Intermixing mechanisms and morphology of the Ge/Si(100) interface investigated by XPD (X-ray photoelectron diffraction) and XAS (X-ray absorption spectroscopy)

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- Ge/Si based devices rely on high quality Ge/Si heterostructures. The atomic morphology and the interdiffusion mechanisms of such heterostructures should be carefully controlled durind their growth.

- These phenomena were investigated by in situ photoelectron diffraction (XPD), electron diffraction (RHEED), XAS (x-ray absorption) and ex-situ techniques (TEM and luminescence).

The intensity anisotropy of Si and Ge photoelectron was used to follow in detail the growth of Ge atoms deposited on Si(001) 2x1 surfaces in an MBE chamber fully operating at the Camerino University

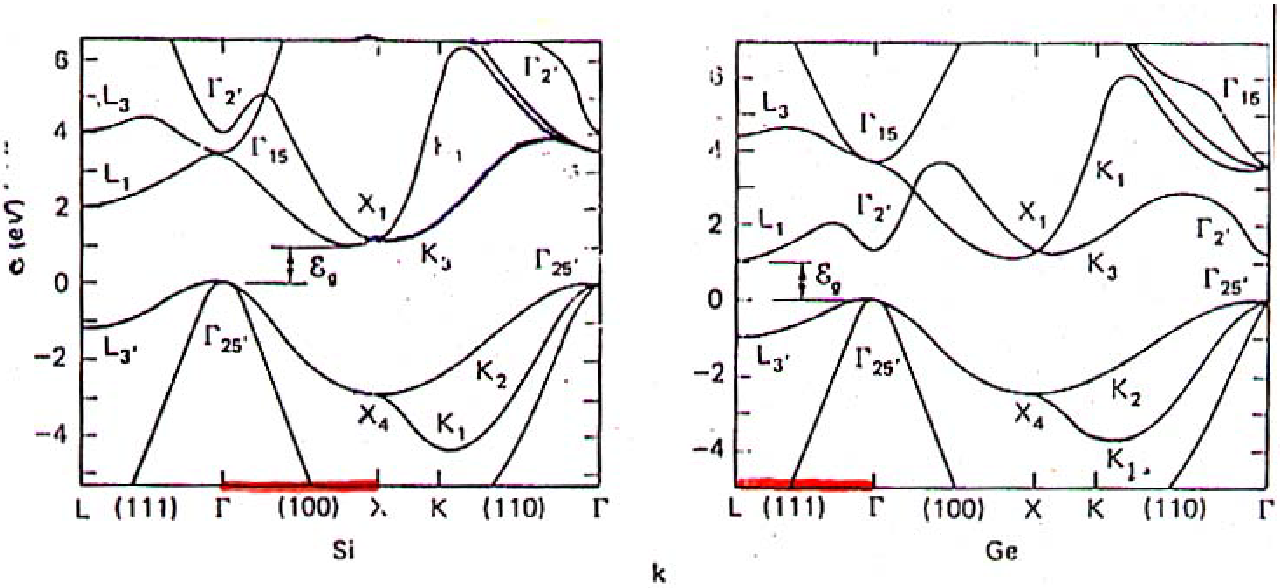


Figure 2.18 Empirical pseudopotential results for the energy bands of the elemental semiconductors Si and Ge. [After M. L. Cohen and T. K. Bergstresser, *Phys. Rev. 141*, 789 (1966).]

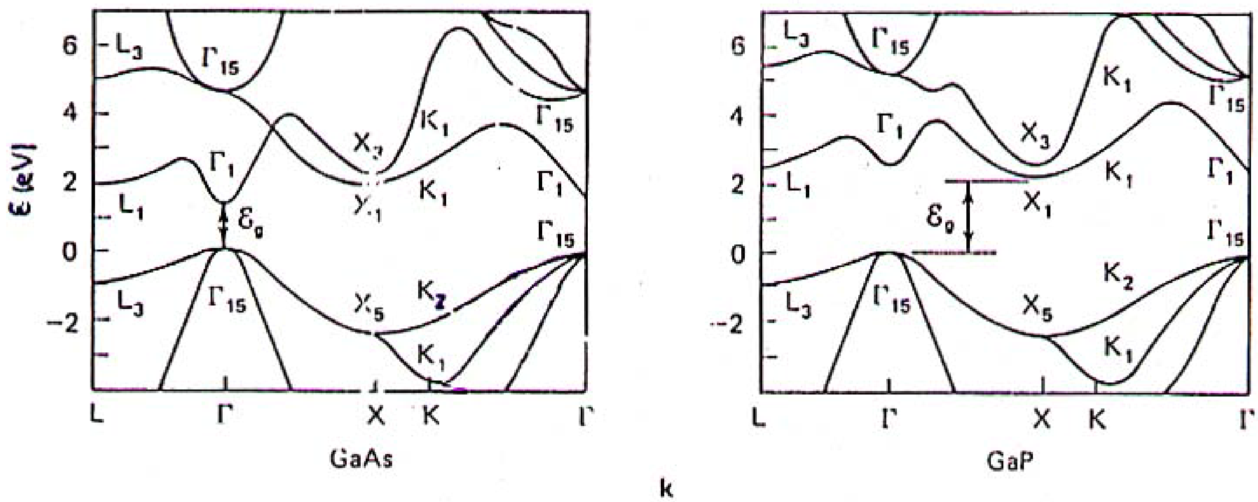


Figure 2.19 Energy bands for the III–V compound semiconductors GaAs and GaP. [After M. L. Cohen and T. K. Bergstresser, *Phys. Rev. 141*, 789 (1966).]

Diamond Structure

The diamond lattice (formed by the carbon atoms in a diamond crystal) consists of two interpenetrating face-centered cubic Bravais lattices, displaced along the body diagonal of the cubic cell by one quarter the length of the diagonal. It can be regarded as a face-centered cubic lattice with the two-point basis **0** and $(a/4)(\hat{x} + \hat{y} + \hat{z})$. The coordination number is 4 (Figure 4.18). The diamond lattice is not a Bravais lattice,

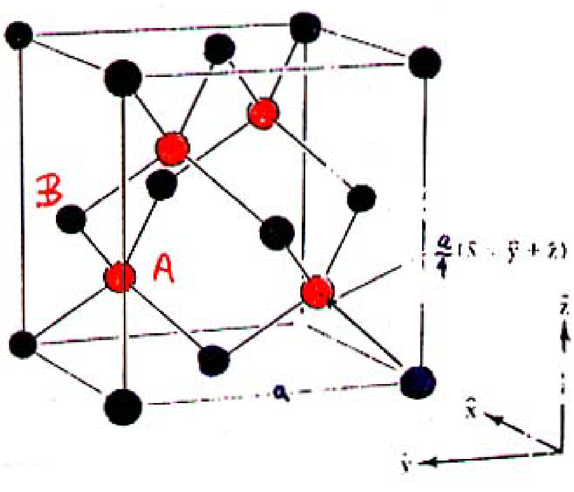
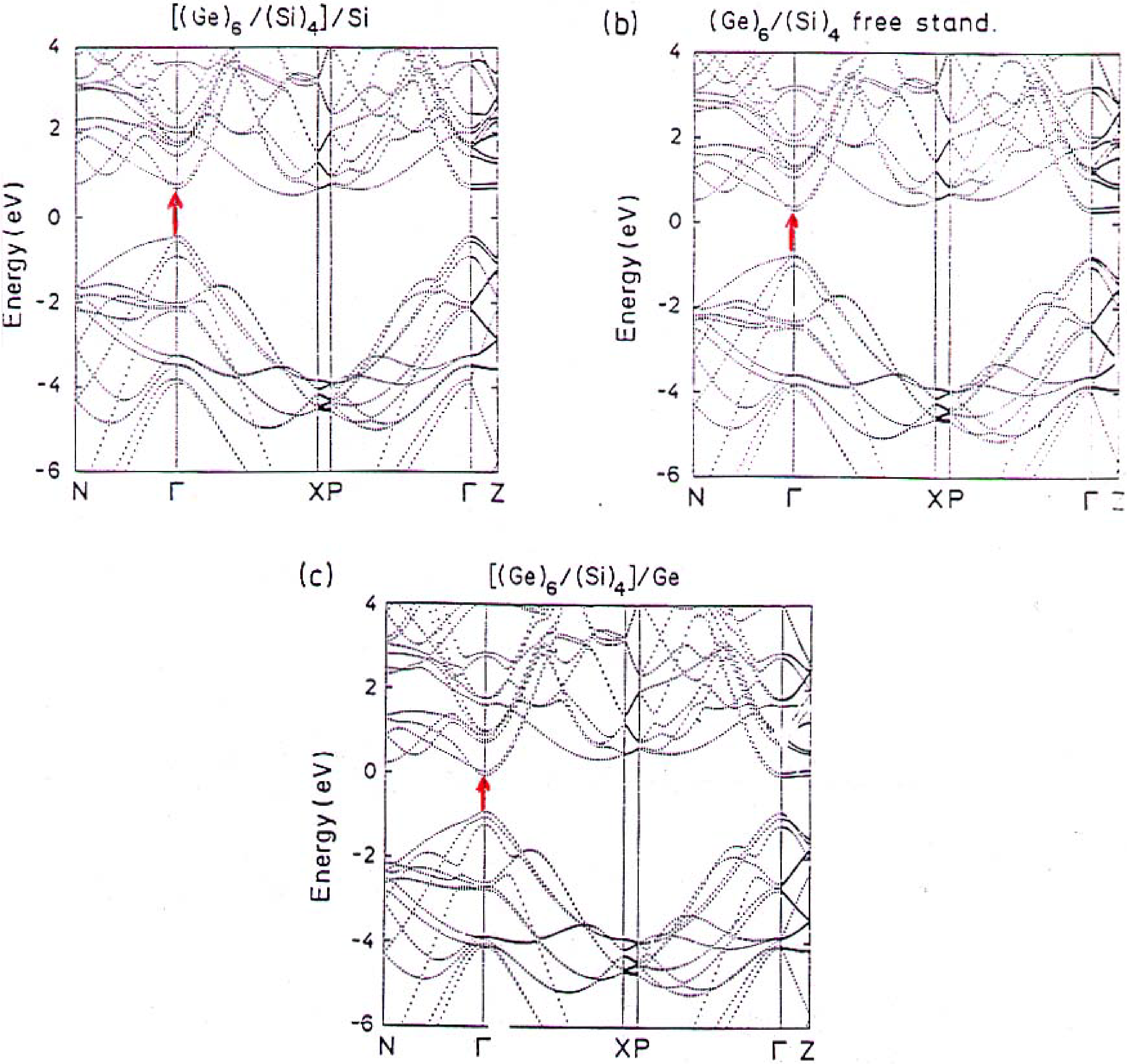


Figure 4.18
Conventional cubic cell of the diamond lattice. For clarity, sites corresponding to one of the two interpenetrating face-centered cubic lattices are unshaded. (In the zincblende structure the shaded sites are occupied by one kind of ion, and the unshaded by another.) Nearest-neighbor bonds have been drawn in. The four nearest neighbors of each point form the vertices of a regular tetrahedron.



U. Schmid, N.E. Christensen, M. Alouani, M. Cardona,
Phys. Rev. B 43, 14597 (1991)

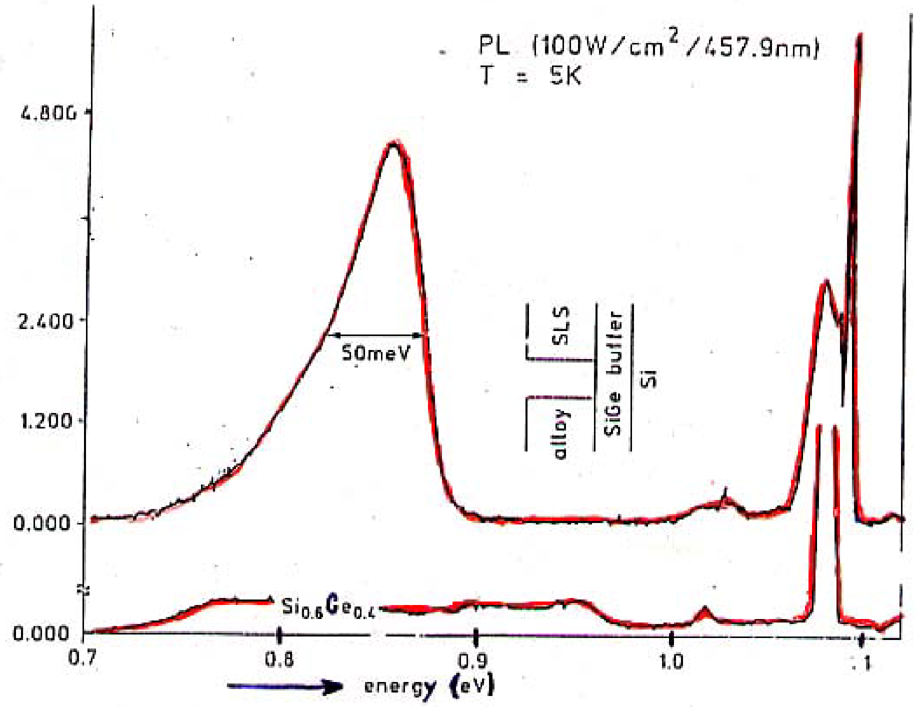


Figure 21. (a) Comparison of the PL signal of a Si_6Ge_4 SLS with a $Si_{0.6}Ge_{0.4}$ alloy sample. The photoluminescence was excited by the blue line ($\lambda = 457.9$ nm) of an Ar^+ laser with an intensity of roughly 100 mW cm^{-2} and measured at T = 5 K. The inset shows the corresponding Raman spectrum where the occurrence of the folded acoustic mode proves the existence of the superlattice periodicity

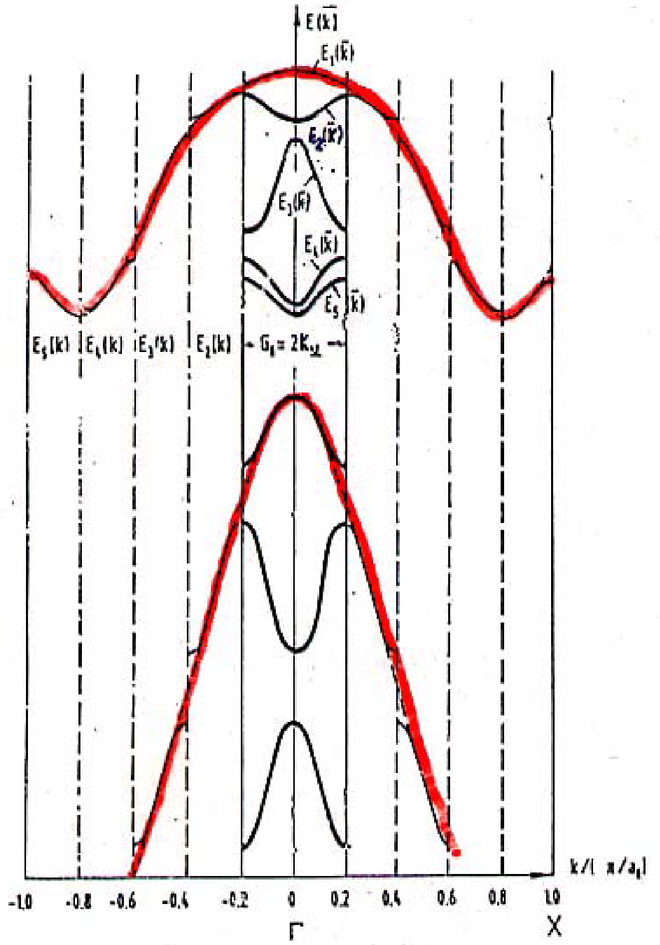
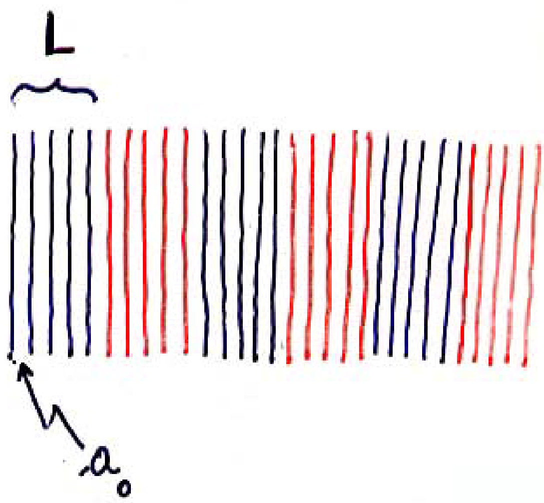
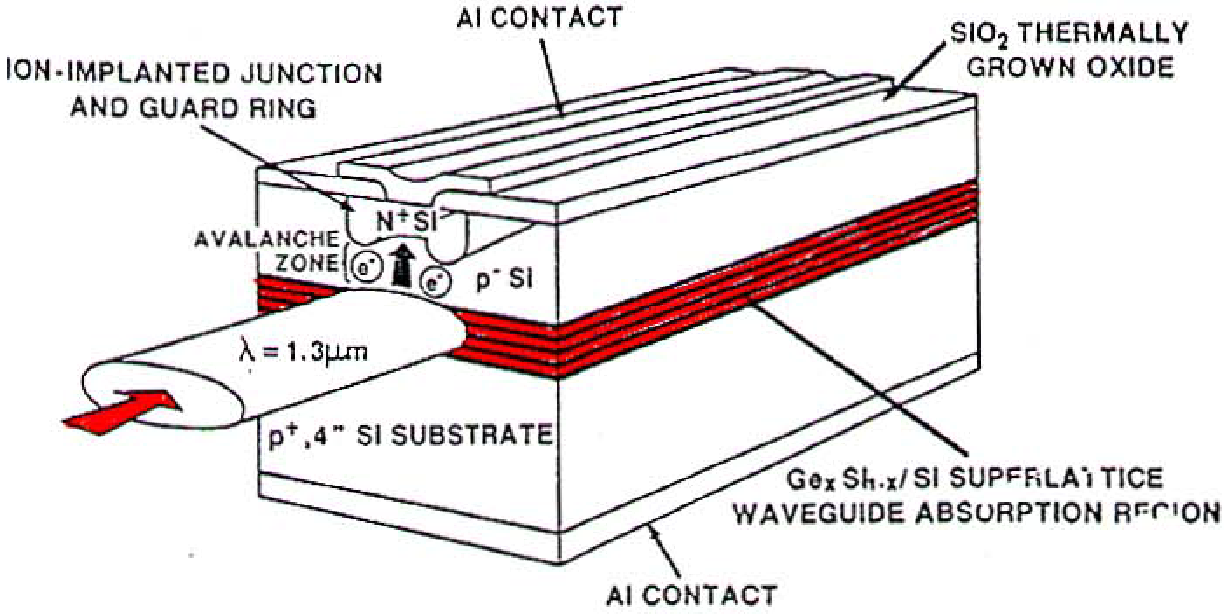


Figure 3: Brillouin zone folding of a Si-like band structure introduced by a superlattice with a period of $L = 5a_0$ ($a_0 = 0.5431$ nm, lattice constant of Si). The band structure is folded into the first minizone (bold curves), which has the extension of $2K_{SL} = 2(\pi/5a_0)$, being 1/5th of the original zone. By this process the original band structure with the indirect bandgap transforms into a band structure with a direct bandgap at $k = 0$.

