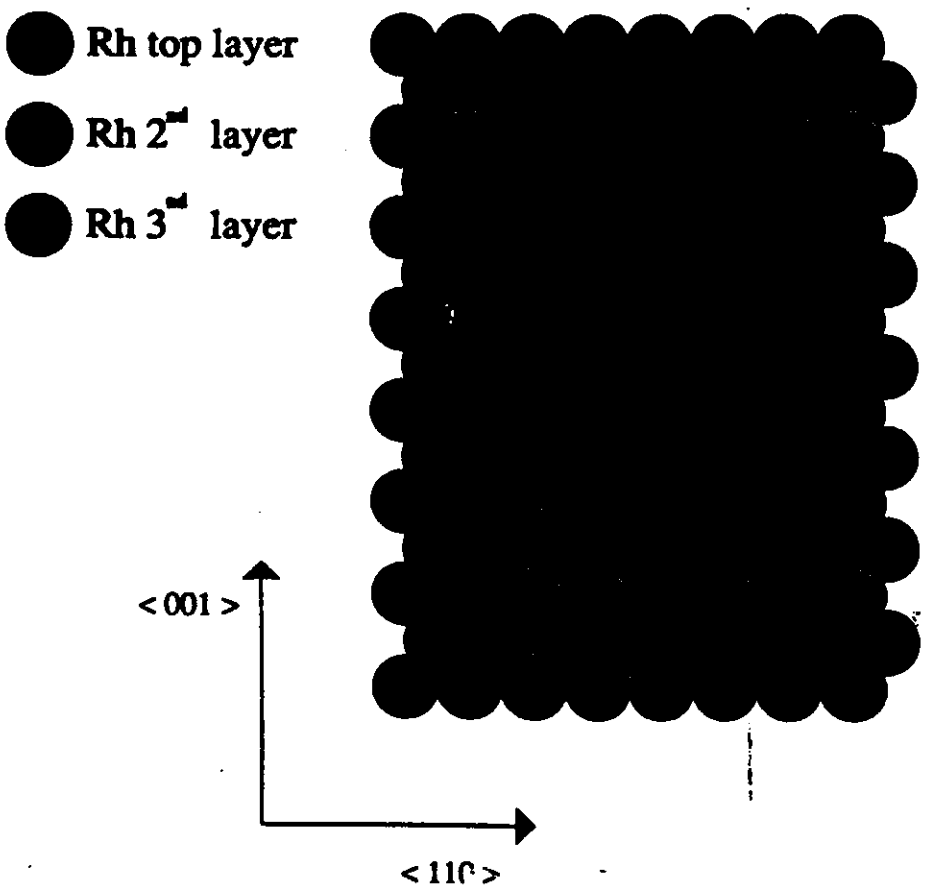


[redacted], T=600K
He beam energy = 18.62 meV
Unit mesh along ΓY = [redacted] Å^{-1}, and along ΓX = [redacted] Å^{-1}





T=600K
He beam energy = 18.62 meV
(0,±1) x 2
(±1,0) x 20
Unit mesh along ΓY = 1.61 Å^{-1} , and along ΓX = 2.32 Å^{-1}



In order to interpret the Diffraction patterns:

- Assume a certain form of the - surface interaction potential.
- Solve the scattering problem.

·) Hard corrugated Wall (HCW)

gives for the corrugation along <0 0 1>:

surface	ξ
(1x1)	0.16 Å
(1x2)	0.8 Å
(2x2)	≈ (0.25 Å)

⇒ Implies the high corrugated "missing row" model

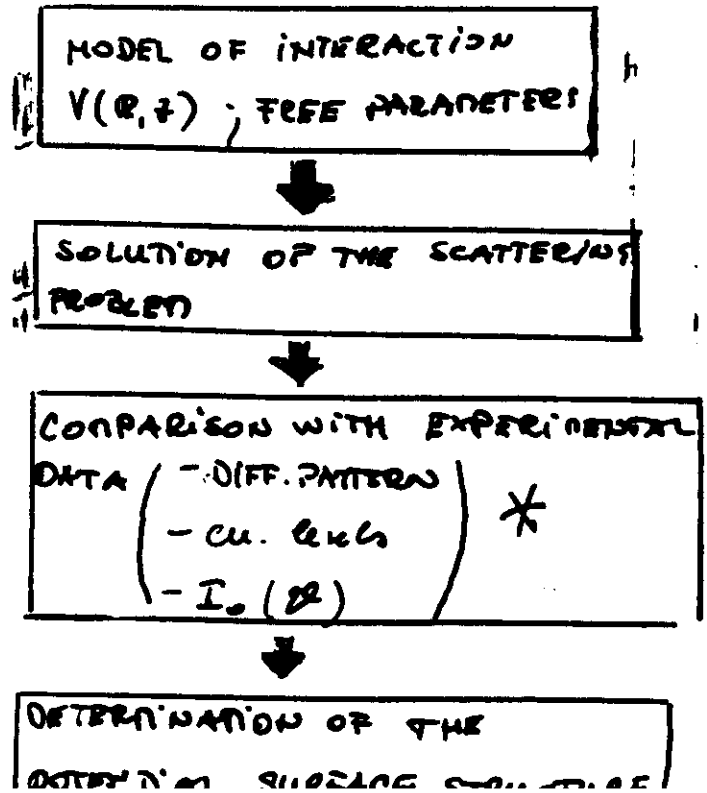
·) Realistic potential:

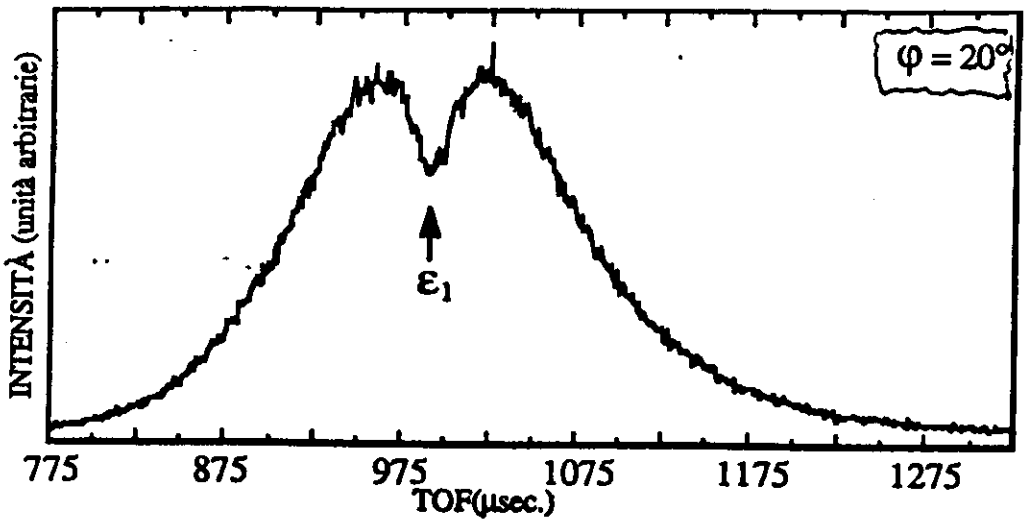
$$V(R,z) = \sum_i U(r_i - r) - \frac{C}{(z-z_i)^3}$$

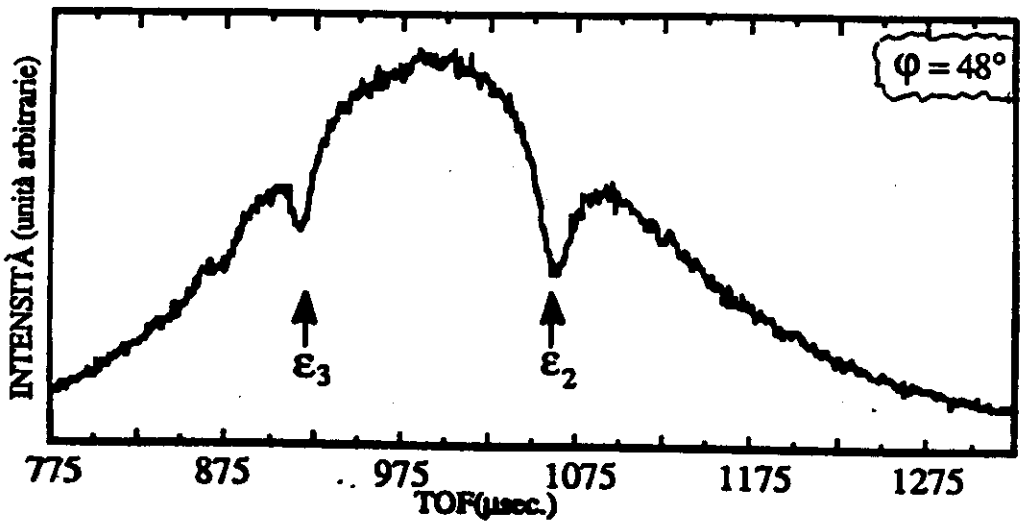
+ C.C.C. calculations!

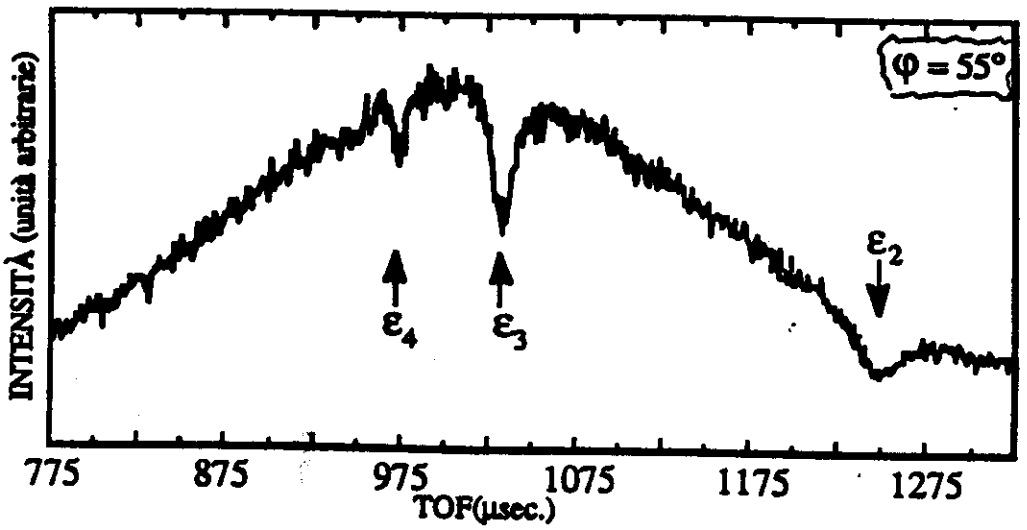
$V_R = \alpha \cdot \bar{u}(R,z)$ ⇒

surface	ξ (corrugation)
(1x1)	0.15 Å
(1x2)	1.6 Å





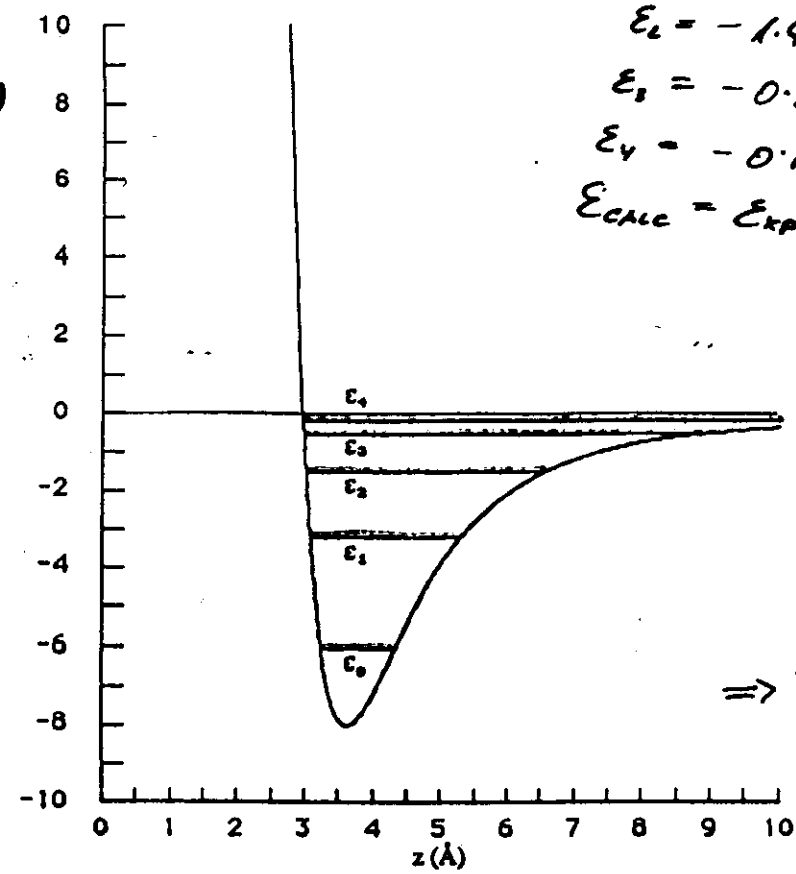




$\frac{\hbar}{2m}\left(|K_i^2 + k_{ii}^2\right) = \frac{\hbar^2}{2m}(K_i + G)^2 + \varepsilon_\nu$

$V(z,s) = V_0(z) + \sum_{G \neq 0} c \cdot V_G(z)$

$V_0(z)$ for the (1×1) surface



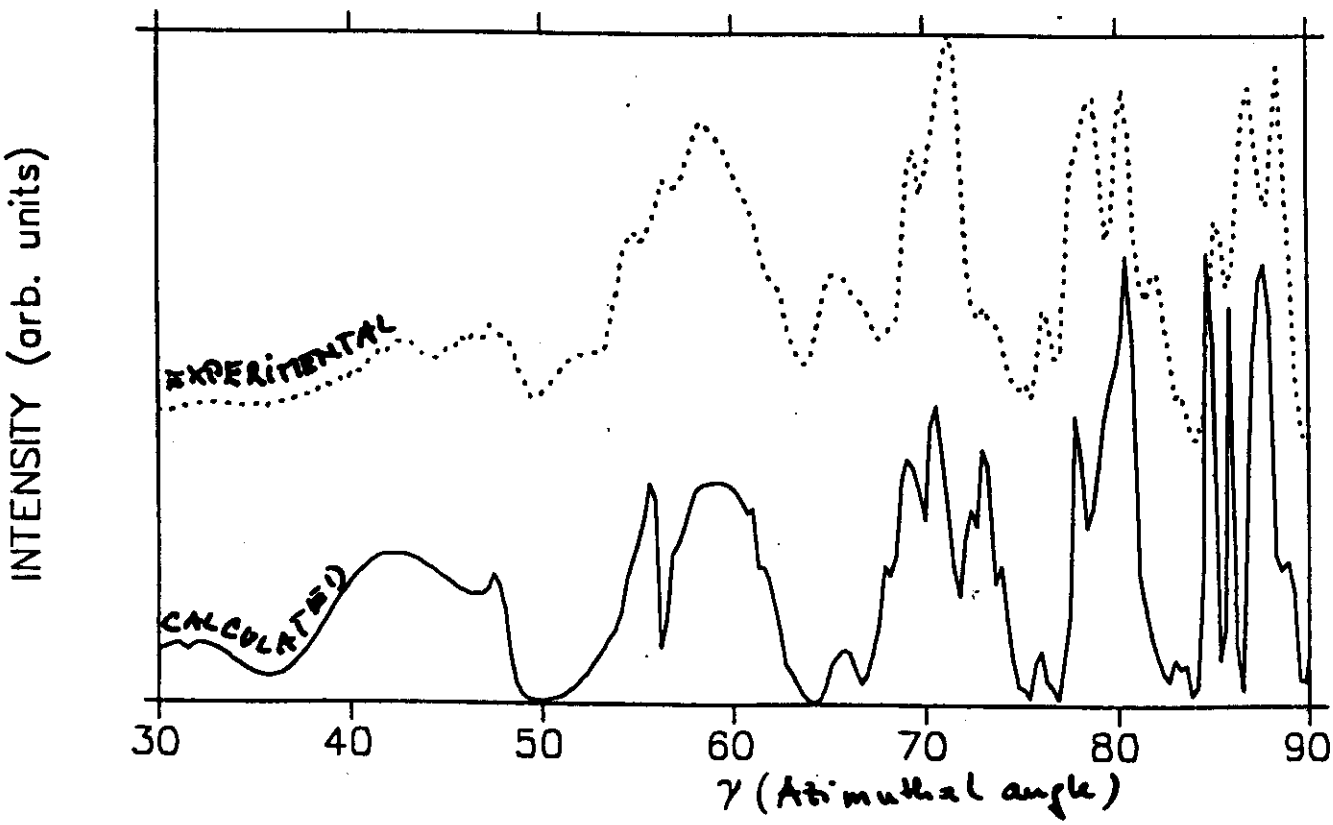
	EXP
ε_1	-3.20 ± 0.02 meV
ε_2	-1.47 ± 0.02
ε_3	-0.55 ± 0.02
ε_4	-0.16 ± 0.02