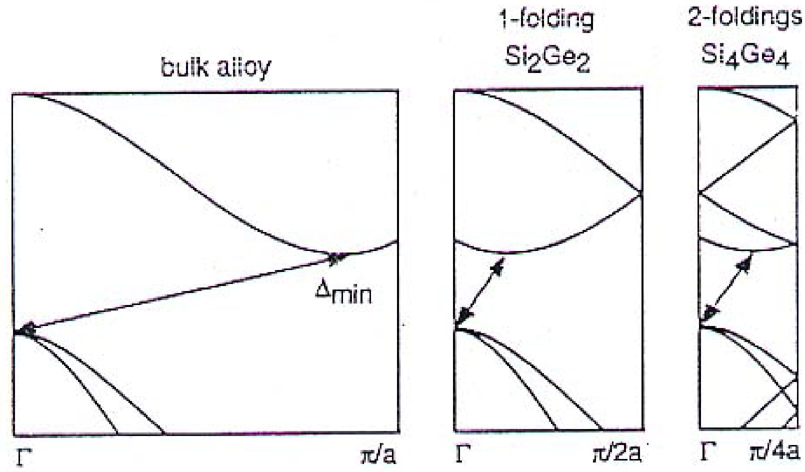


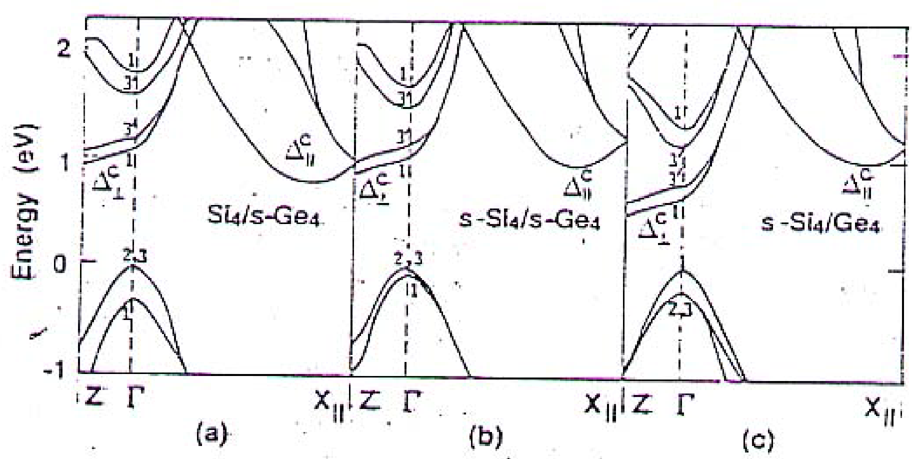
Zachai et al.
PRL 64 (1990) 1055

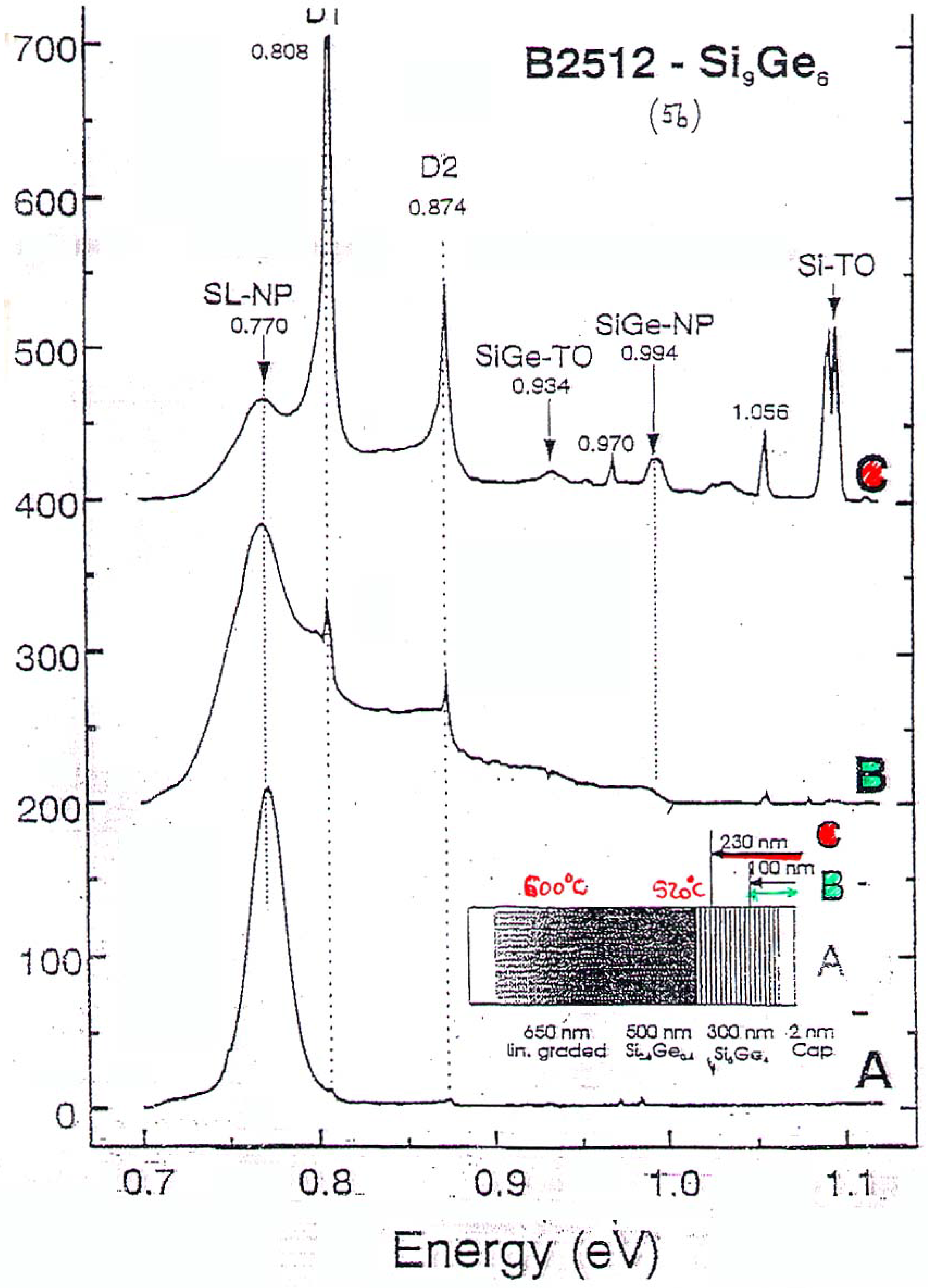
PLANAR, LONG-WAVELENGTH WAVEGUIDE AVALANCHE PHOTODIODE WITH SEPARATE ABSORPTION AND MULTIPLICATION REGIONS

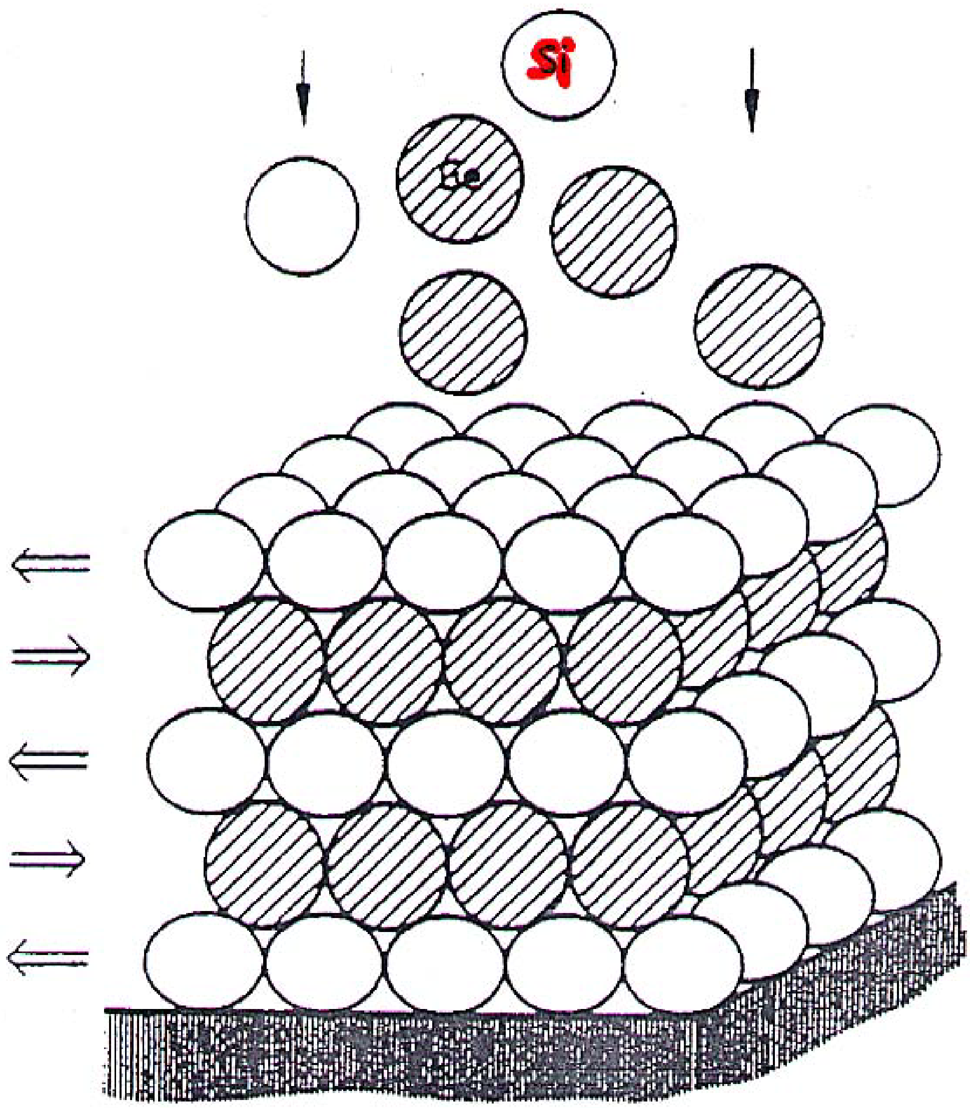


Short period superlattices





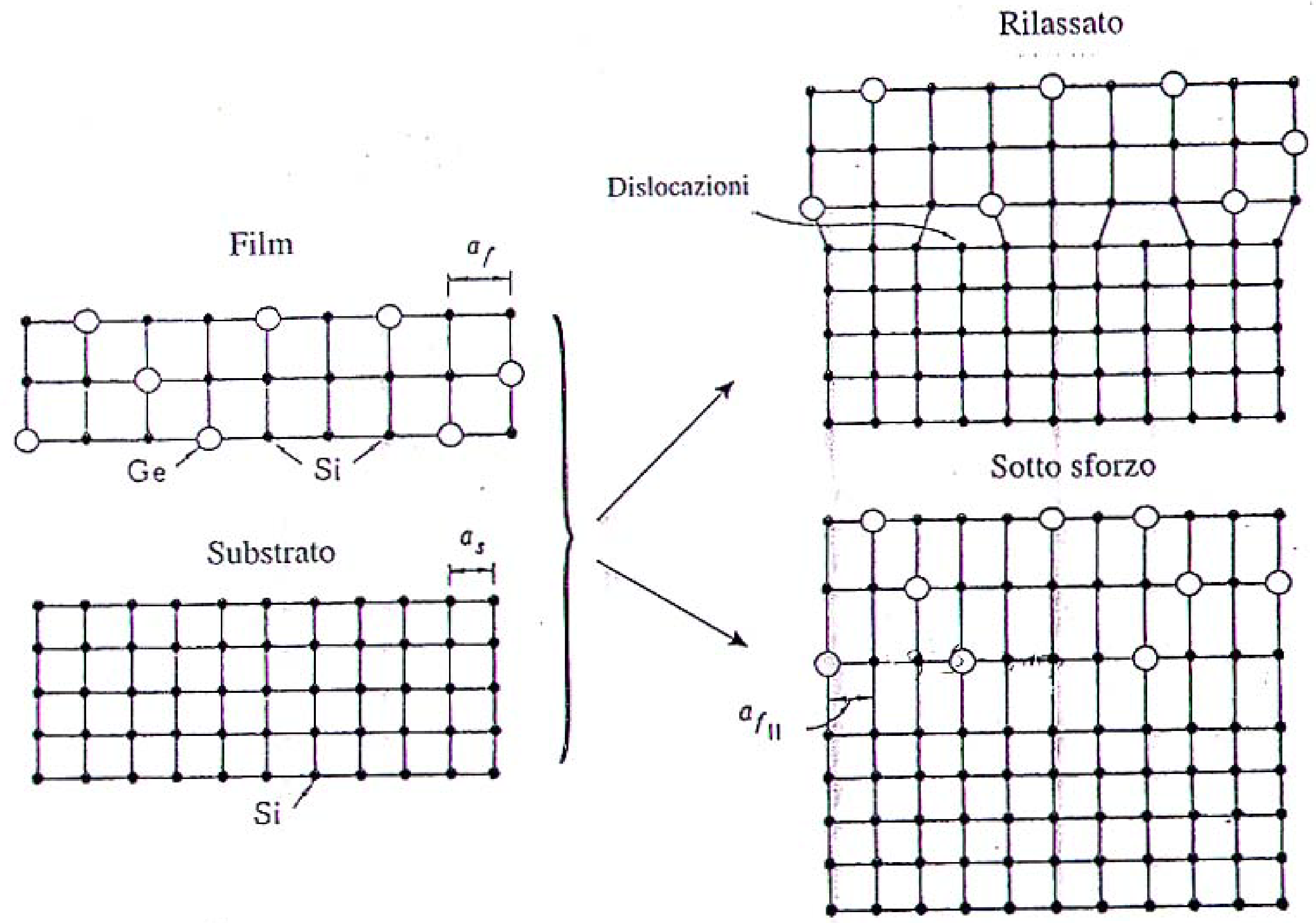

B2512 - Si9Ge6
(5b)
D1
0.808
D2
0.874
SL-NP
0.770
SiGe-TO
0.934
SiGe-NP
0.994
0.970
1.056
Si-TO
C
B
A
230 nm
100 nm
600°C
520°C
650 nm lin. graded
500 nm
300 nm
2 nm Cap
700
600
500
400
300
200
100
0
0.7
0.8
0.9
1.0
1.1
Energy (eV)



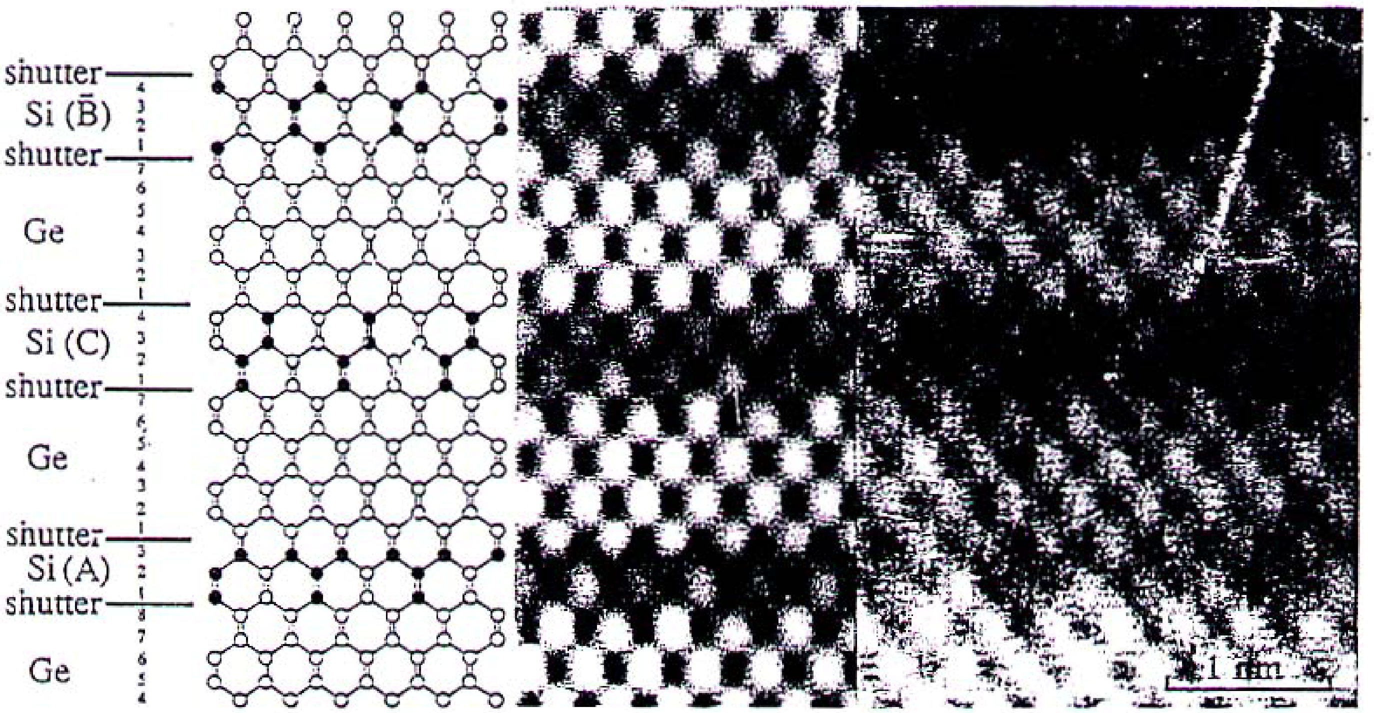
Costante reticolare planare del sistema : $a_{\parallel}$

$$a_{\parallel} \cong a_{Si}$$

$$a_{\parallel}(Ge) \rightarrow a_{\parallel}$$



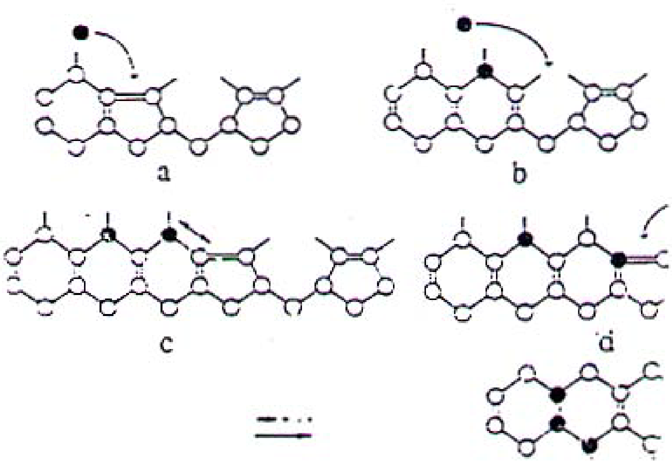
Film
a_f
Ge
Si
Substrato
a_s
Si
Rilassato
Dislocazioni
Sotto sforzo
$a_{f_{||}}$