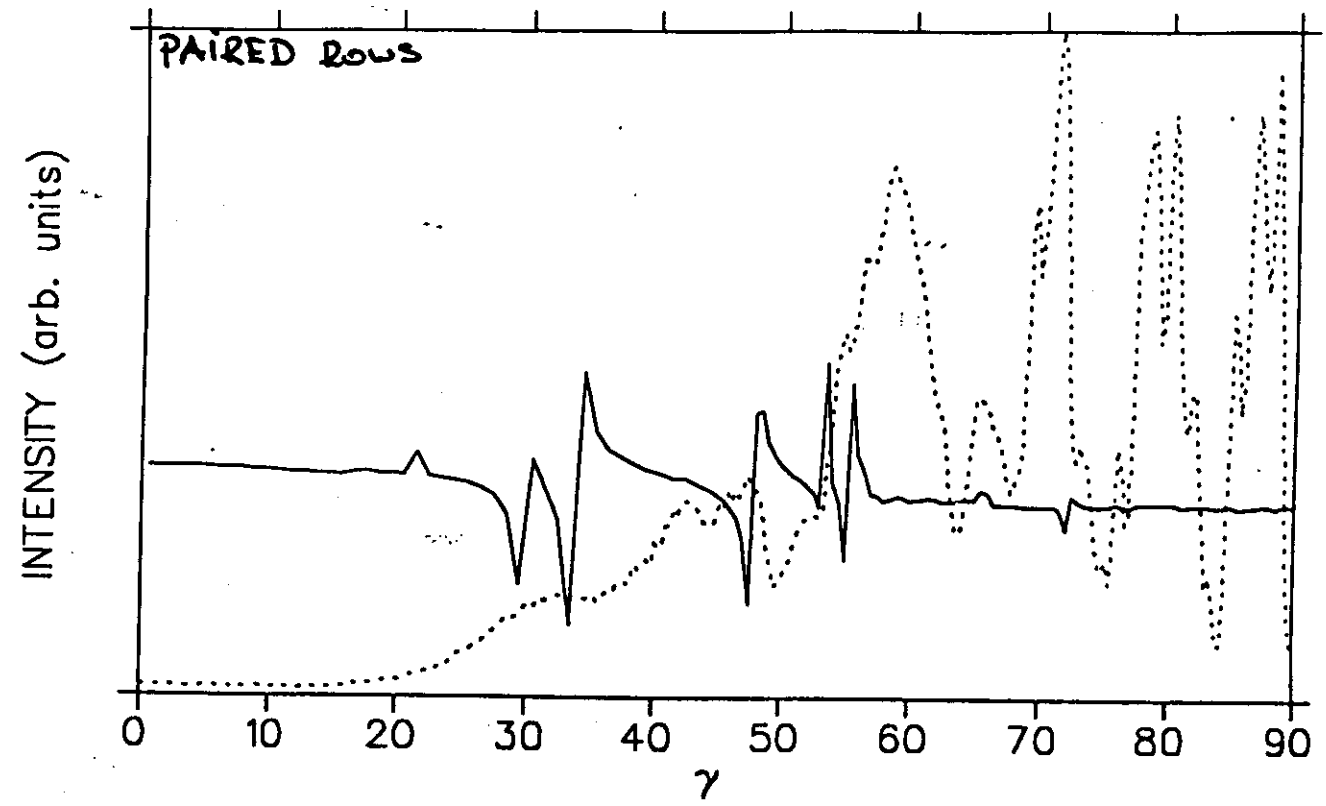
$\varepsilon_{CALC} = \varepsilon_{EXP}\ (1 \pm 0.02)$

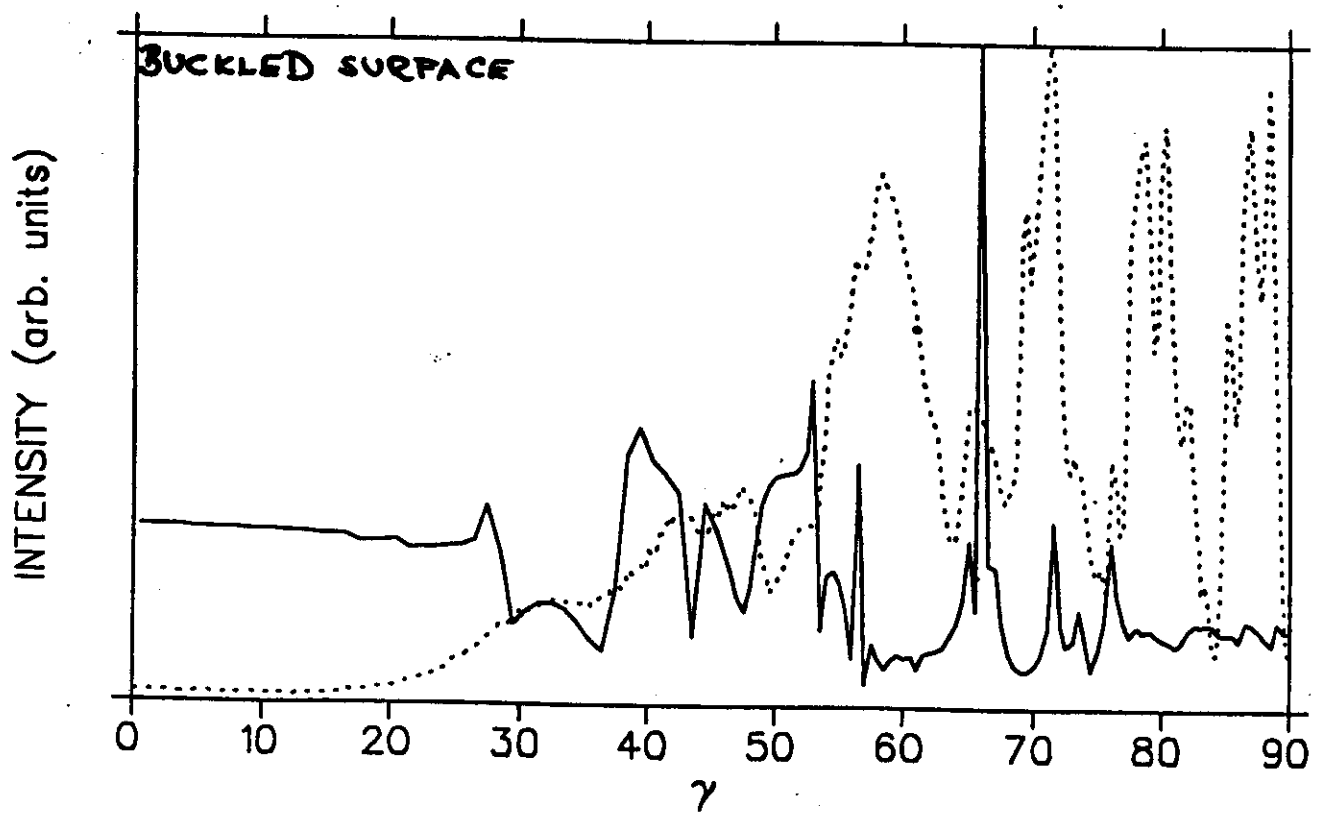
⇒ DETERMINE SOME PARAMETERS OF THE POTENTIAL!