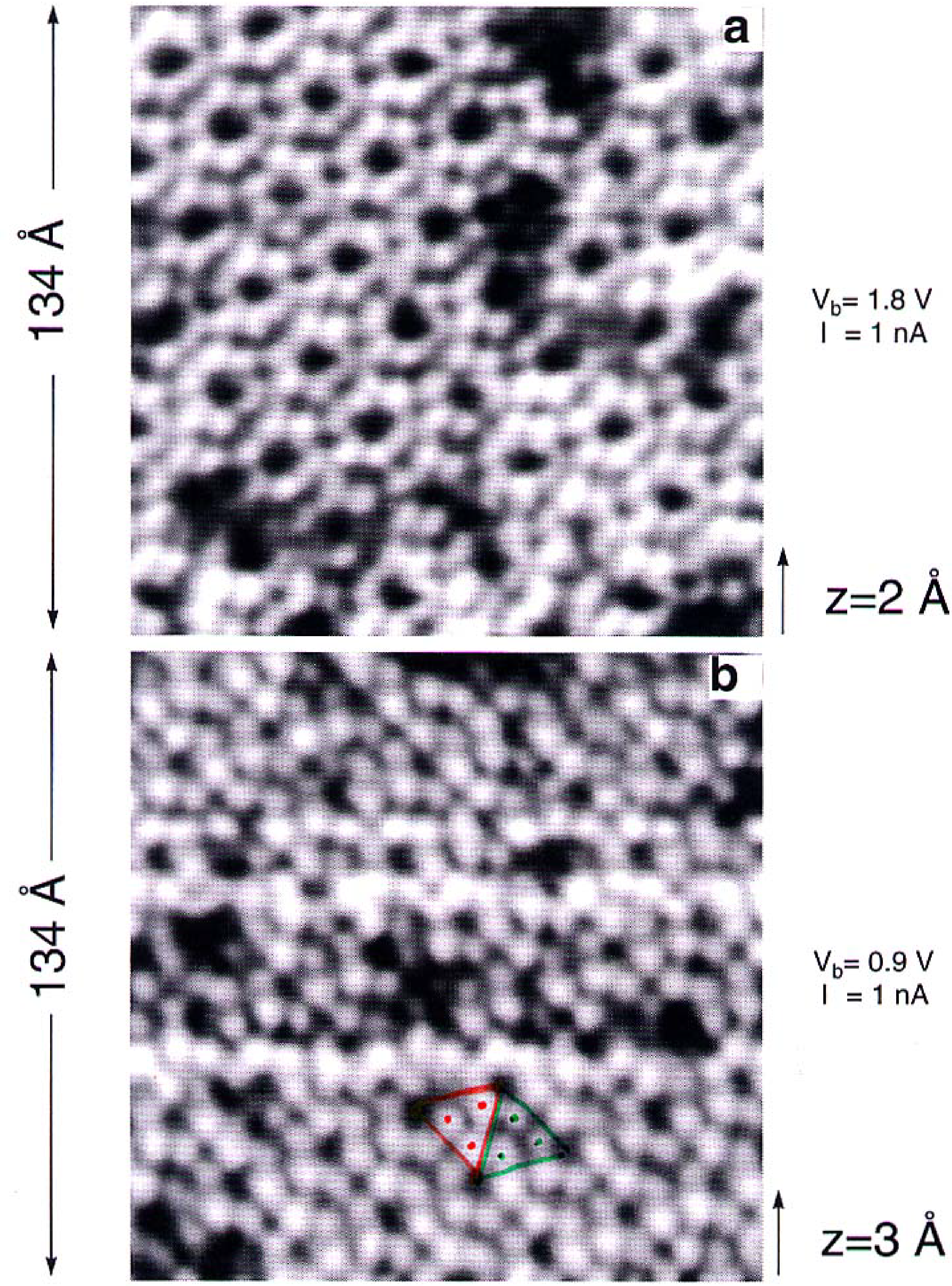
Z-contrast STEM image of a nominal $(Si_4Ge_8)_{24}$ superlattice showing interfacial ordering. The [001] g top of the image with the sample thickness increasing toward the lower left-hand corner. Our interpre ure based on the image simulation indicates the sequential deposition of Si and Ge layers together witi d A resulting from the atom pump mechanism. Open circles represent Ge columns; solid circles, Si y columns. Simulation parameters are $C_s = 1.3$ mm, convergence angle $= 10.3$ mrad, and defocus =

for all of the various image forms and e asymmetric interfacial abruptness. The own in Fig. 1 was grown by MBE directly strate at 350 °C with a deposition rate of he presence of significant quantities of Ge s is therefore of considerable surprise for erature growth. Strain-enhanced interdif- to Si is expected to be small or negligible n temperature[12] and the alternative ex- e islanding during growth can be immedi- from the compositional uniformity of our low temperatures the surface diffusion onsiderably smaller than the typical dis- steps so that growth occurs via monolay- nd formation and the consecutive inter- ×1) and (1×2) domains.[13] At 350 °C this

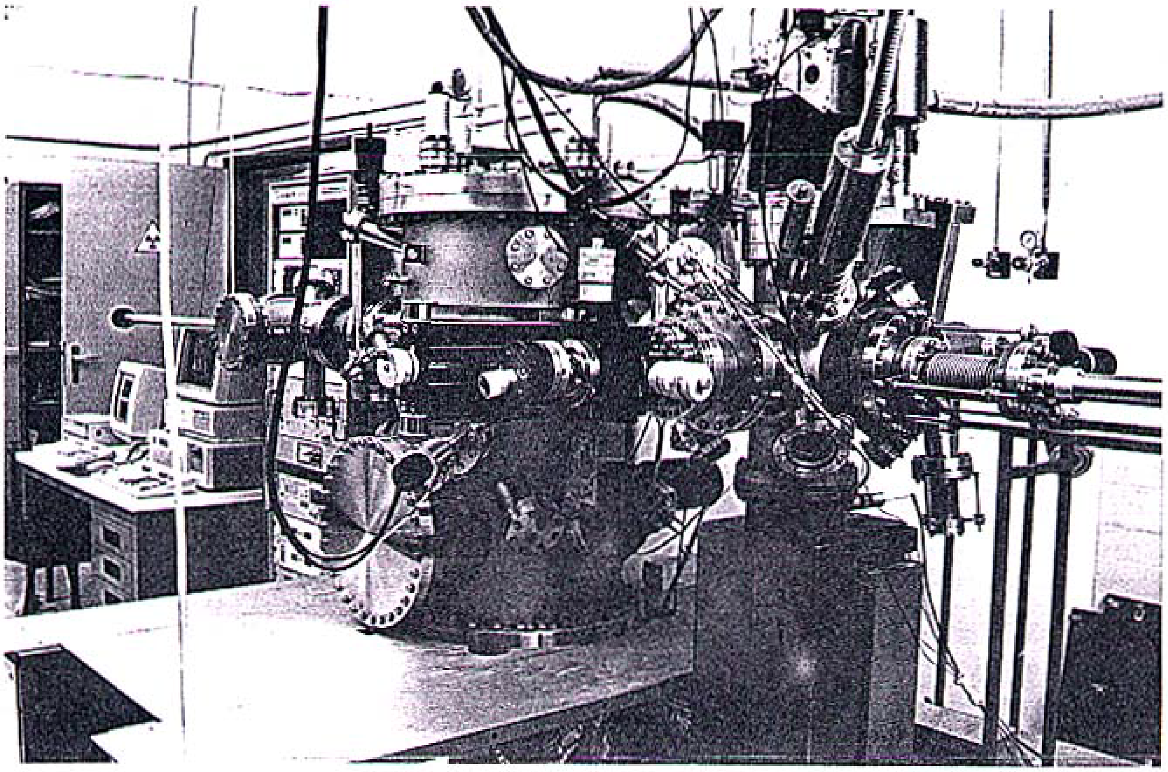
the interchange of relatively weakly bou neighbor atoms at the step edge. We note, h an interchange of Si and Ge atoms at the Fig. 2(b) will not significantly affect the str reduce the number of unsaturated bonds,



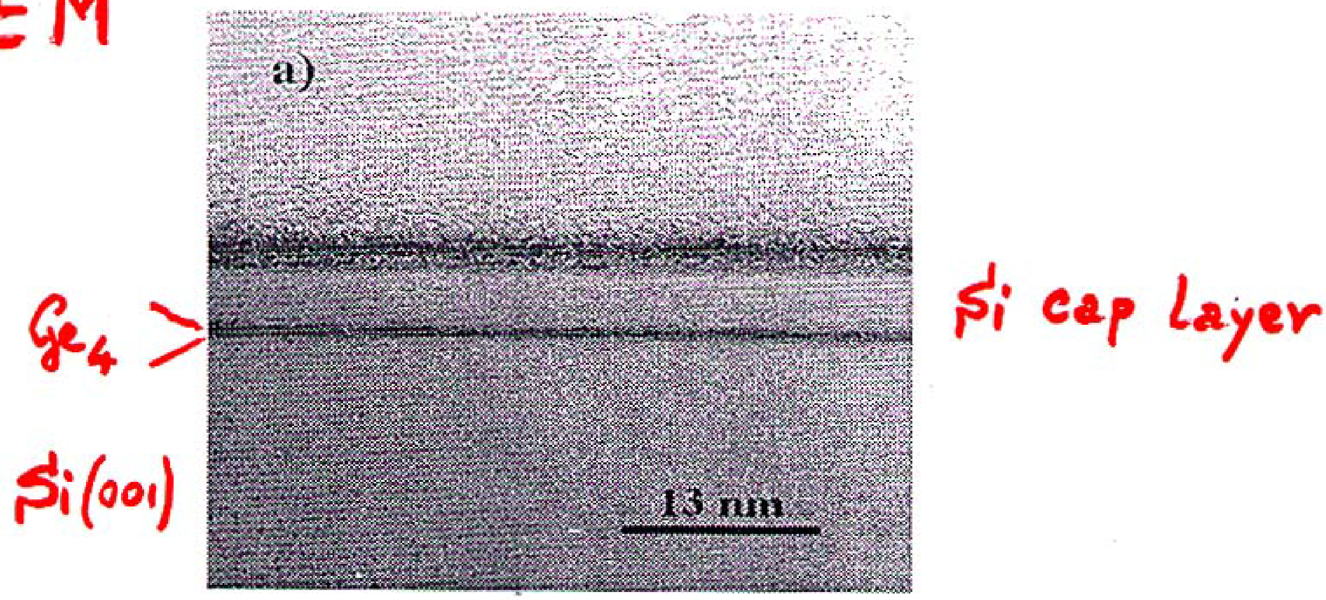
Formation of the GeSi alloy: 5x5 reconstruction