$I_0(\vec{k})$ for (1×2) "missing row" structure

⇒ relaxation of (0–10%)



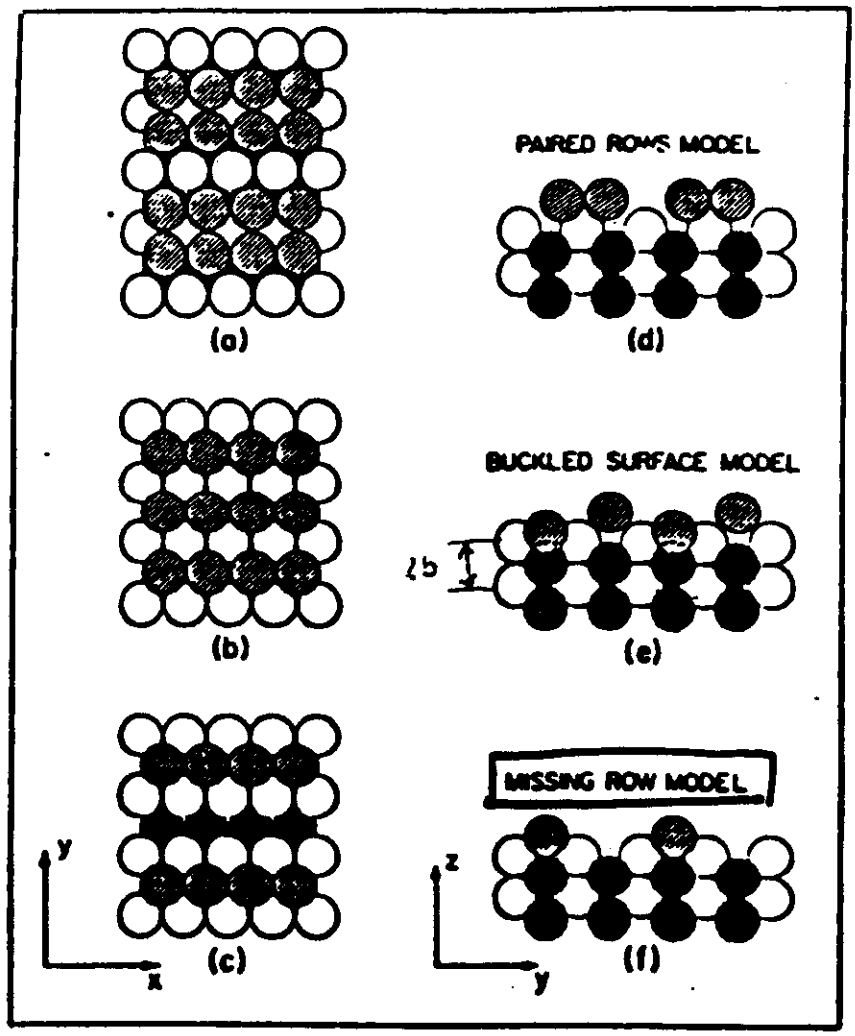

PAIRED ROWS
INTENSITY (arb. units)
0
10
20
30
40
50
60
70
80
90
γ


BUCKLED SURFACE
INTENSITY (arb. units)
0
10
20
30
40
50
60
70
80
90
γ

VARIOUS MODELS OF THE (1x2)

10) SURFACE.

Thick: $a = 3.80$



$a_1 = 3.40$ Å

$a_2 = 4.20$ Å

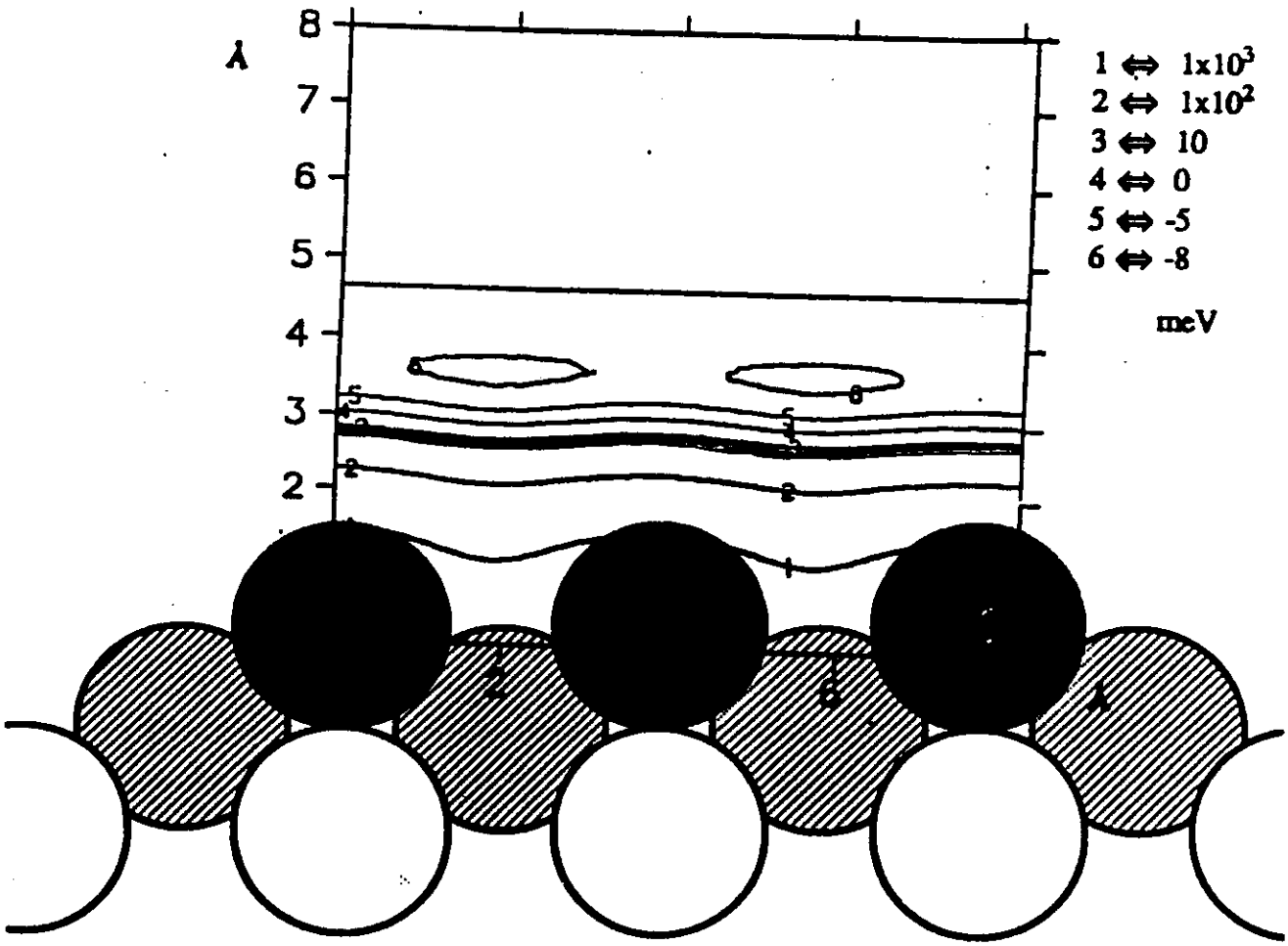
$b_1 = 1.15\ b$

$b_2 = 0.85\ b$

FROM HCW MODEL:

ALTA CORRUGAZIONE $\Rightarrow$ "MISSING ROW"