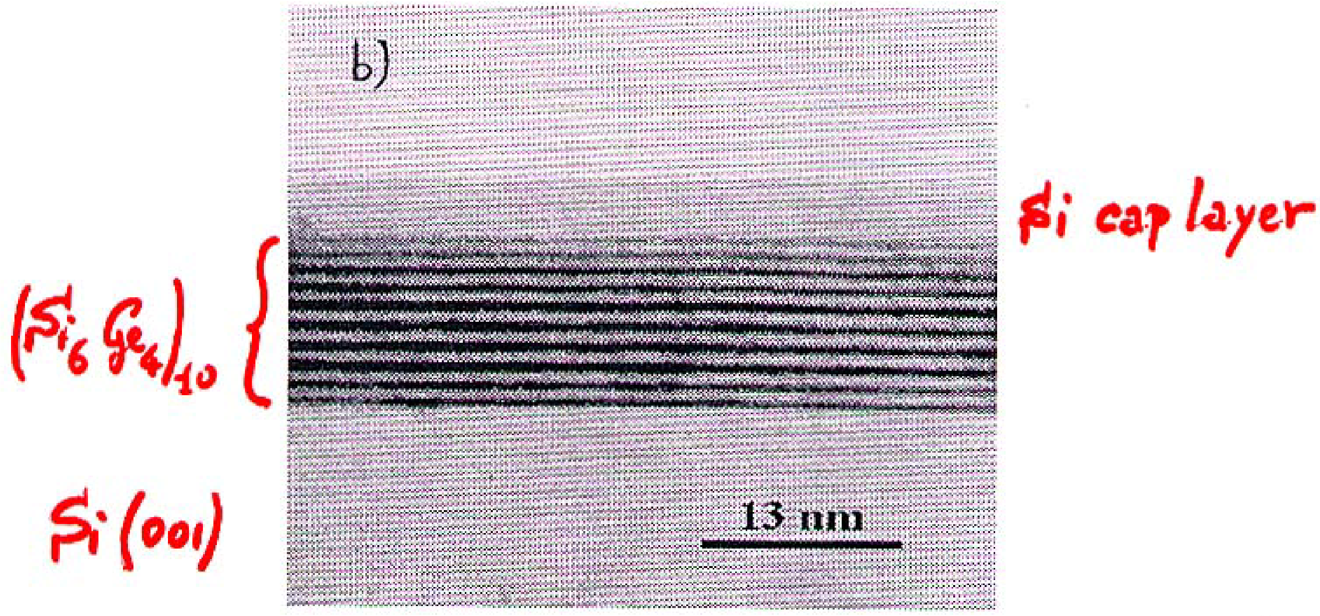


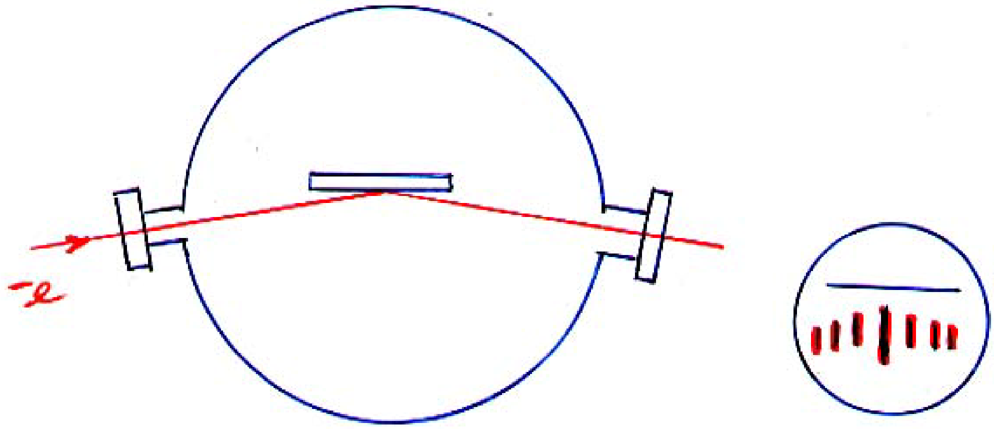
Si (111) 7x7 + 5Å Ge + annealing 790 C



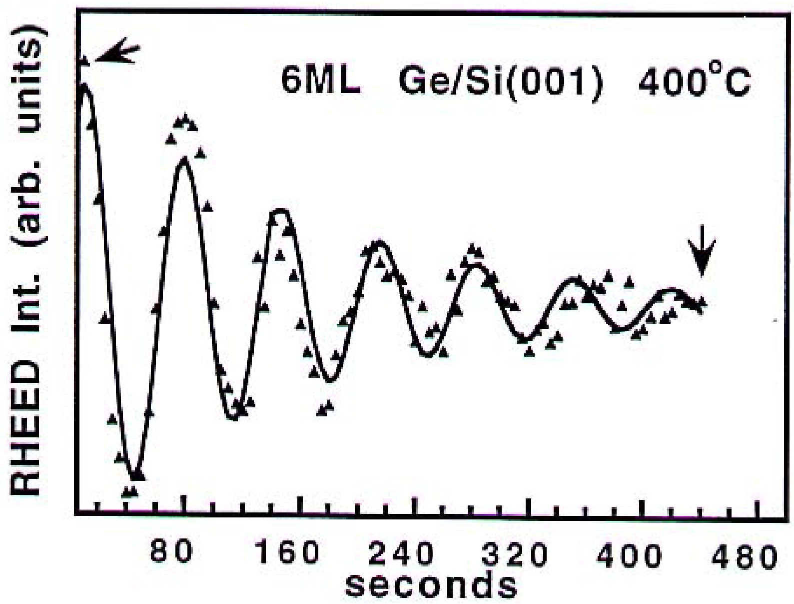
TEM


a)
Ge4
Si cap layer
Si(001)
13 nm

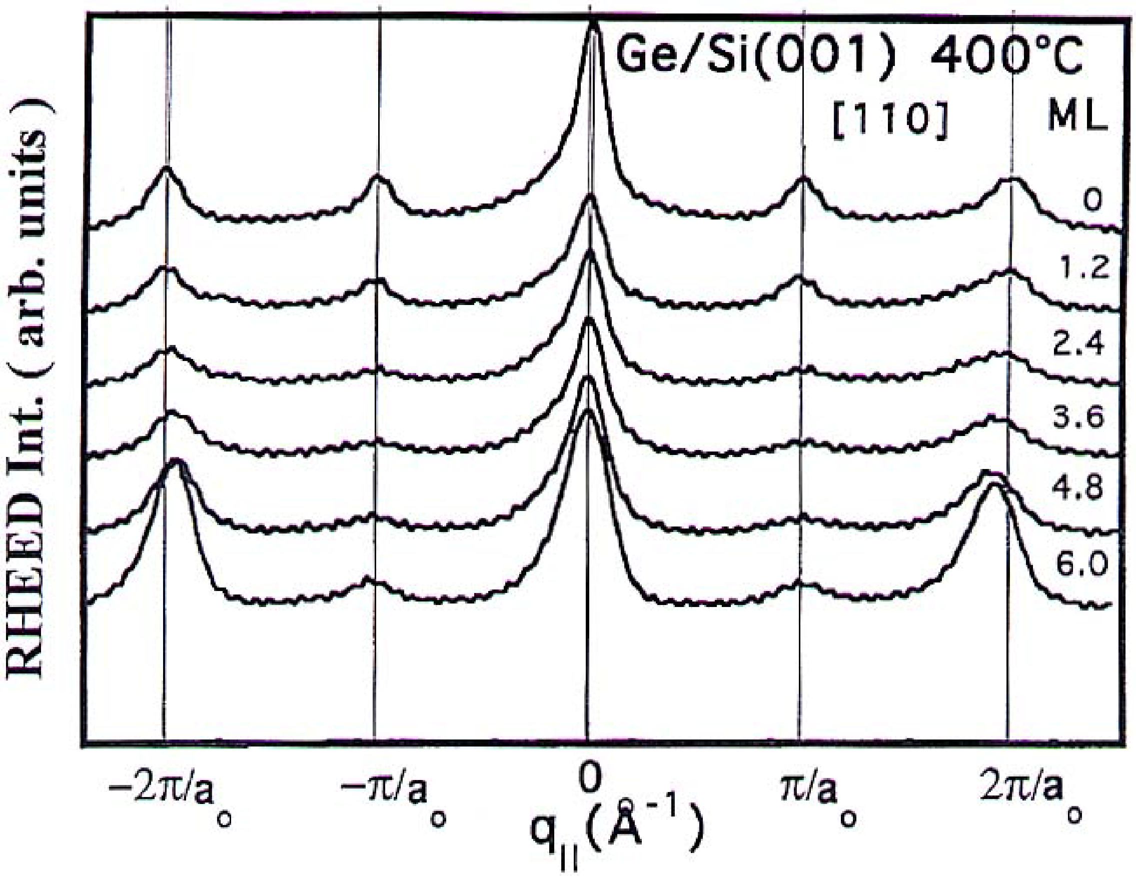

b)
Si cap layer
(Si6 Ge4)10
Si(001)
13 nm



Reflected
High
Energy
Electron
Diffraction



R. Gunnella et al. Fig. 4



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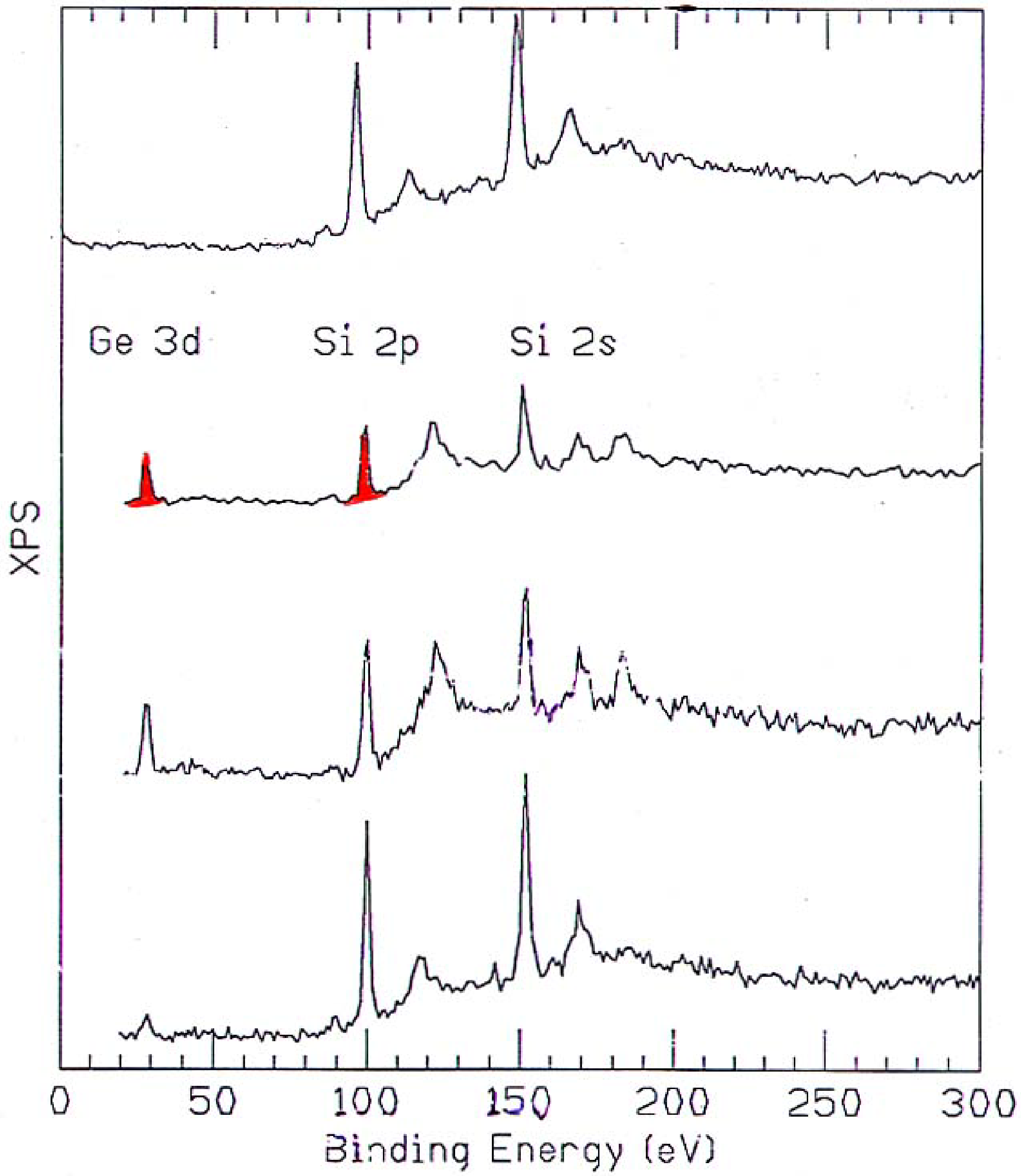
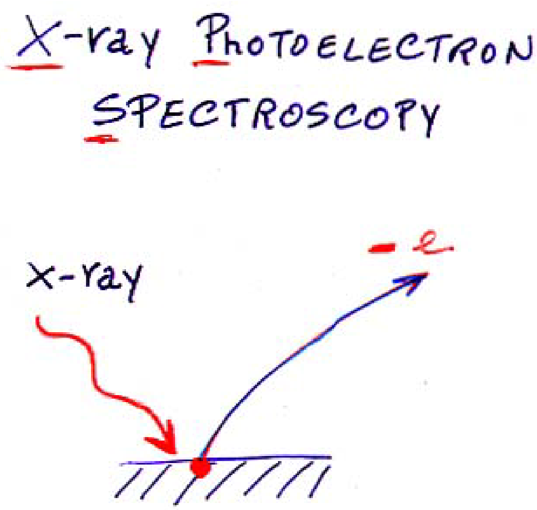
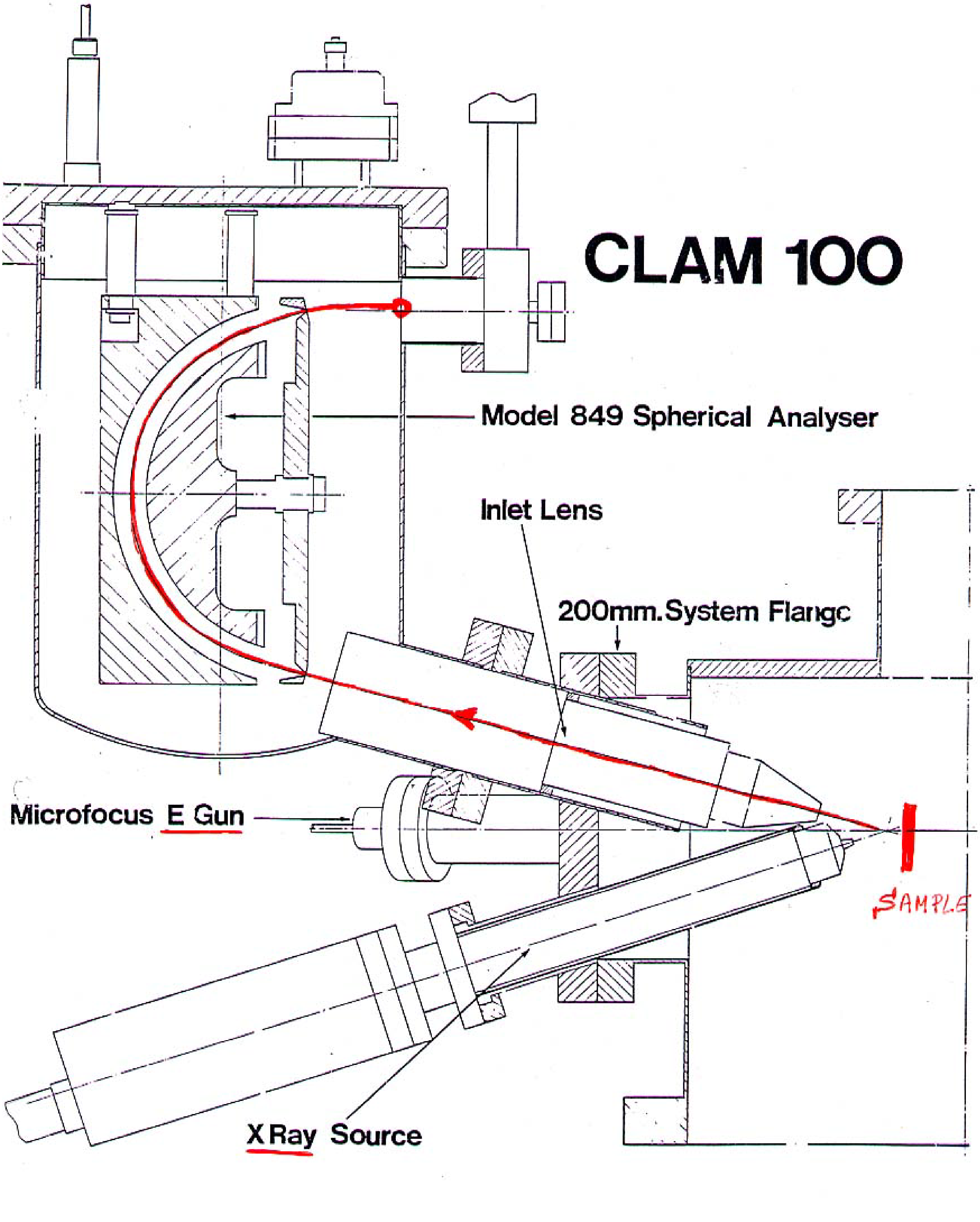
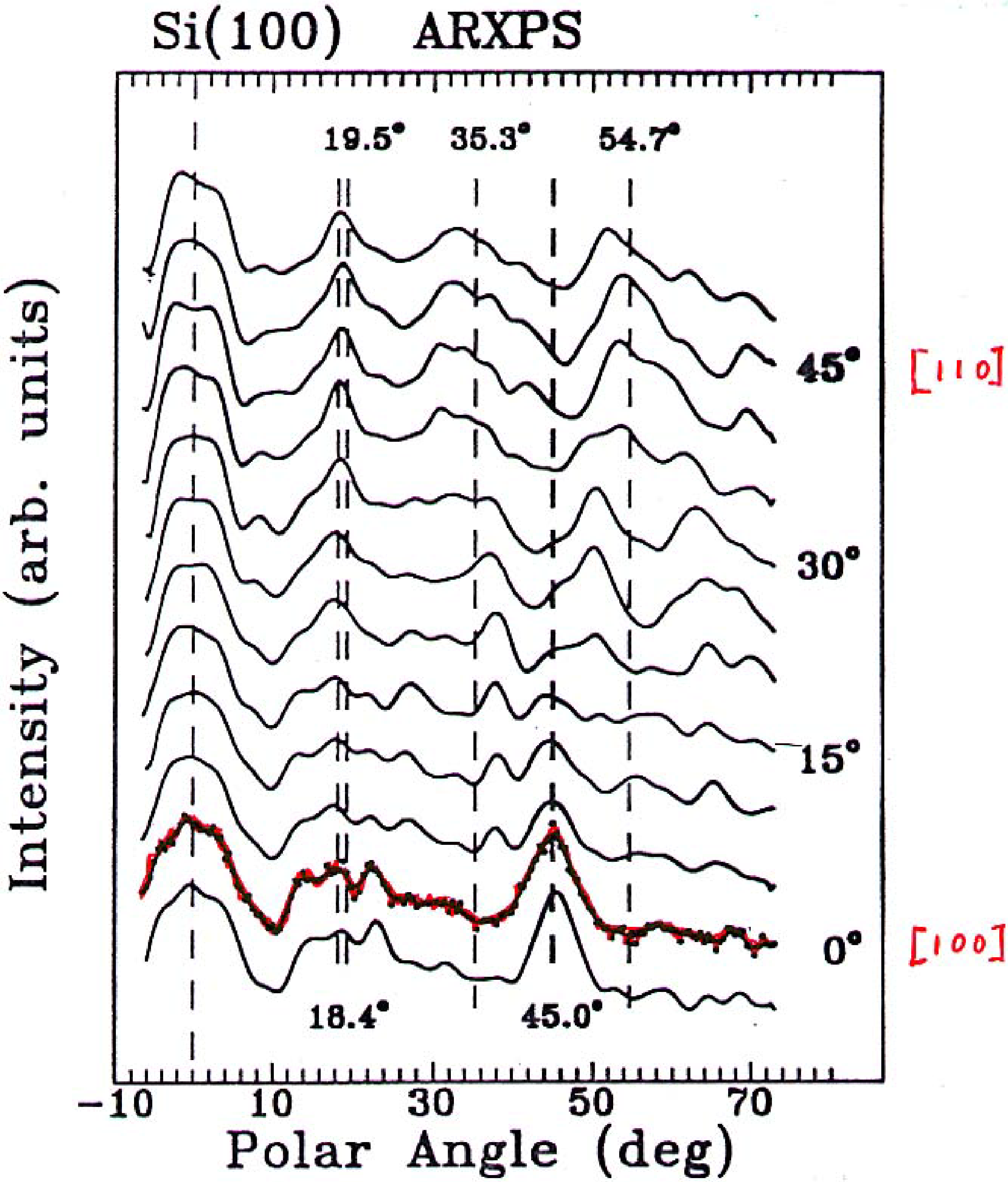


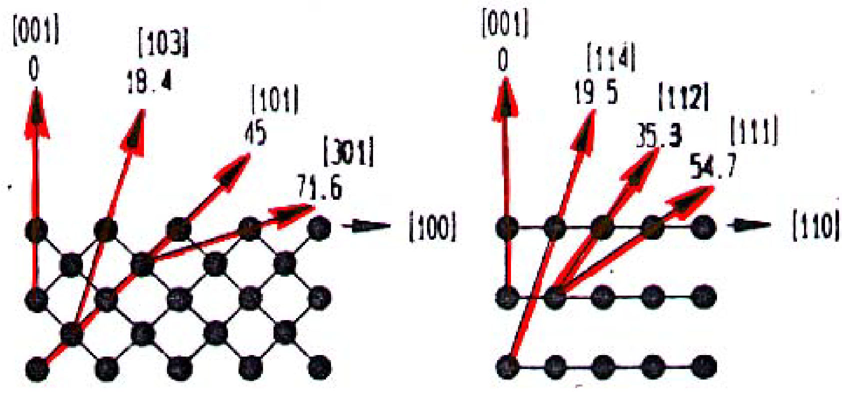
Ge 3d
Si 2p
Si 2s
XPS
0
50
100
150
200
250
300
Binding Energy (eV)



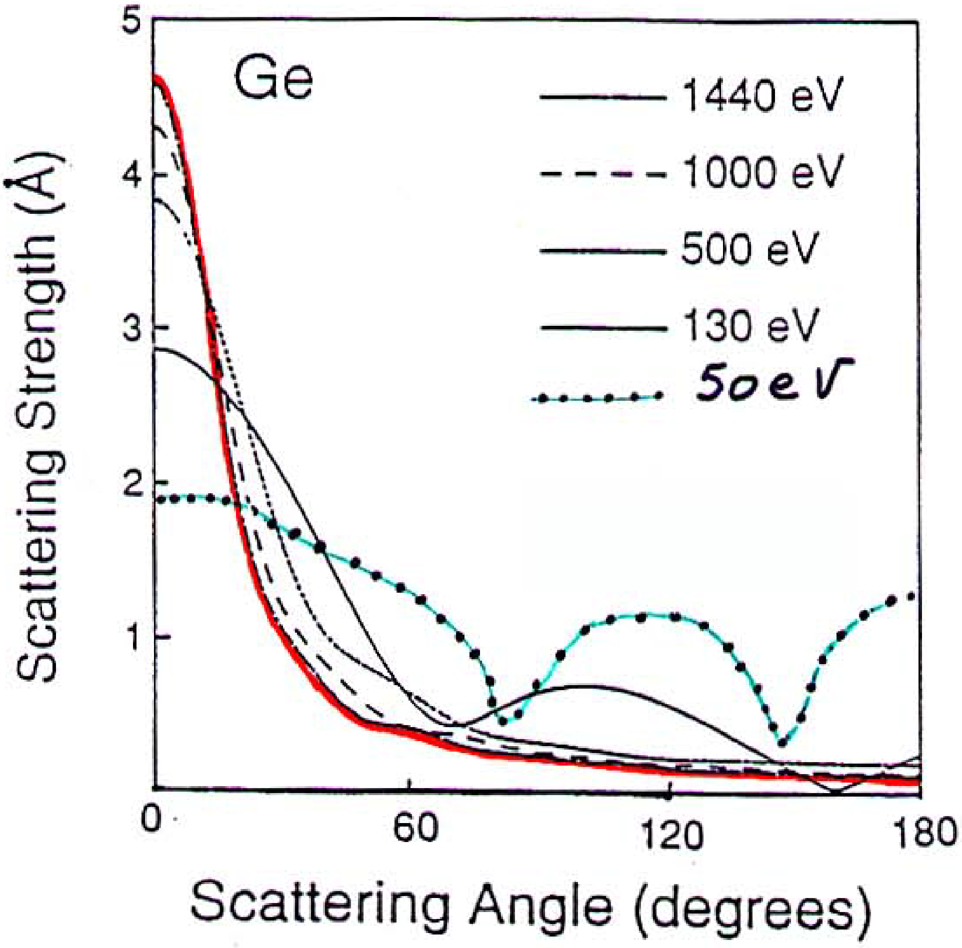
X-ray Photoelectron Spectroscopy
X-ray
e

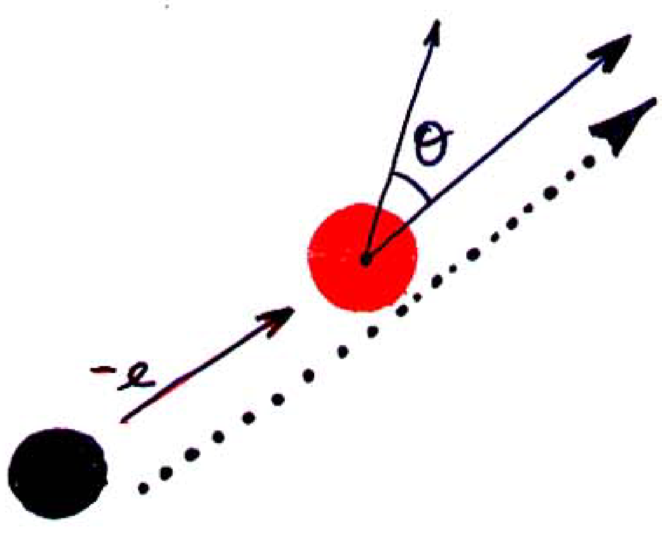

CLAM 100
Model 849 Spherical Analyser
Inlet Lens
200mm. System Flangc
Microfocus E Gun
SAMPLE
X Ray Source


Si(100) ARXPS
19.5°
35.3°
54.7°
45°
[110]
30°
15°
0°
[100]
18.4°
45.0°
−10
10
30
50
70
Polar Angle (deg)
Intensity (arb. units)

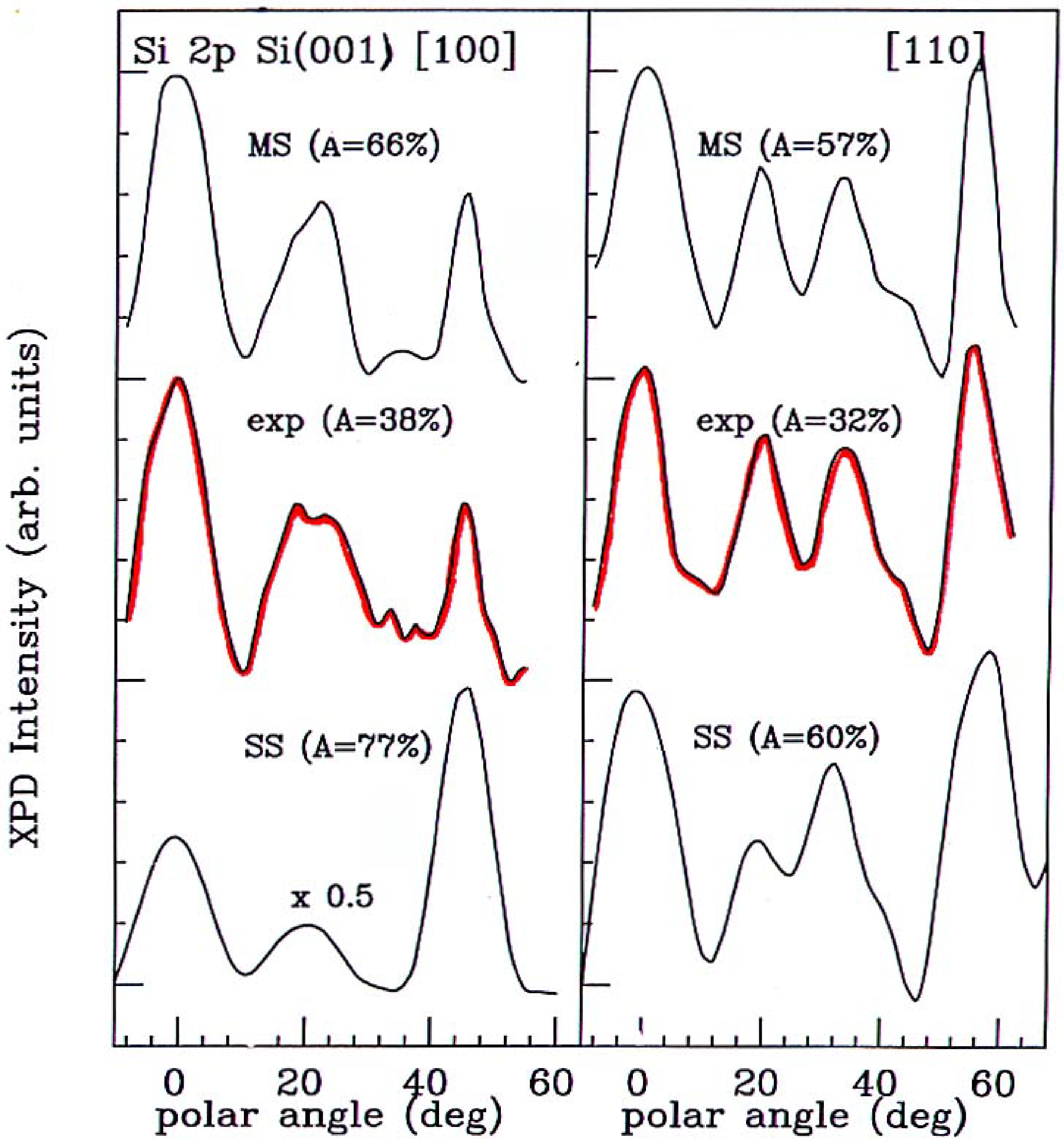

[001]
0
[103]
18.4
[101]
45
[301]
71.6
[100]
[001]
0
[114]
19.5
[112]
35.3
[111]
54.7
[110]

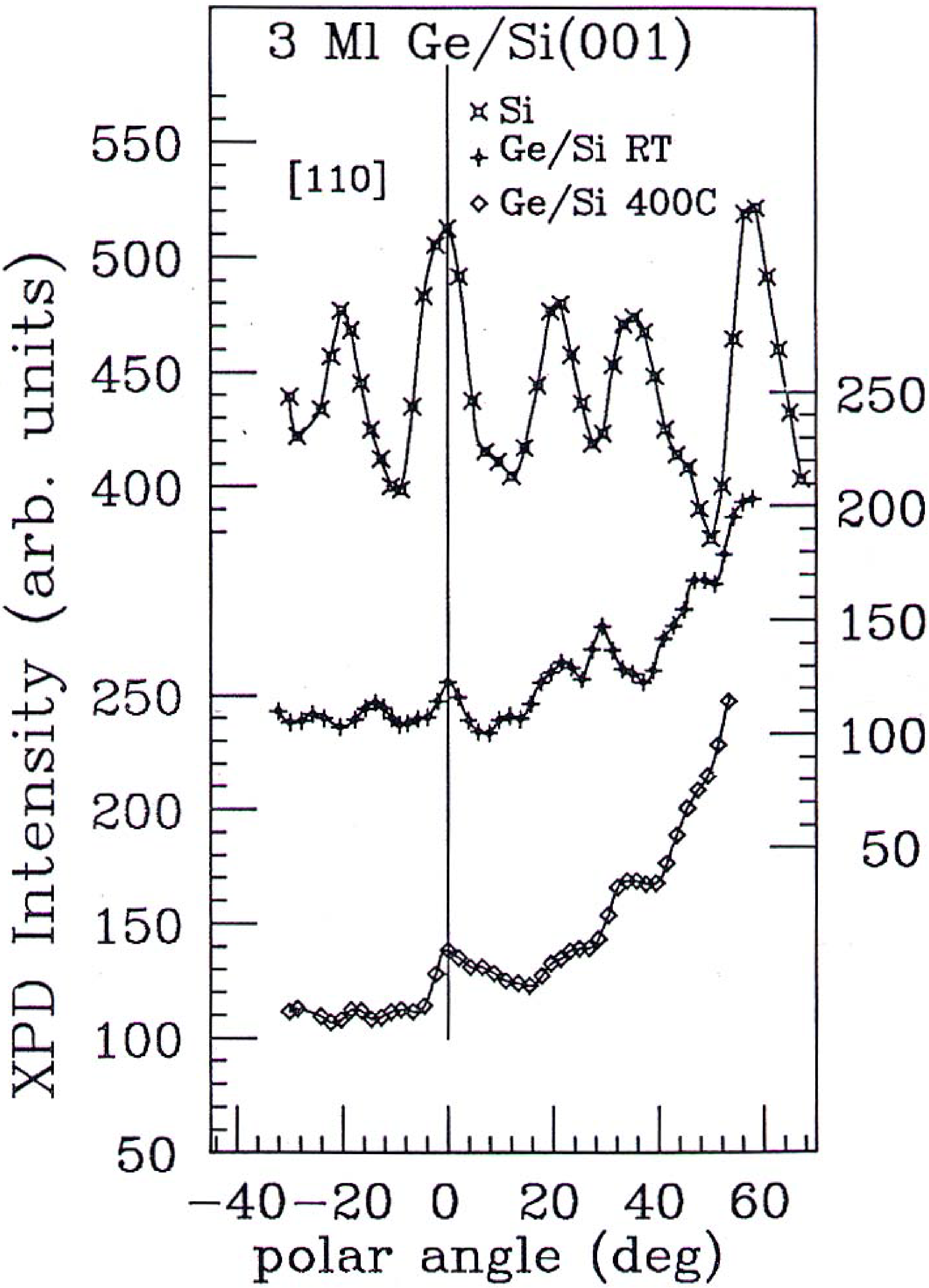
$$f(\theta) = \frac{1}{k} \sum_{0}^{\infty} (2l+1) e^{i\delta_l} P_l(\cos\theta)$$