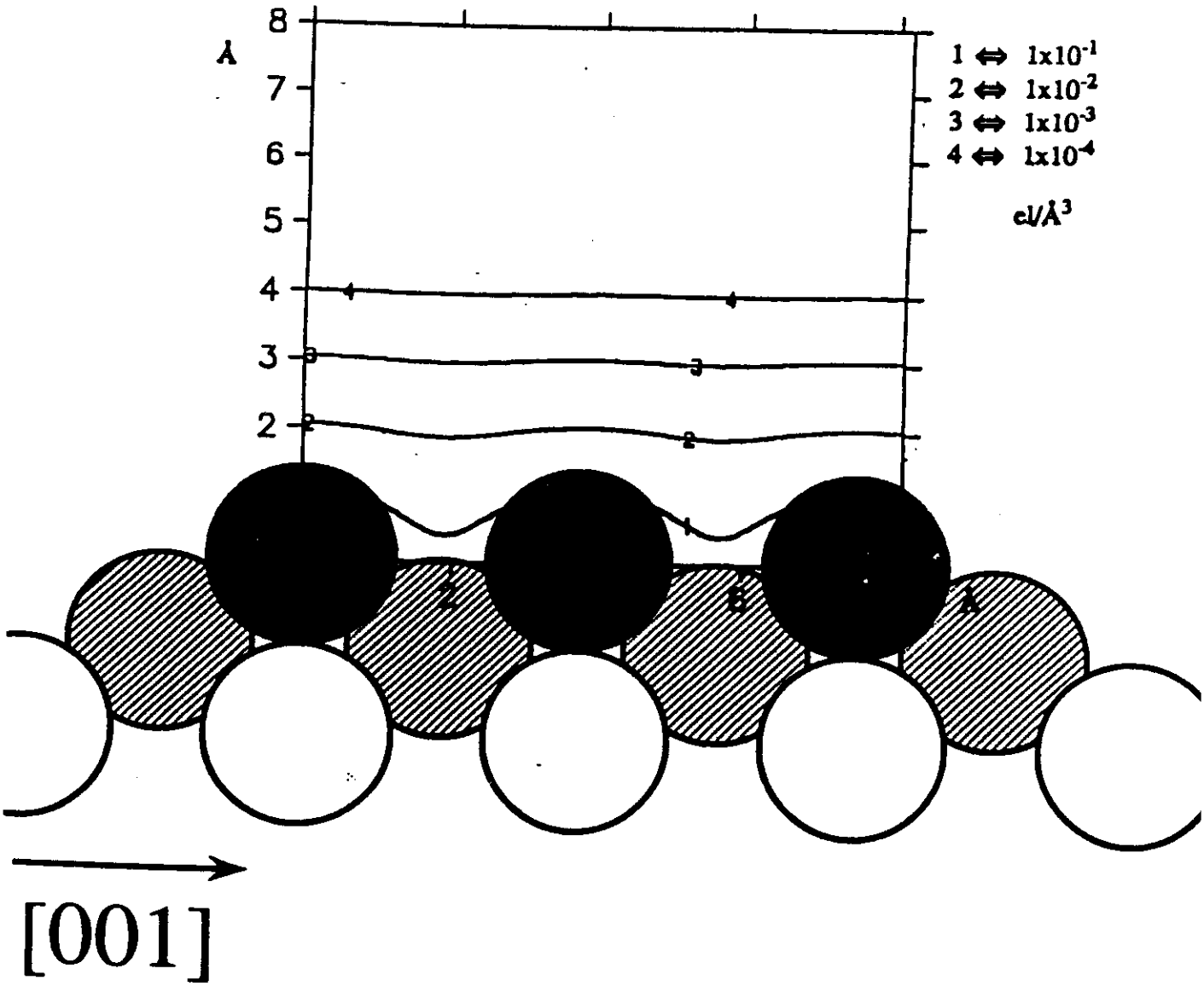
CURVE EQUIPOTENZIALI



[001]

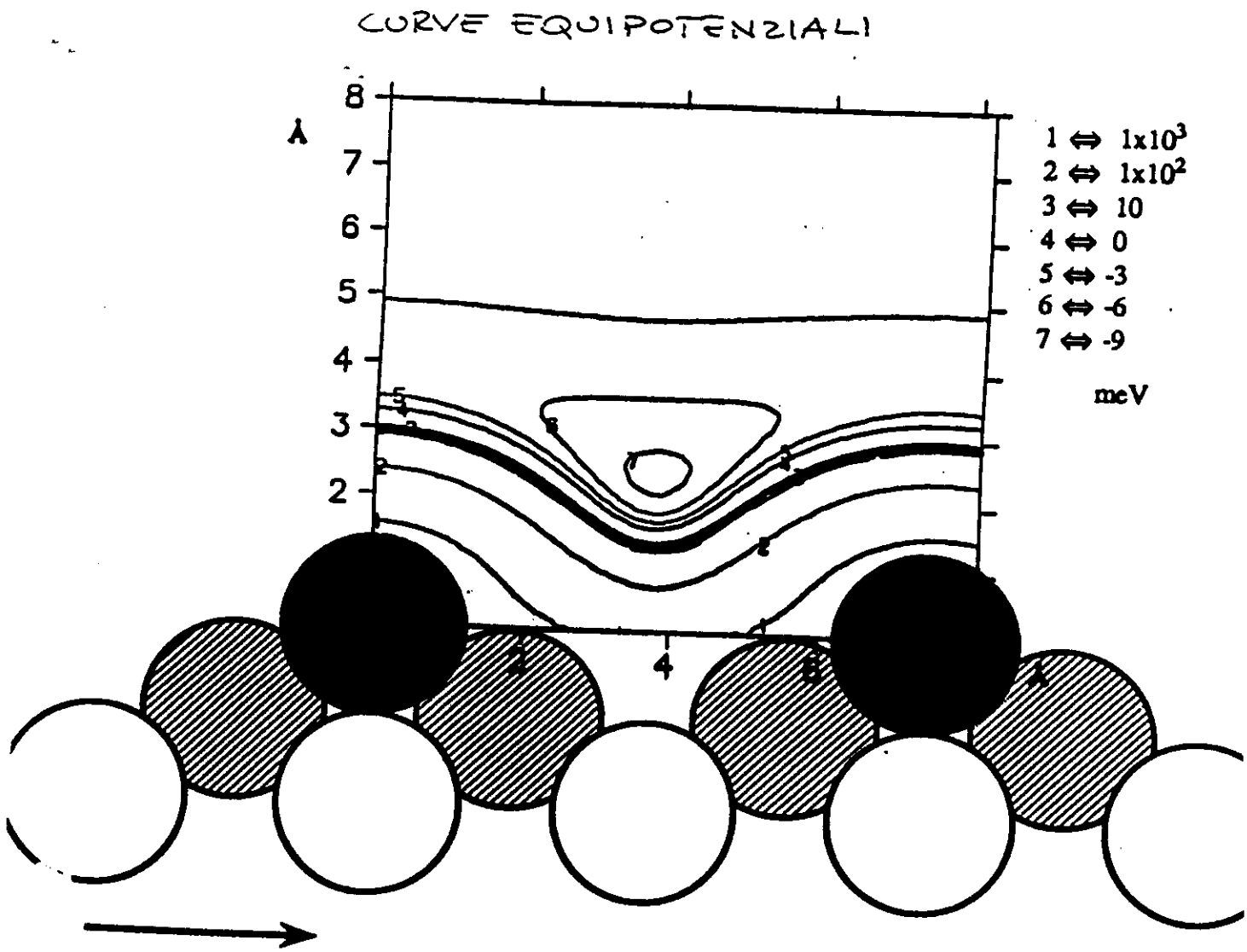
Rh(110)(1x1) structure 7%

CURVE DI ISODENSITÀ ELETTRONICA.



Rh (110) (1x1) structure 7 % = REL.

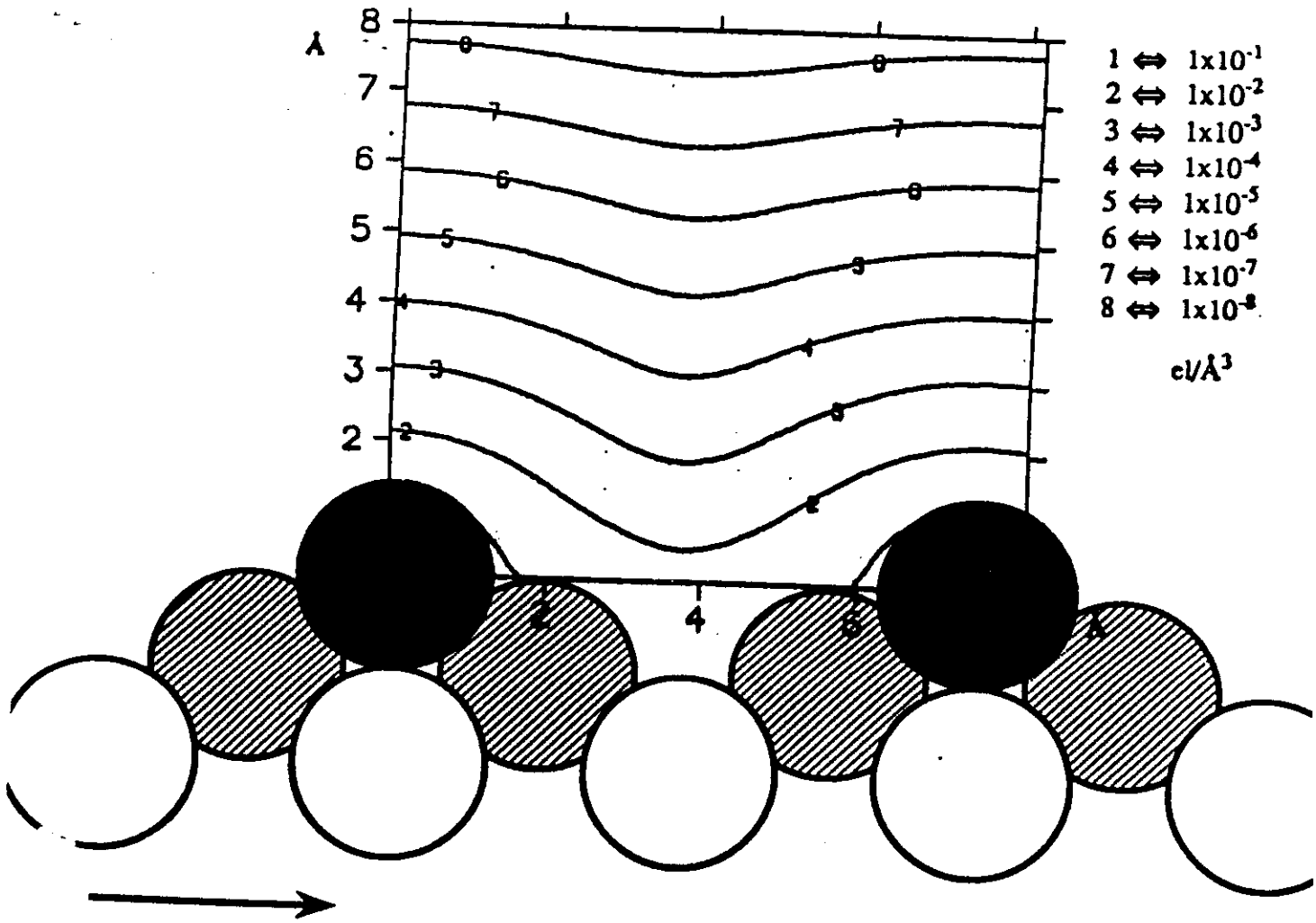
(1x2) Rh (110) "missing row" surface structure