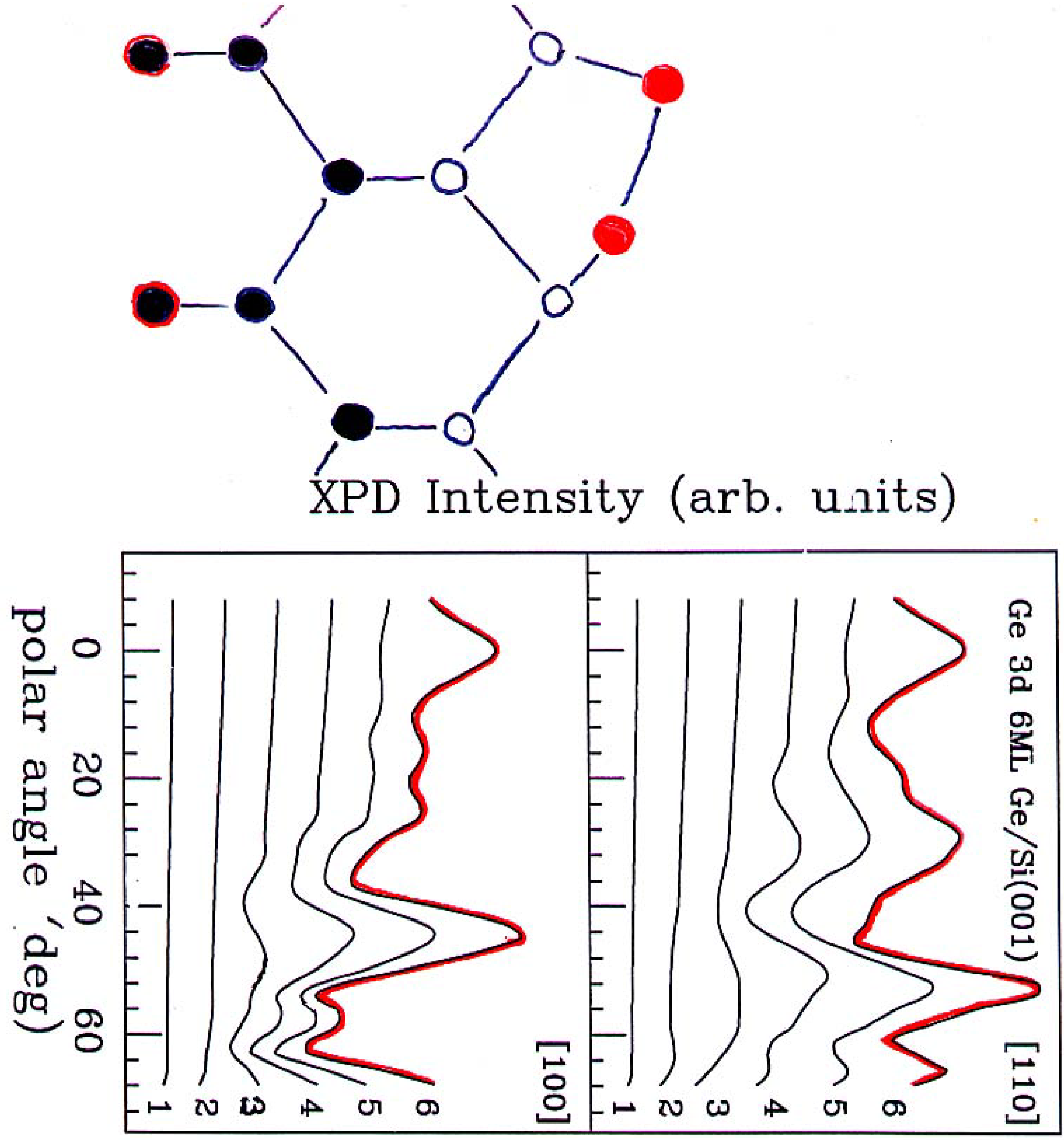




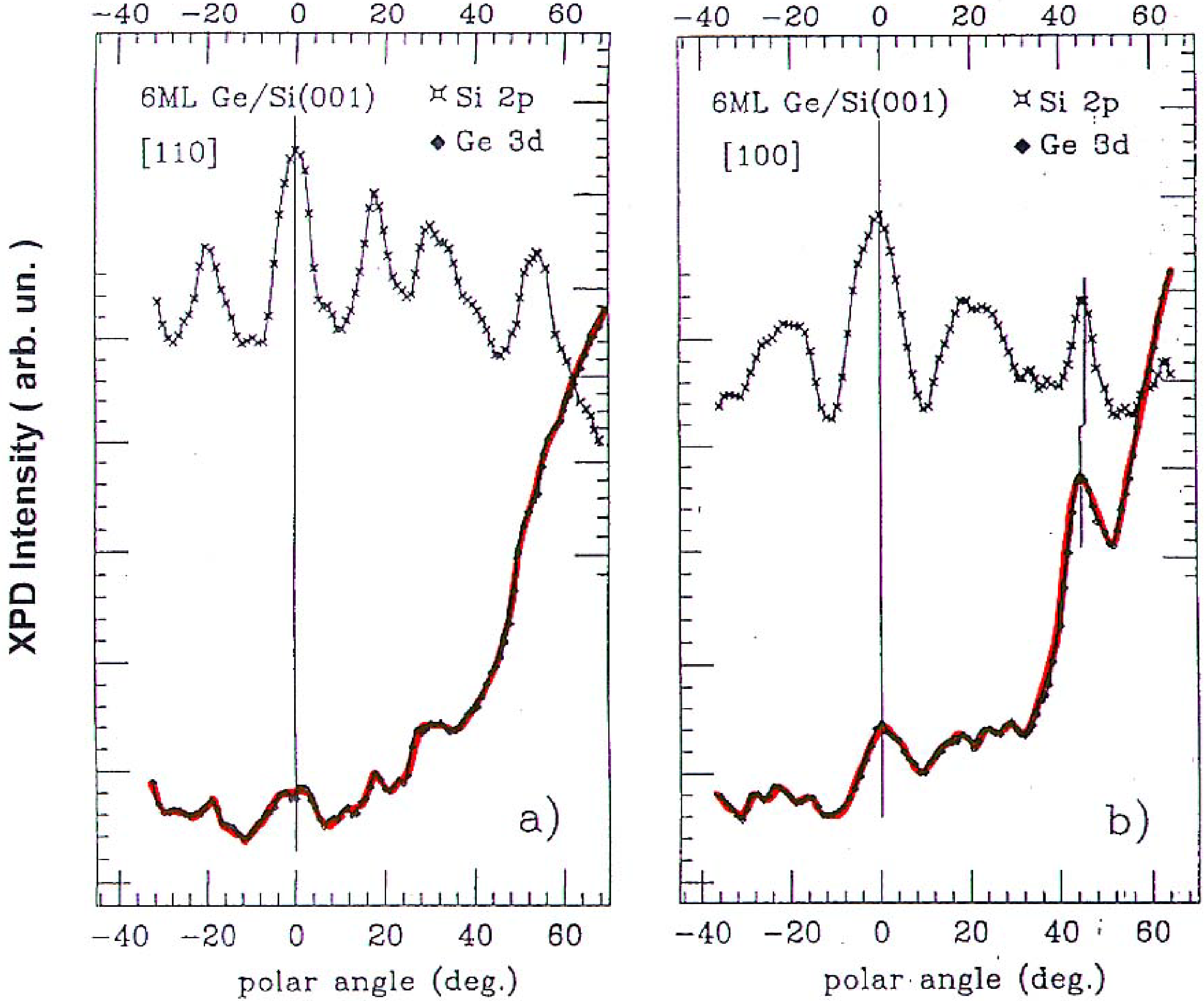
R. Gunnella et al. Fig. 2



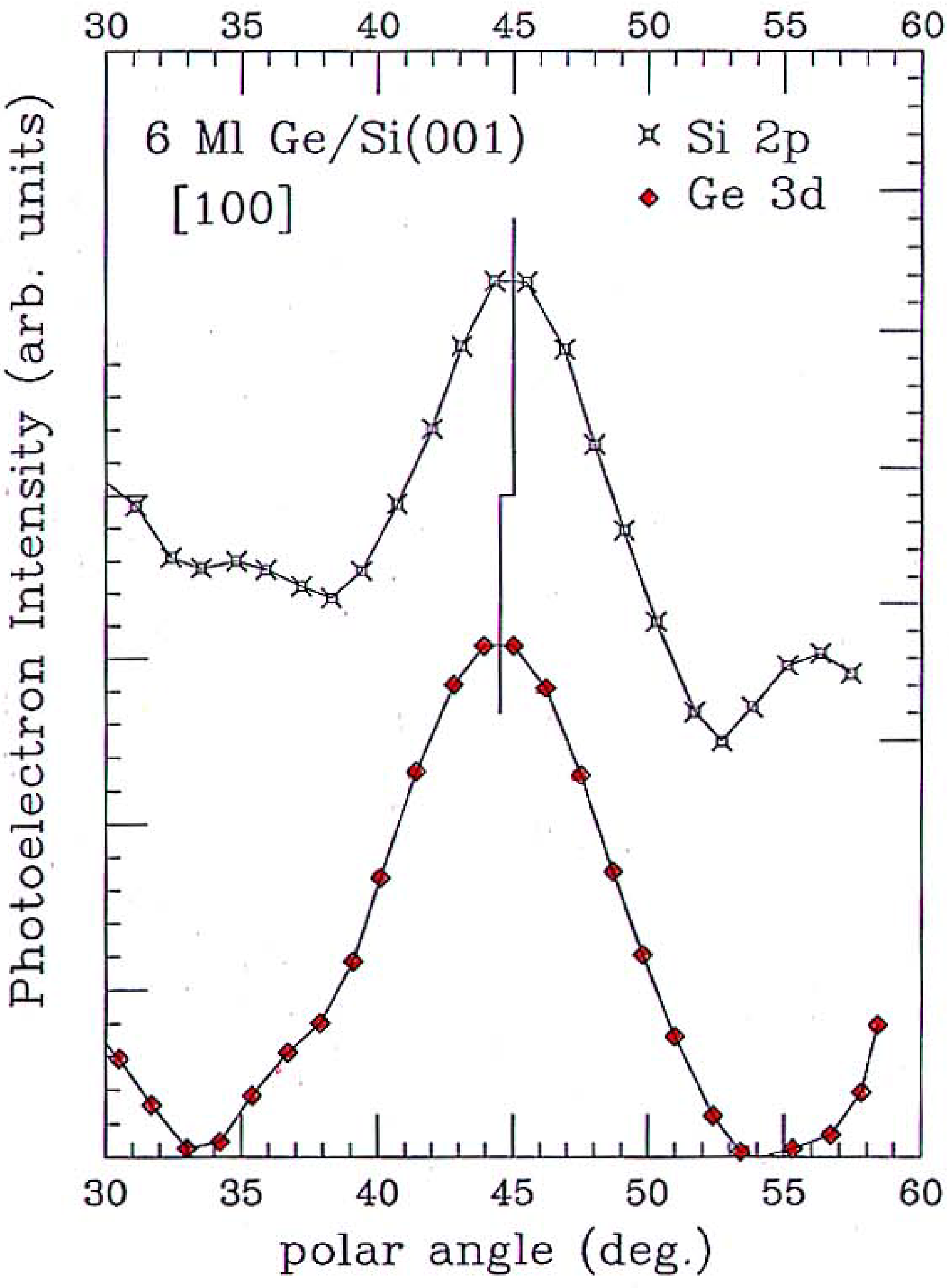

3 Ml Ge/Si(001)
Si
Ge/Si RT
Ge/Si 400C
[110]
XPD Intensity (arb. units)
polar angle (deg)
550
500
450
400
250
200
150
100
50
250
200
150
100
50
−40
−20
0
20
40
60



R. Gunnella et al. Fig. 8

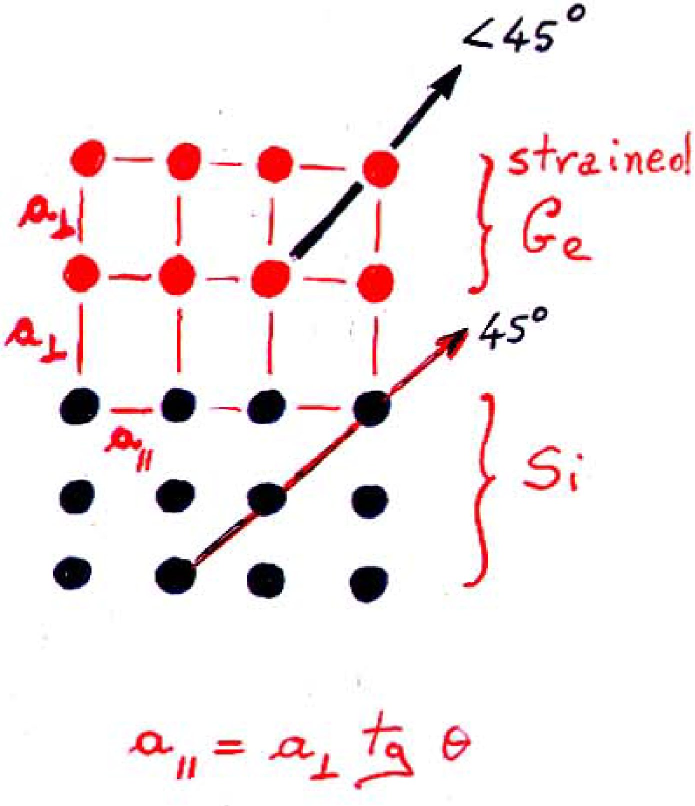


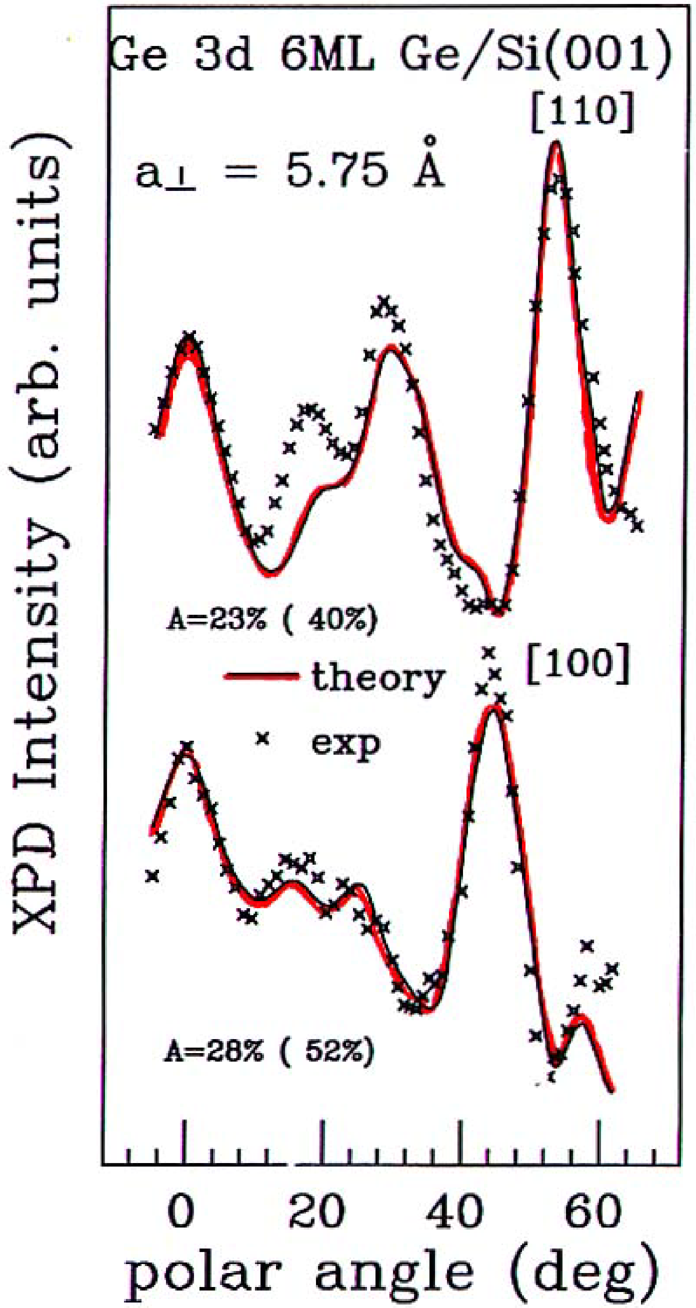
XPD Intensity (arb. un.)
6ML Ge/Si(001)
[110]
Si 2p
Ge 3d
a)
polar angle (deg.)
6ML Ge/Si(001)
[100]
Si 2p
Ge 3d
b)
polar angle (deg.)