(1x2) "MR" surface relaxation (0-10%)

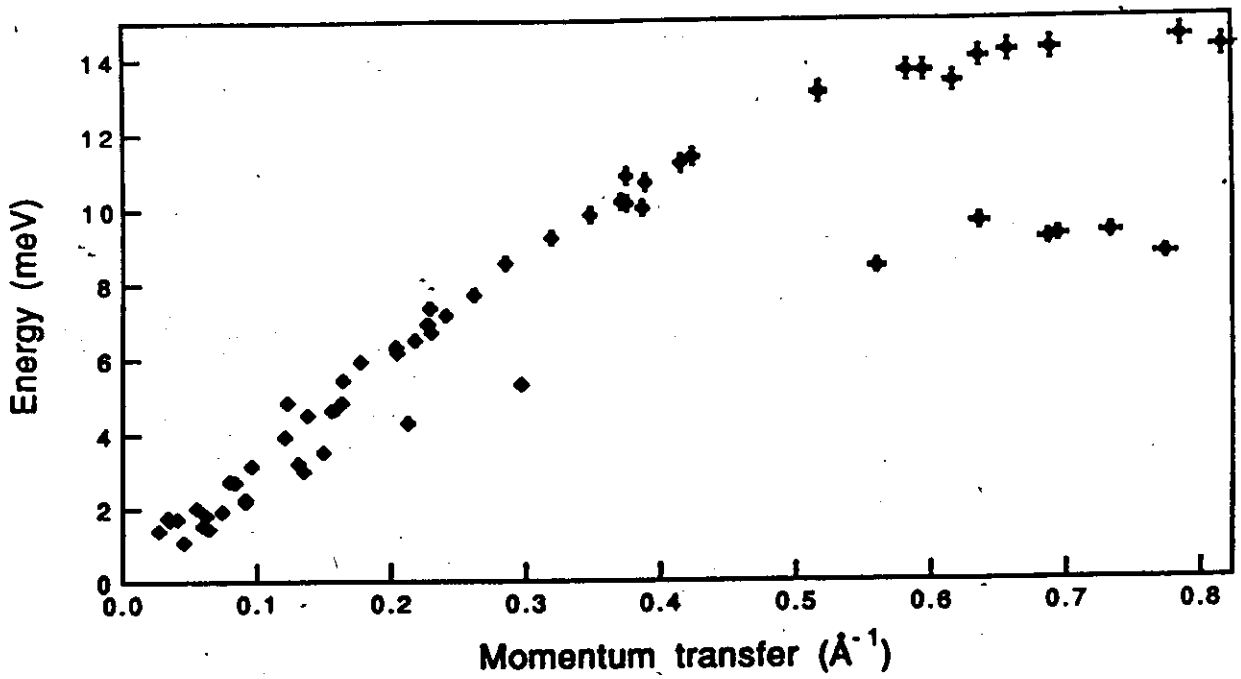
(1x1)

CURVE DI ISODENSITÀ ELETTRONICA

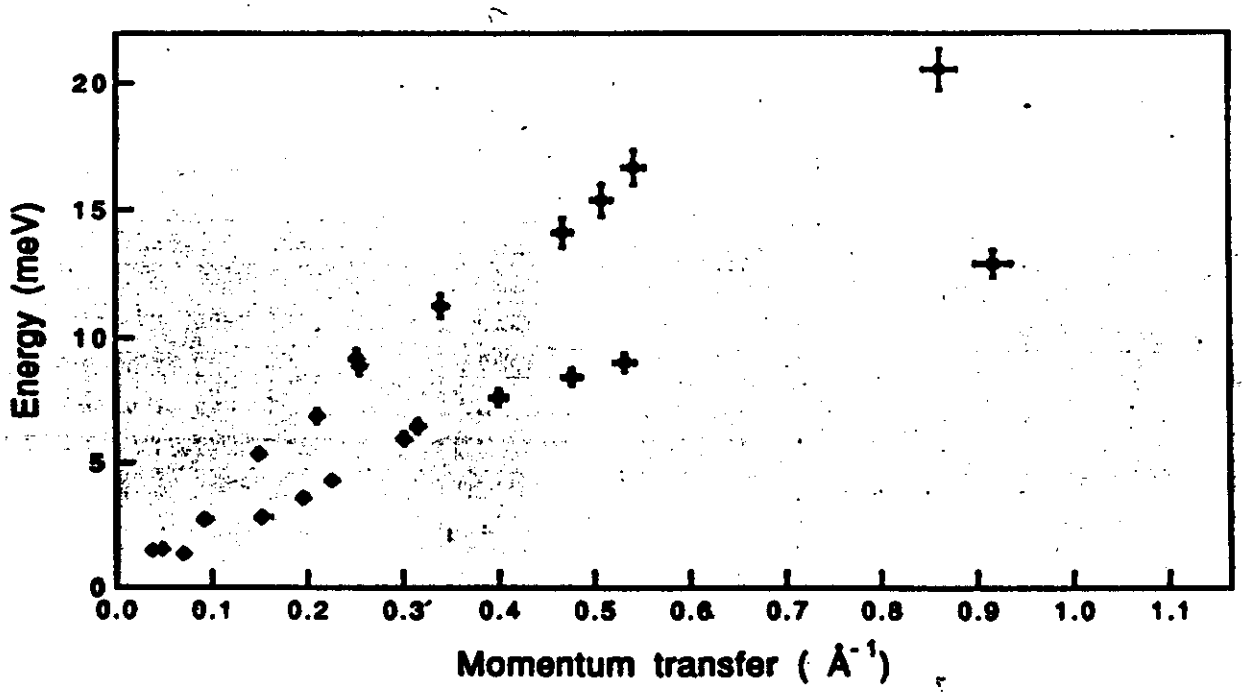


[001]