$a(Ge) = 5.657$ Å

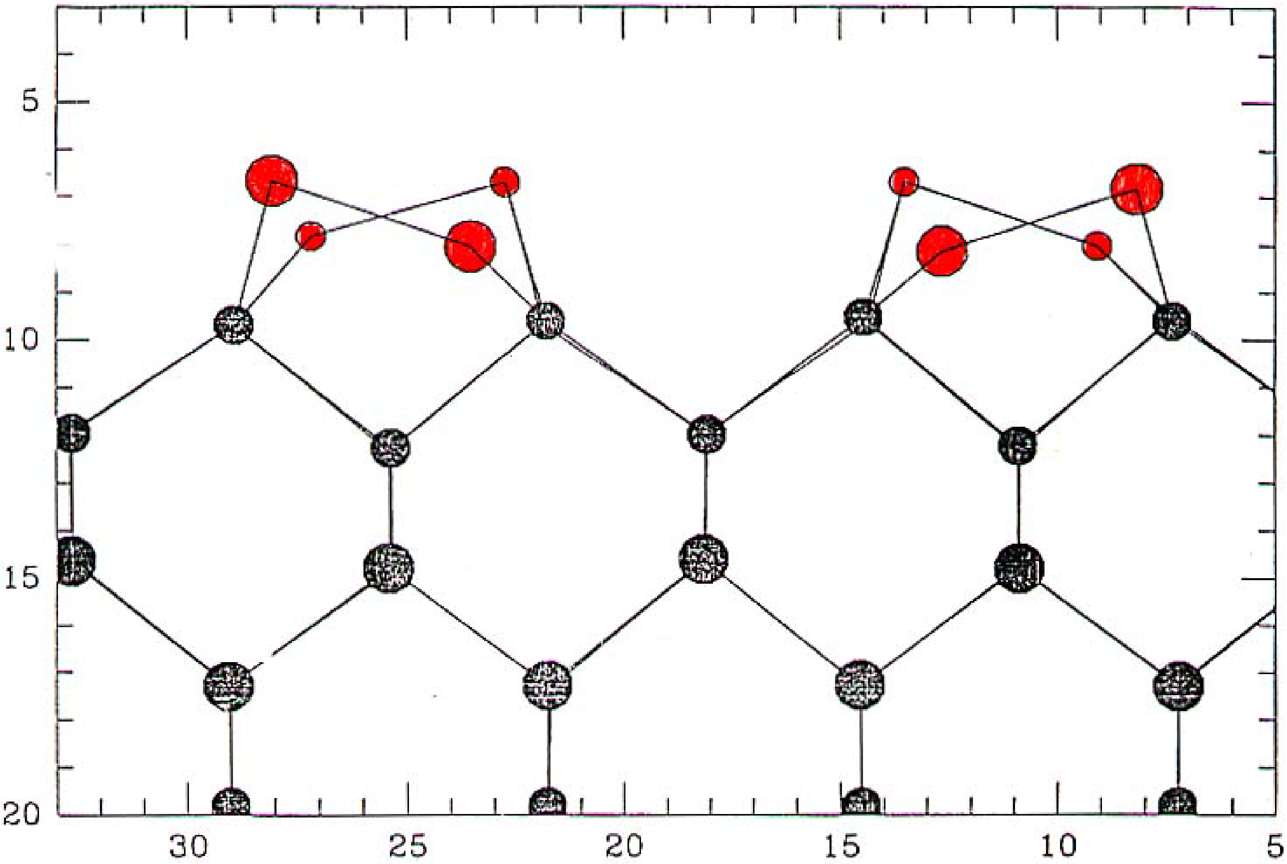
$a(Si) = 5.431$ Å

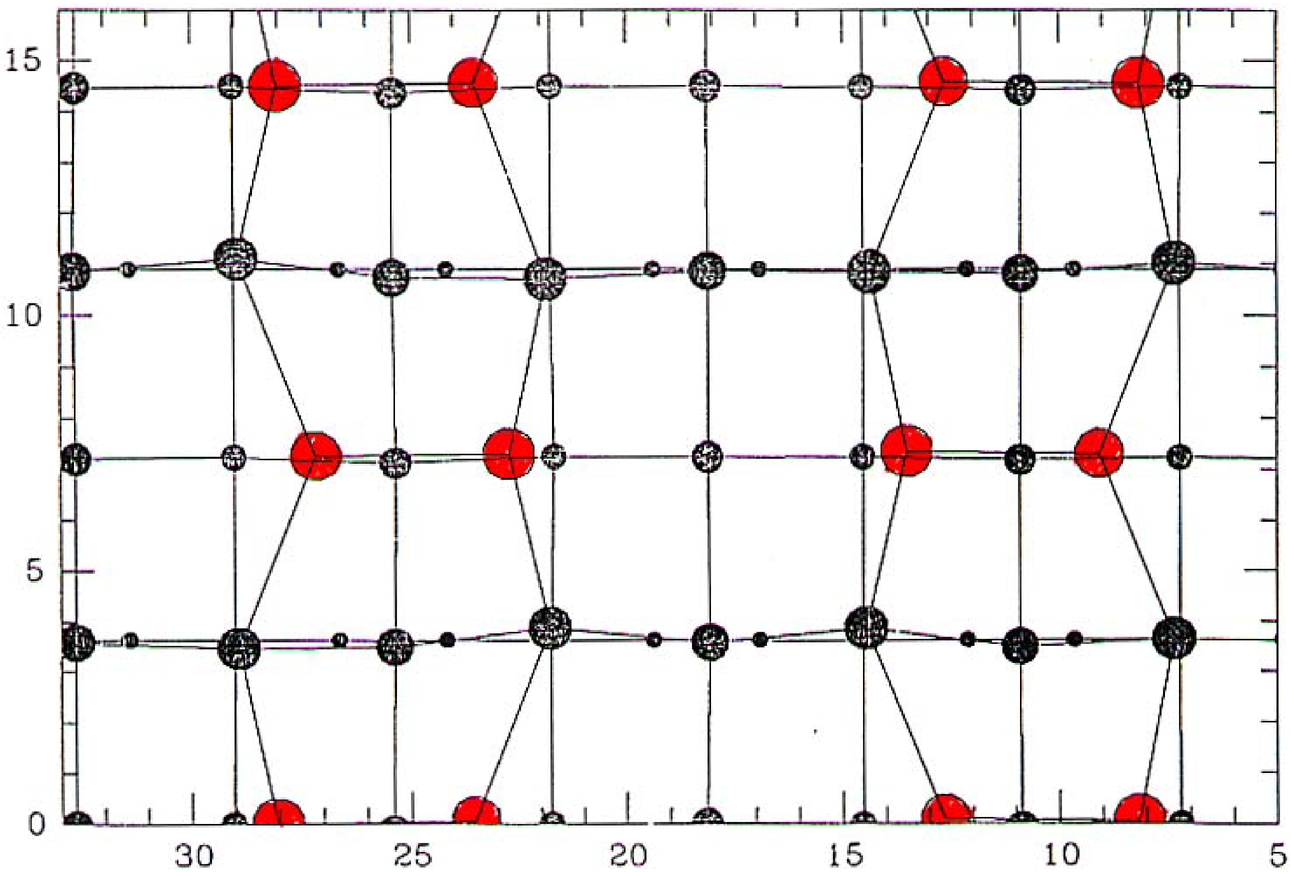




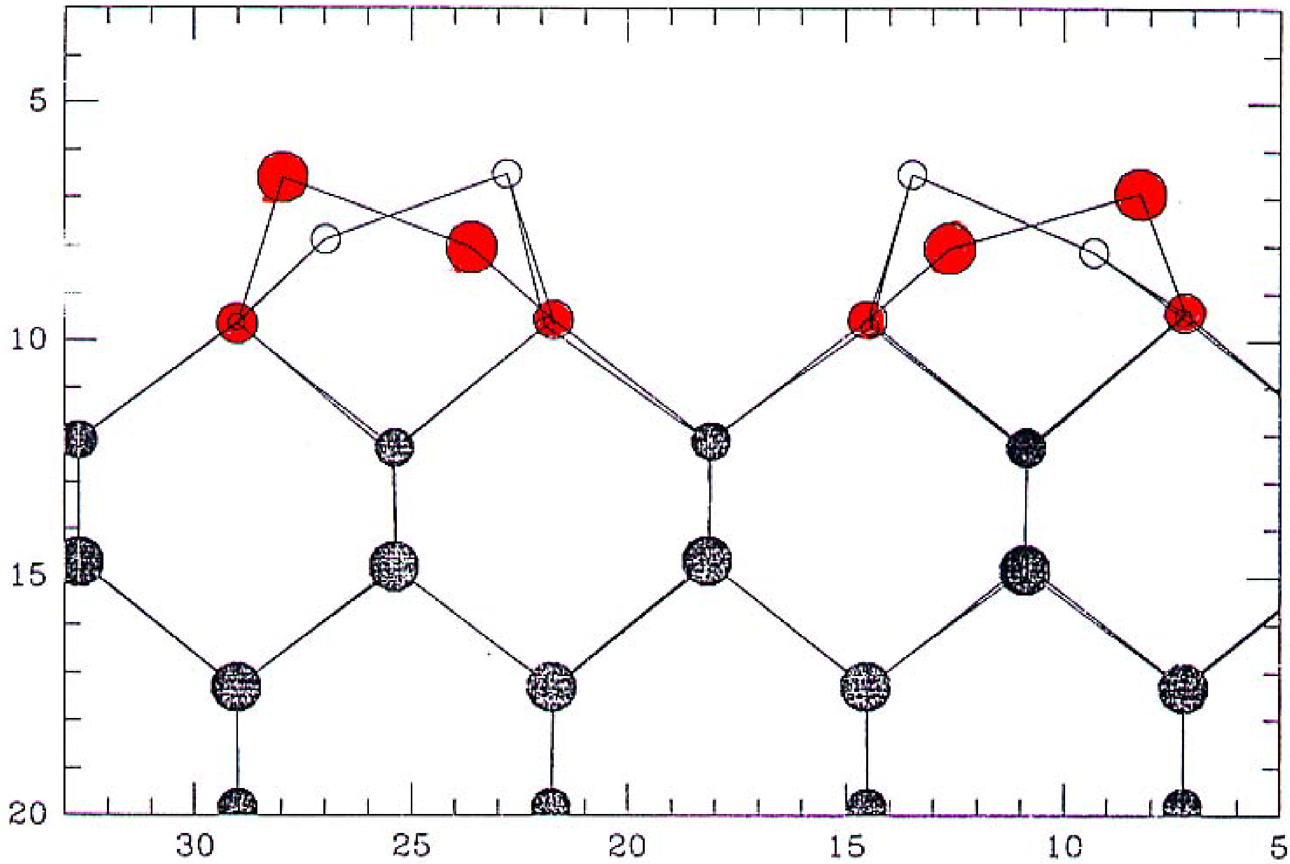
R. Gunnella et al. Fig. 9

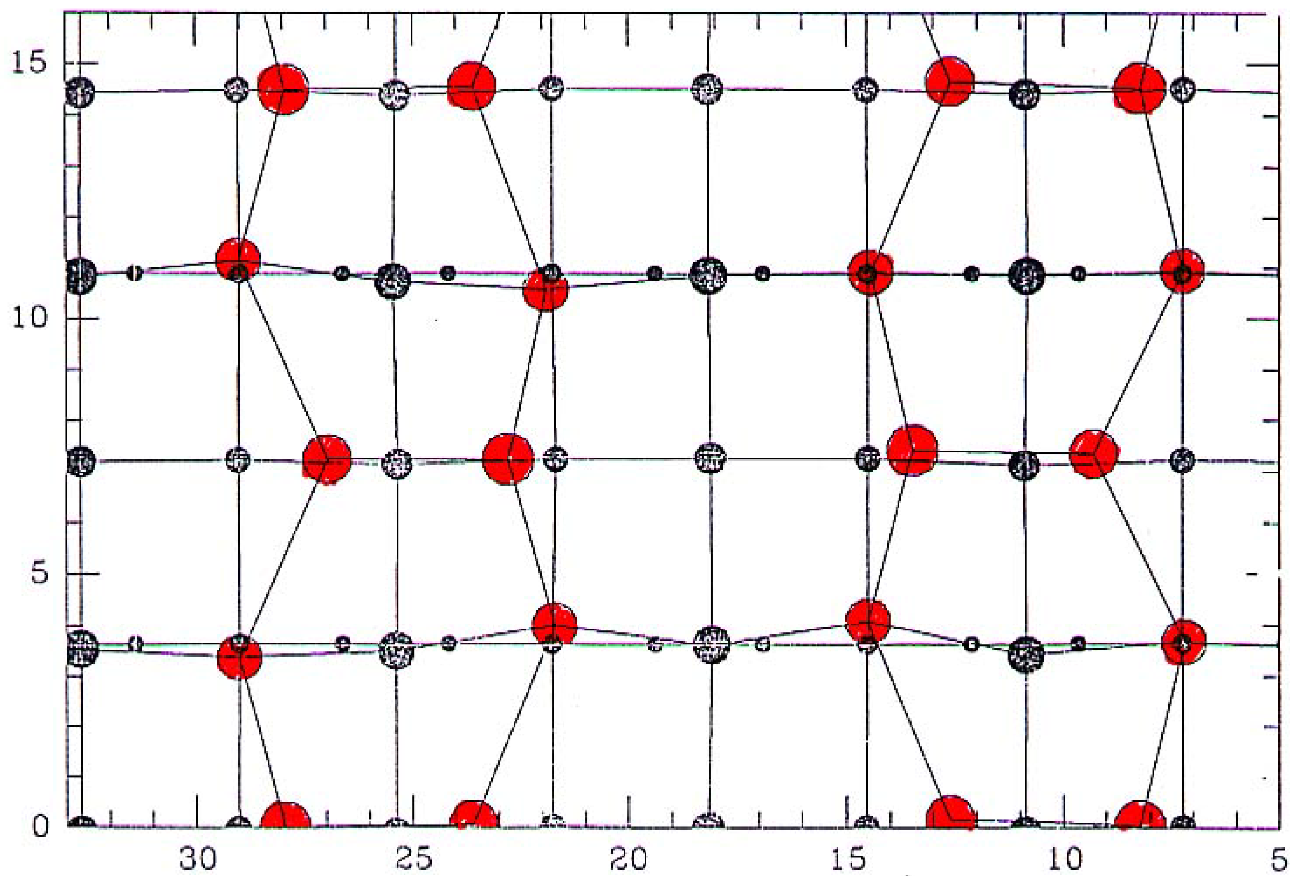
1 ML Ge/Si(100)



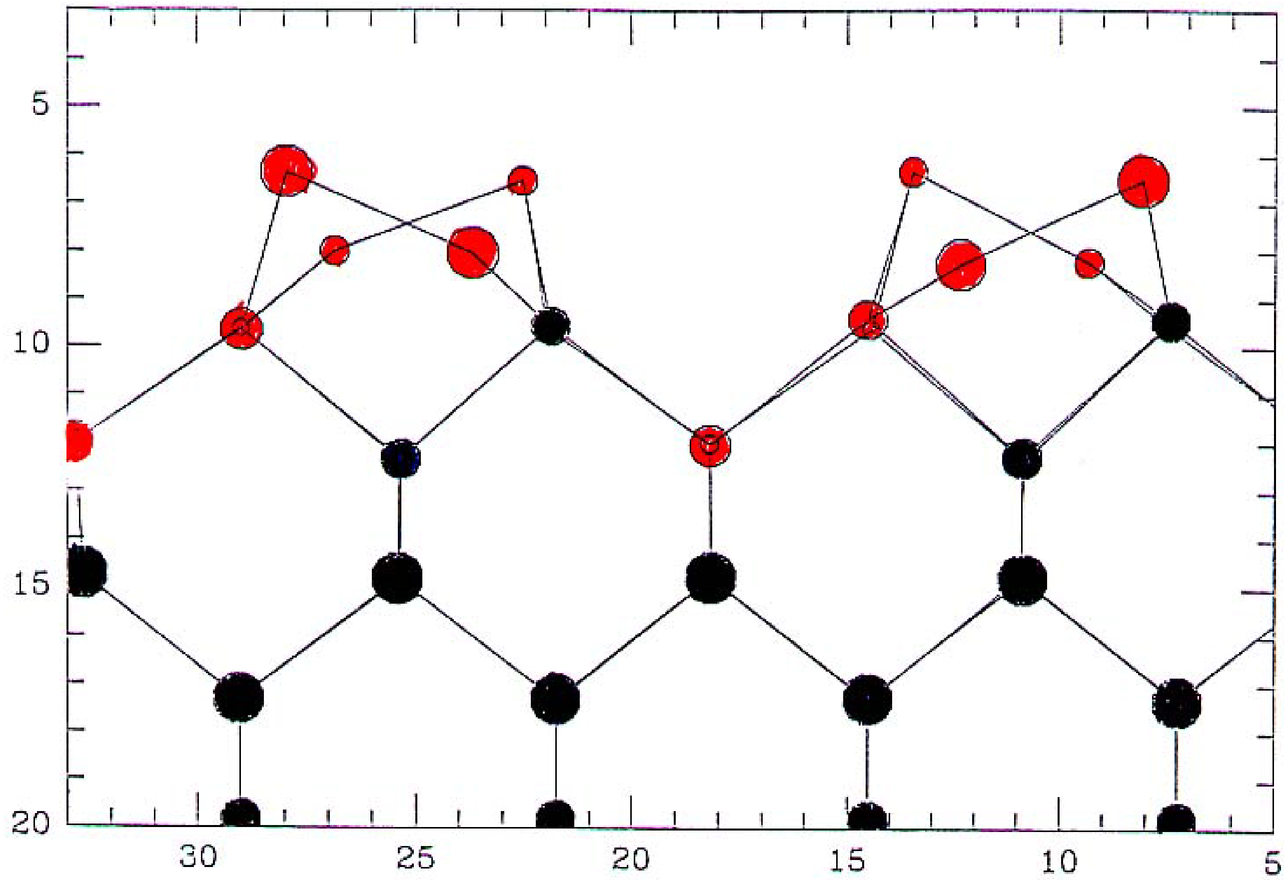


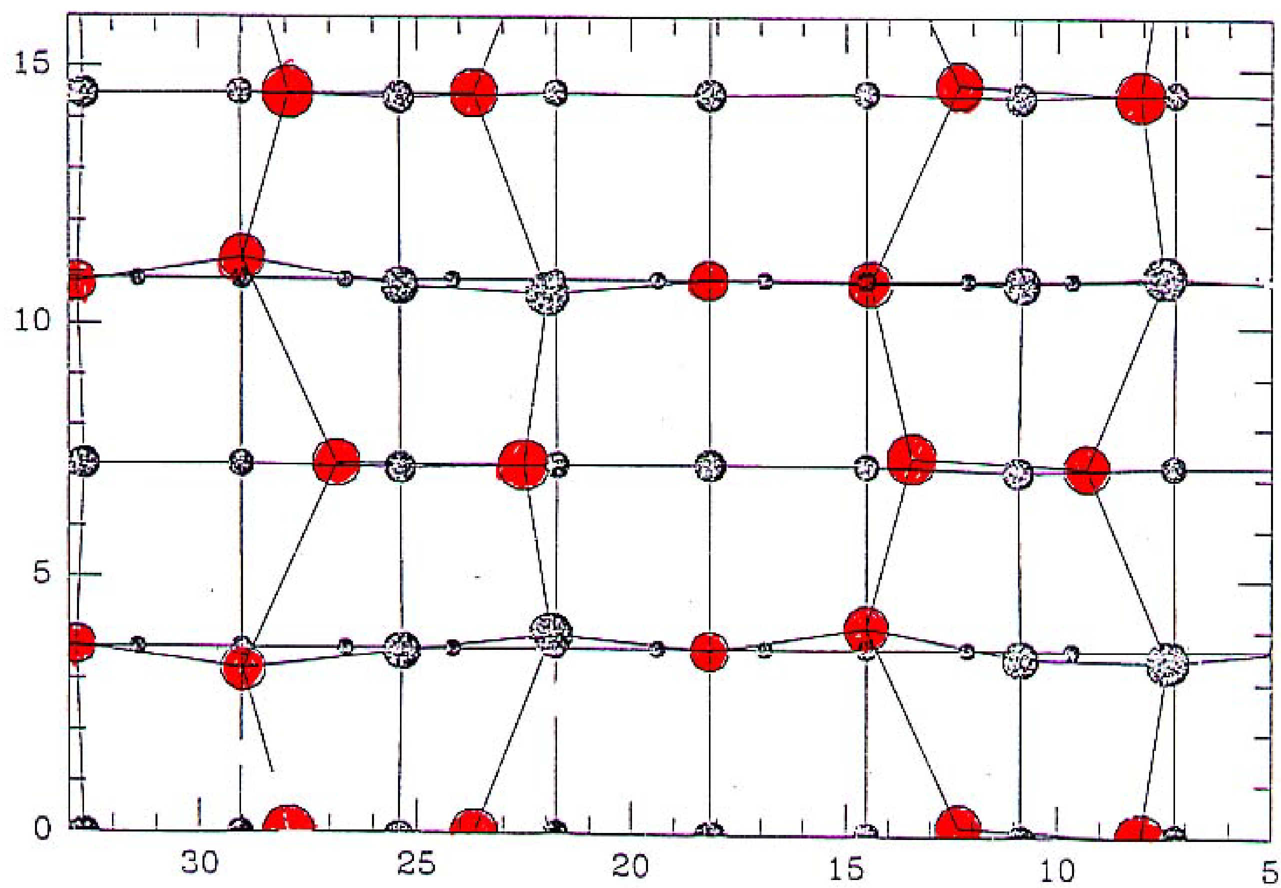
Ge 2 Monolayers / Si (100)

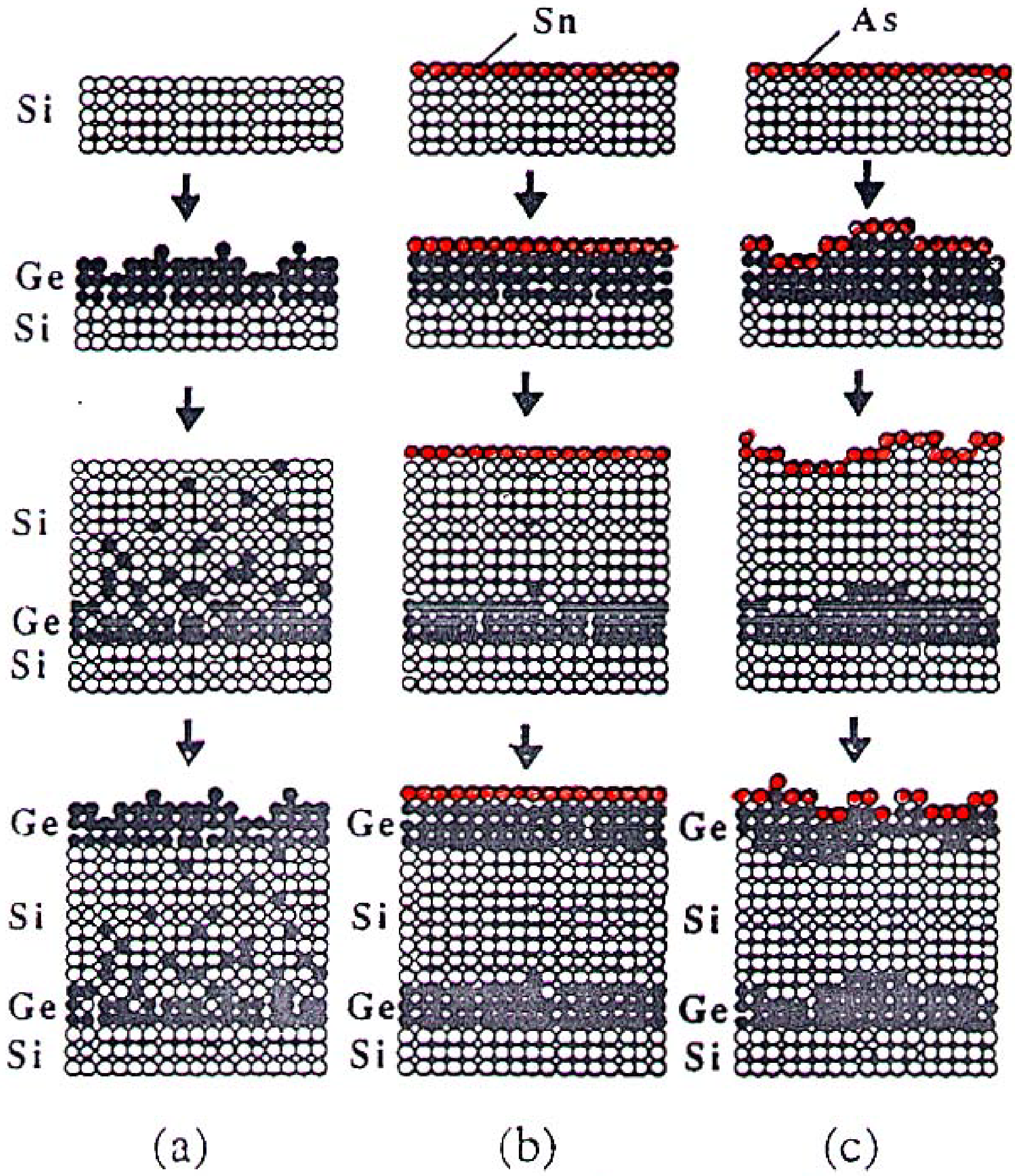




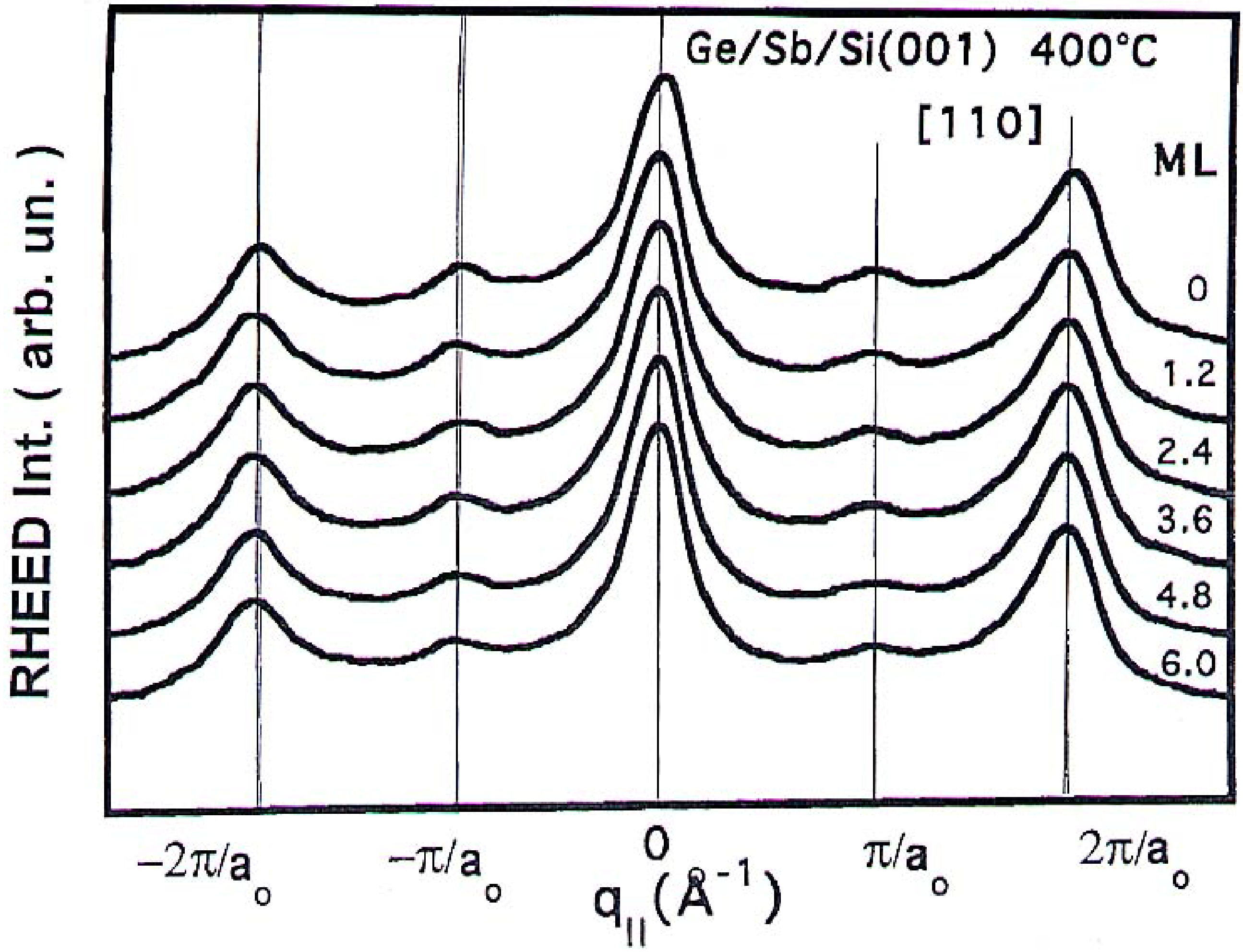
02-05-95 comb_mix_2_n.out, → comb_ge2_si4_new_mix.dat