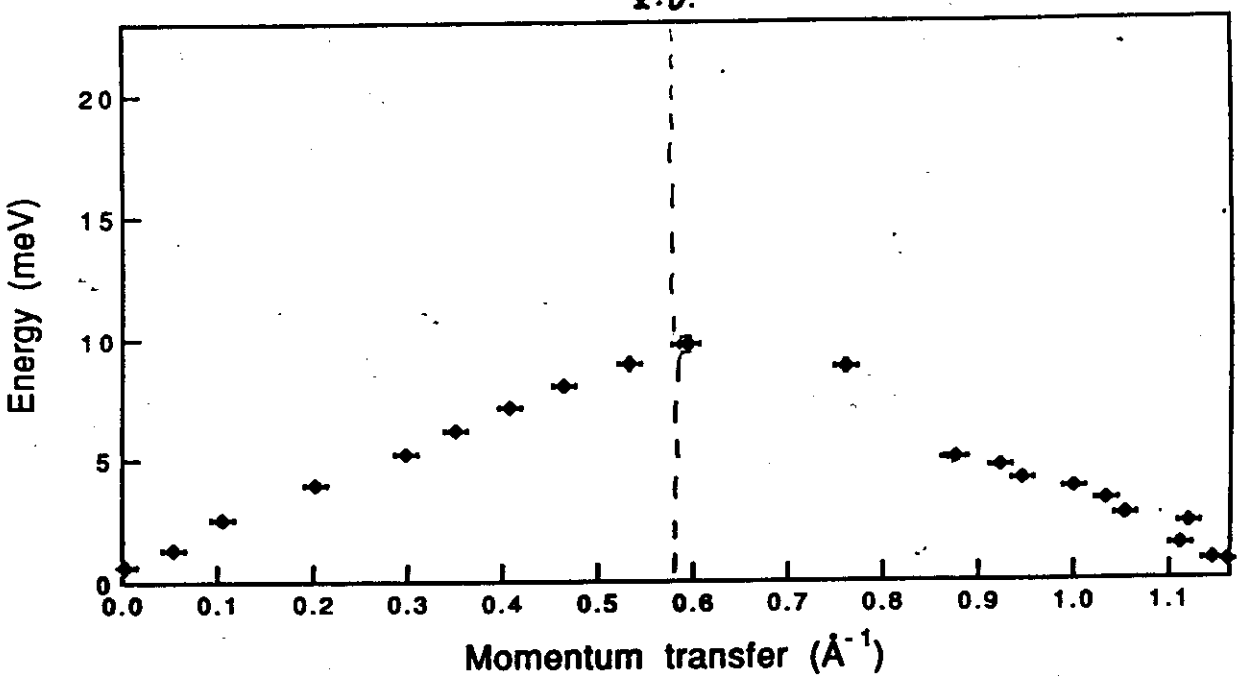
(1x2) "HR" SURFACE RELAXATION (0-10%)



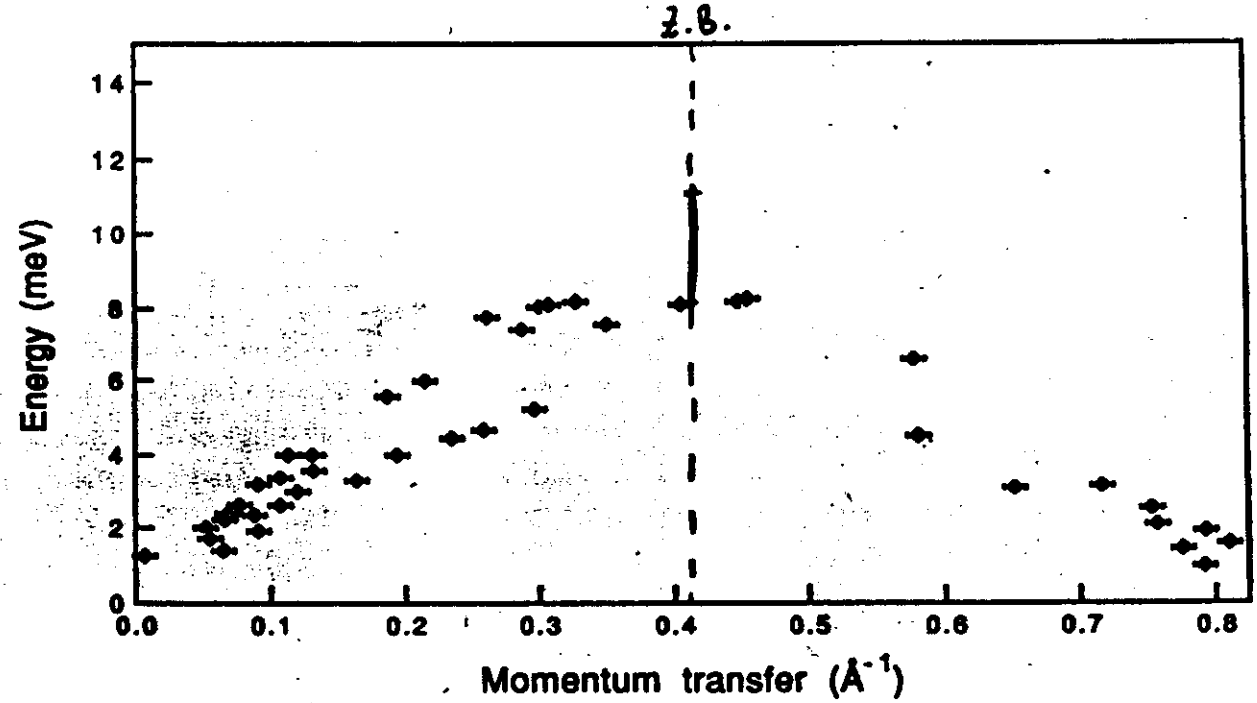
[redacted] Phonon dispersion curve along [redacted]
He beam energy = 18.62 meV, T=600K,
Zone boundary, $G_y/2$ = 0.824 Å^{-1}
sampling time = 10 min. per point



[redacted] Phonon dispersion along [redacted]
He beam energy = 18.62 meV, T=600K
(1x1) Zone boundary, $G_x/2$ = 1.165 Å^{-1}
sampling time = 20 min. per point

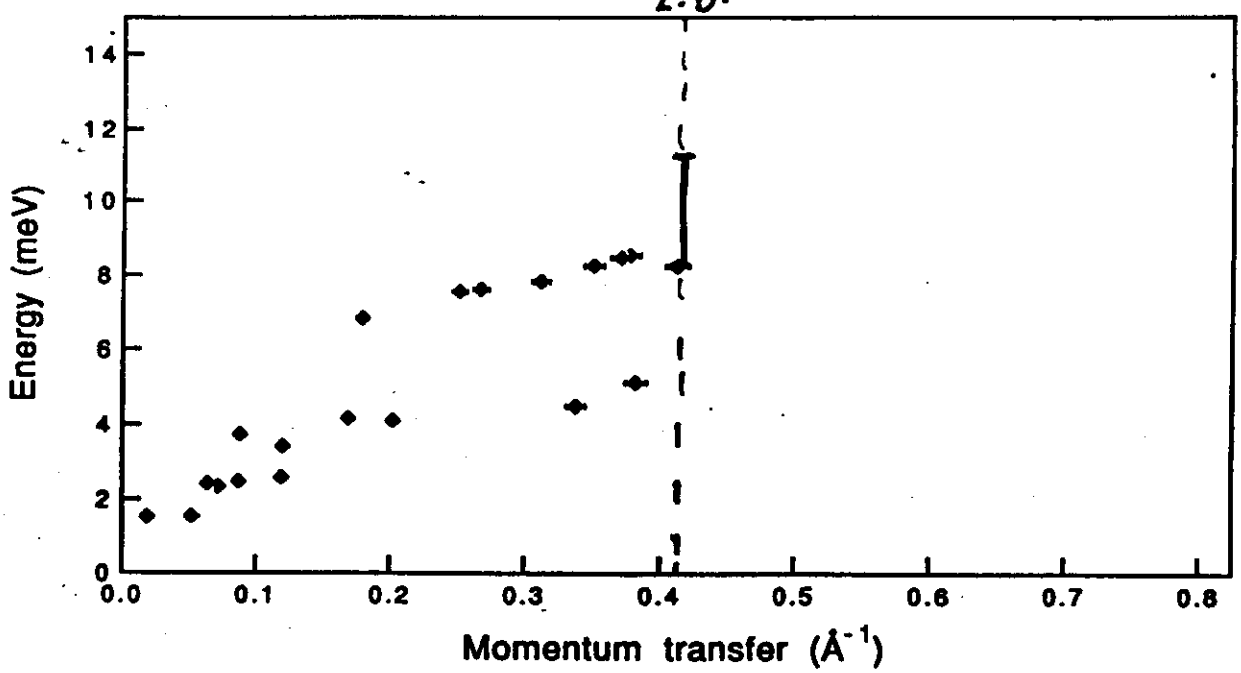


[redacted] Phonon dispersion curve along [redacted]
He beam energy = 18.62 meV, T=600K,
(2x2) zone boundary, $G_x/2$ = 0.5825 Å^{-1},
sampling time ... min. per point.



[redacted] Phonon dispersion curve along [redacted]
He beam energy = 18.62 meV, T=600K,
(2x2) zone boundary, $G_y/2$ = 0.412 Å^{-1},
sampling time 20 min. per point.

Z.B.



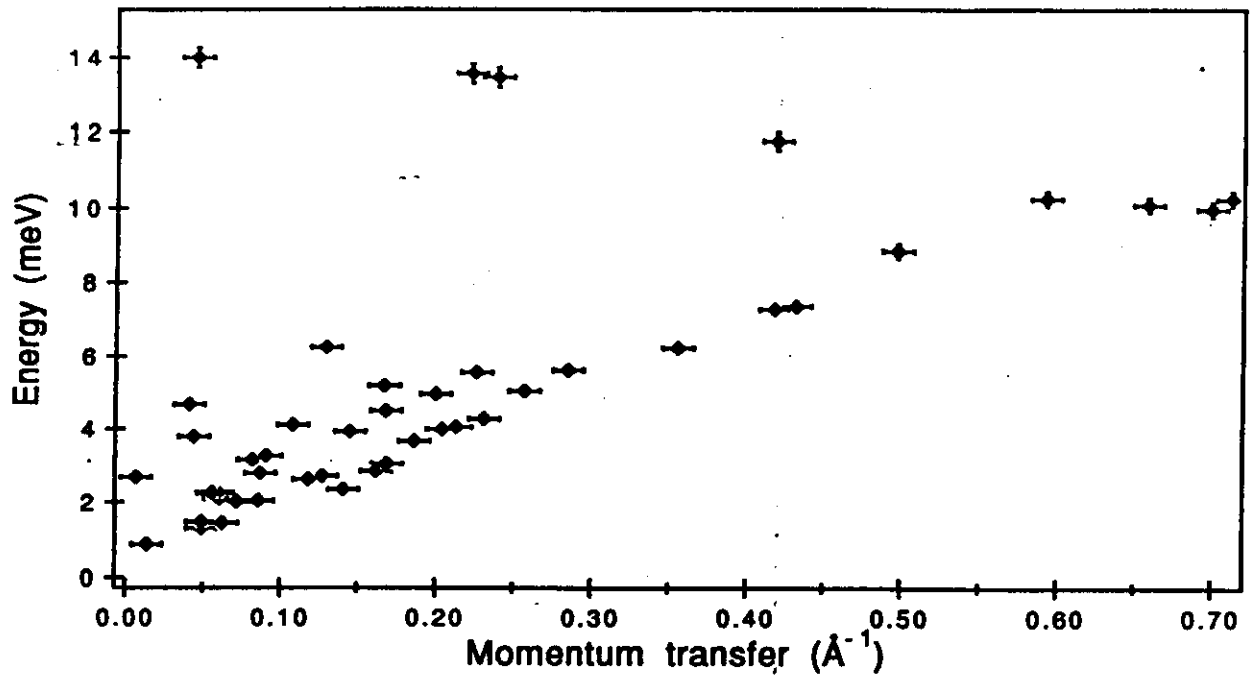
[redacted] Phonon dispersion along [redacted]
He beam energy = 18.62 meV, T=370K
(1x2) Zone boundary, $G_y/2$ = 0.412 Å^{-1}
sampling time = 20 min. per point

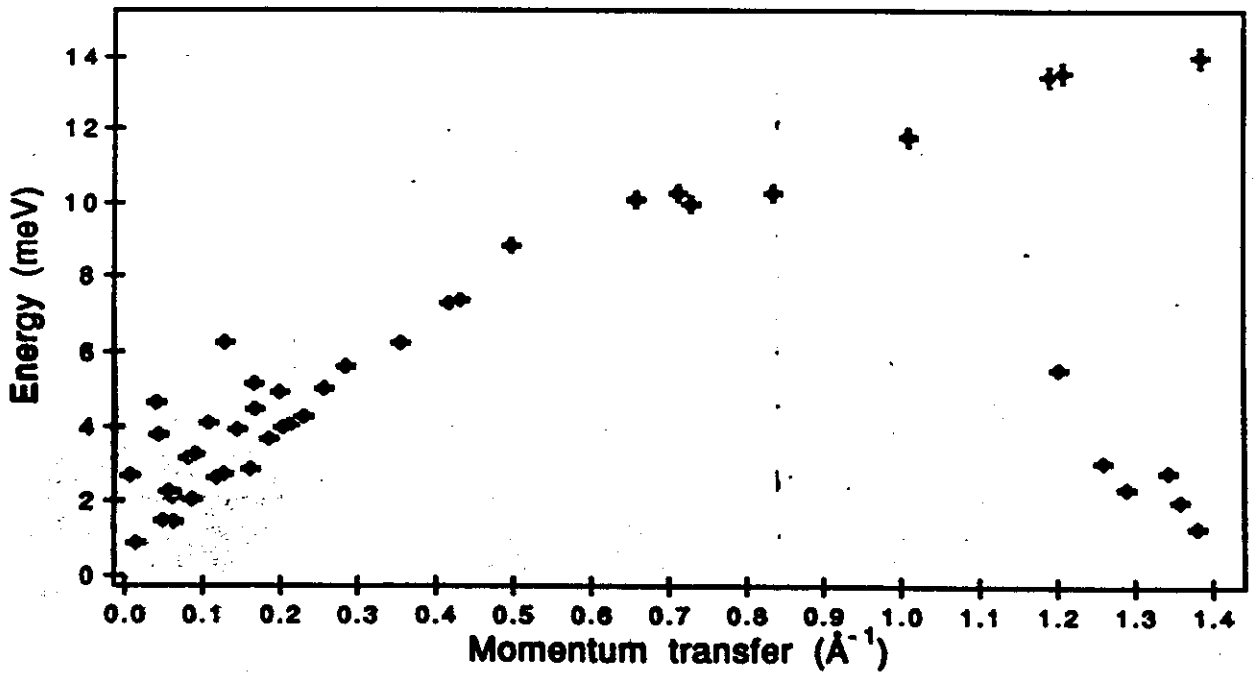
Summary: (1x1) No bulk phonon measurements
No bulk phonon calculations
Surface phonon calculations in progress

Rh (1x2); ΓY: - Substantial softening at the Z.B.
- No folded dispersion curve

O/Rh (2x2); ΓY: - Perfectly matching the 1x2 spectra
(No effect due to oxygen)

ΓX: - No changes with respect to (1x1) case (apart from lower symmetry! (lower bound)





[redacted] Phonon dispersion curve along [redacted]
He beam energy = 18.62 meV, T=600K
S point at 1.427 Å^{-1},
sampling time = ... min. per point.

Atom-Surface Interaction Potential

Long-range polarization attraction:

$$V_{long}(r) \propto - \frac{C}{z^3}$$

[Zaremba and Kohn, 1976]

Short-range repulsion:

$$V_{short}(r) = \alpha\, n(r)$$

whith $\alpha = 30$ eV Å^3

[Esbjerg and Nørskov, 1980]

problem: $V(r) = V_{short}(r) + V_{long}(r)$

Sum of pairvise terms $u_j(r)$:

$$V(r) = \sum_j u_j(r)$$

$$V(r) = V_{0,0} + \sum_G V_G(z)\, e^{(iGR)}$$

Atom Surface Interaction Potential from Empirical Data

- Solving the Schrœdinger Equation: the solutions have lateral Bloch-wave character:

$$\psi_K(\mathbf{r}) = \sum_G c_G(z)\ e^{i(K+G)\cdot R}$$

and the Schr. eq. becomes a sistem of coupled differential equations in the incognitæ $c_G(z)$, given the Fourier components $V_G(z)$ of the interaction potential.

- **Analysis of diffraction intensities within the Hard Corrugated Wall Model: corrugation function $\zeta(R)$**

$$V(r) = 0 \qquad \text{for } z > \zeta(R)$$

$$V(r) = \infty \qquad \text{for } z \leq \zeta(R)$$

- Bound State Resonance Data

levels of $V_{0,0}(z)$

POTENZIALE ATOMO - SUPERFICIE

$$V(R,z) = \sum_{kem}{}' U(r - r_{kem}) - \frac{C}{(z-z_0)^3 + \sigma^3 \exp\left(-\frac{1}{2}\left(\frac{z-z_0}{\sigma}\right)^3\right)}$$

CORTO RAGGIO

LUNGO RAGGIO

POTENZIALE ATOMO - ATOMO TOMMASINI et al. Phys. Rev.

$$U(\rho_{kem}) = \eta_x \eta_y A \exp(-\beta \rho_{kem}) \left\{ 1 - \exp[0.36\beta(\rho_{kem} - \sigma)] \right\}$$

$$\rho_{kem} = \sqrt{(z-z_k)^2 + \eta_x^2 (x - x_{kem})^2 + \eta_y^2 (y - y_{kem})^2}$$

η_x, η_y Parametri di anisotropia

A, β • POTENZIALE A CORTO RAGGIO

C, z_0 • POTENZIALE A LUNGO RAGGIO

σ • ATTRAZIONE A CORTO RAGGIO
• REPULSIONE A LUNGO RAGGIO

POSIZIONI ATOMICHE.