surfactant
effect



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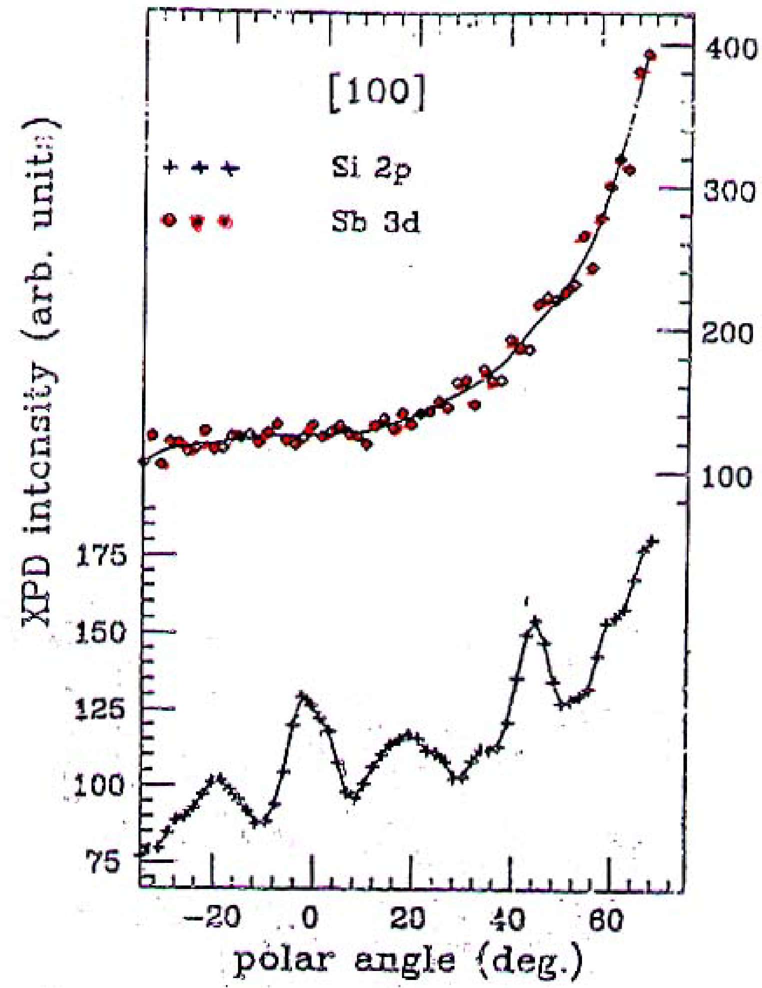
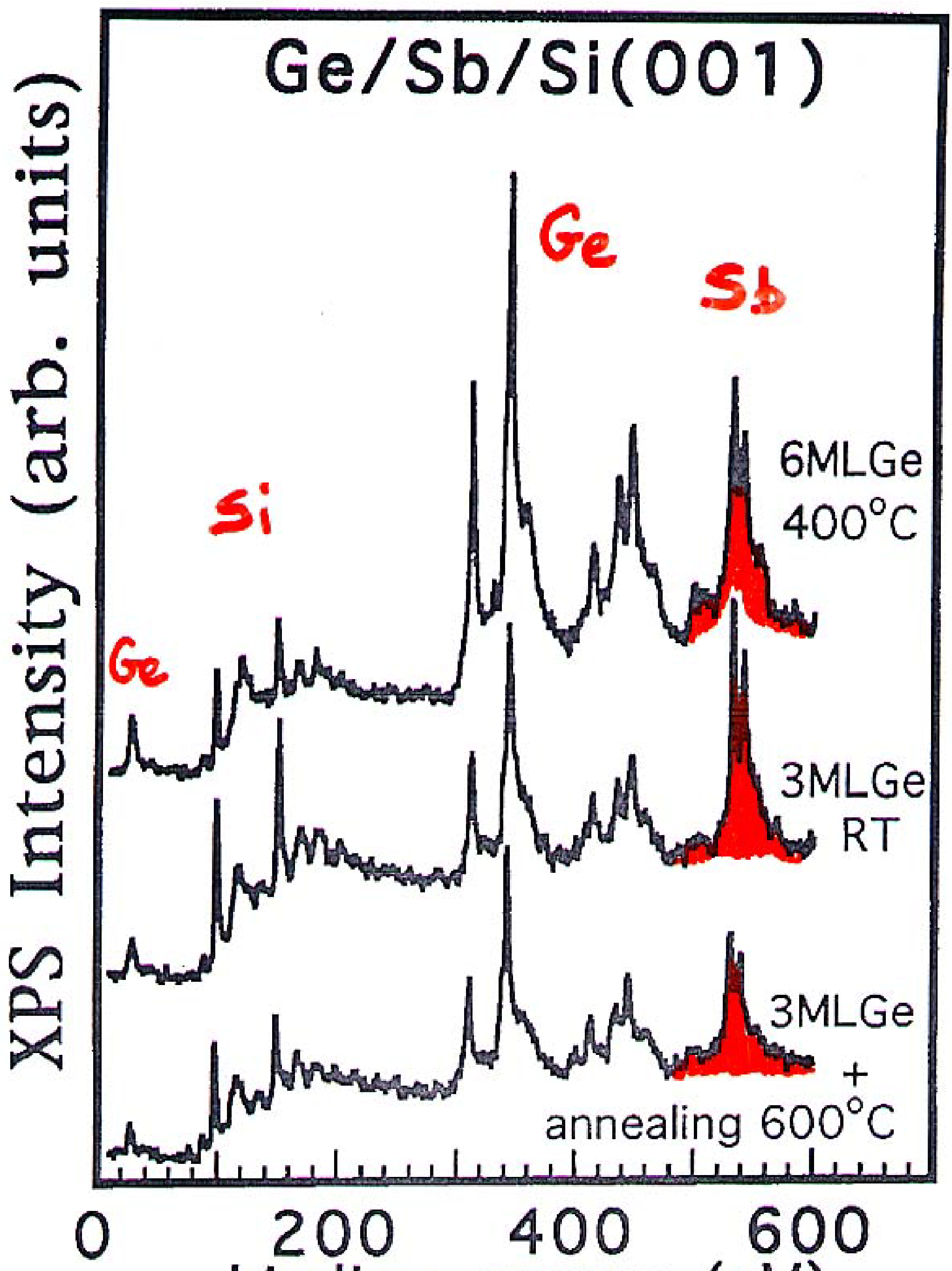
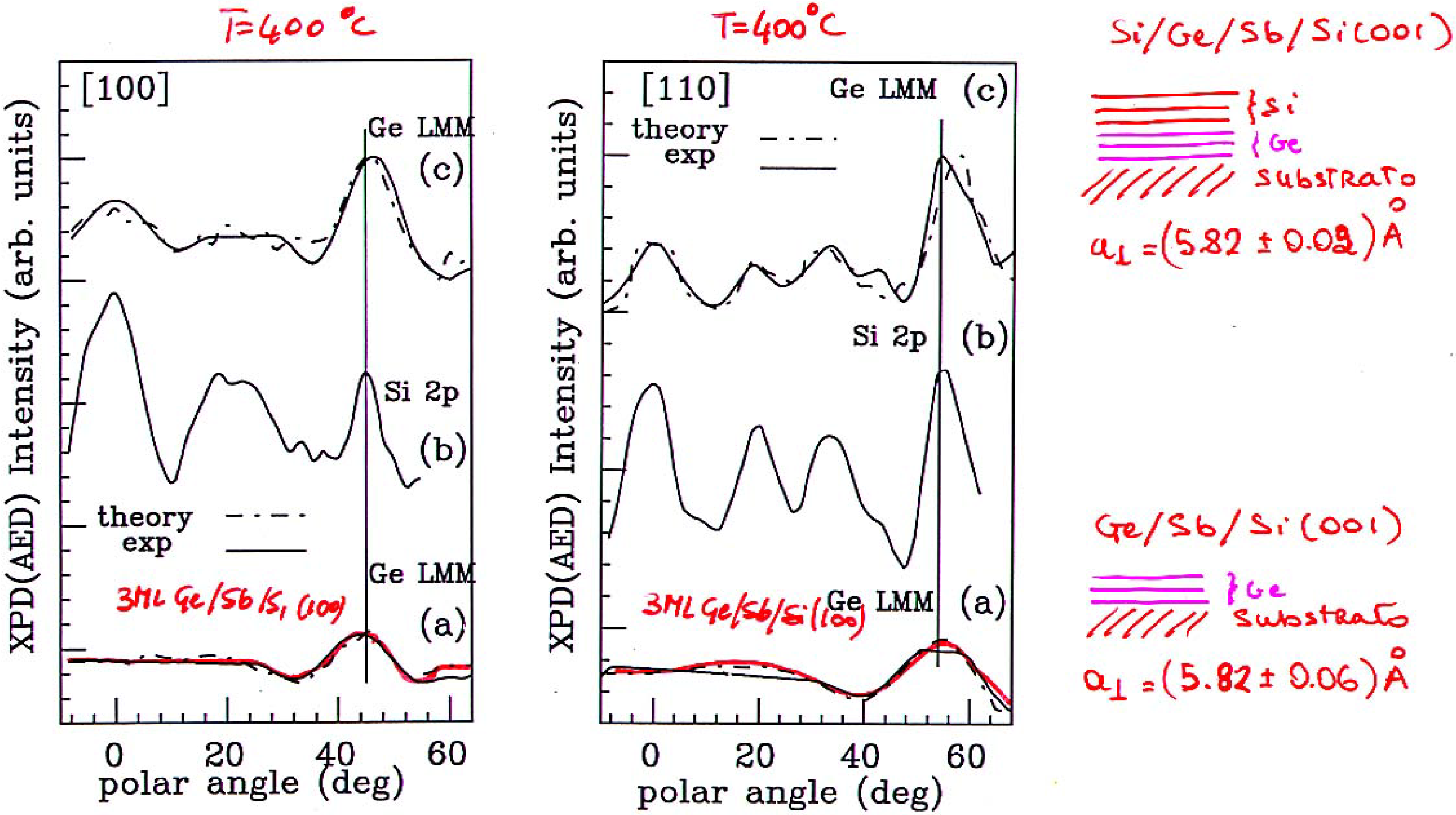
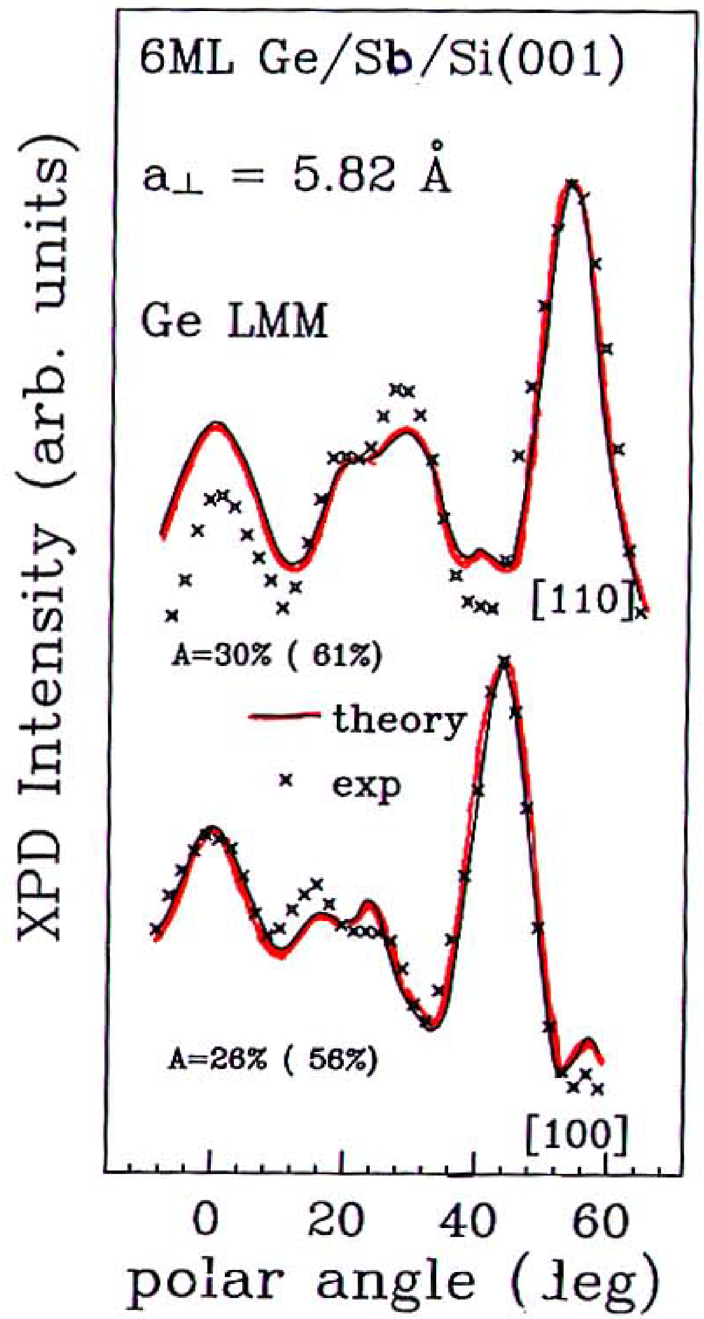


Fig. 1. XPD of 1 ML Sb/Si(001). The top curve represents the instrumental response of the apparatus only as no diffraction features can be observed on the polar diagram of Sb 3d. In the lower curve is reported the diagram of the Si 2p. The direction of emission is the [100].

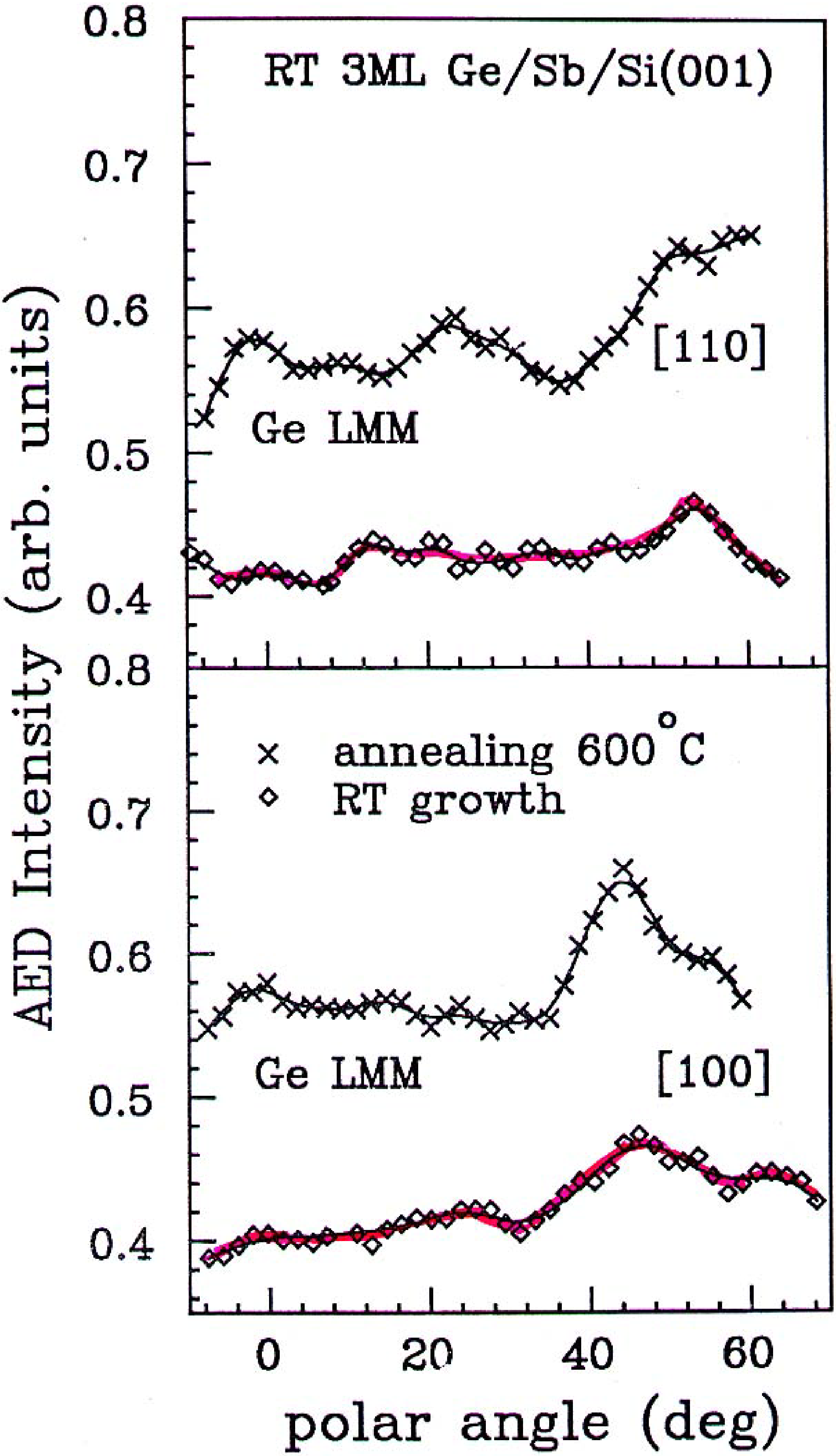


Ge/Sb/Si(001)
XPS Intensity (arb. units)
Ge
Sb
Si
Ge
6MLGe
400°C
3MLGe
RT
3MLGe
+
annealing 600°C
0
200
400
600
binding energy (eV)

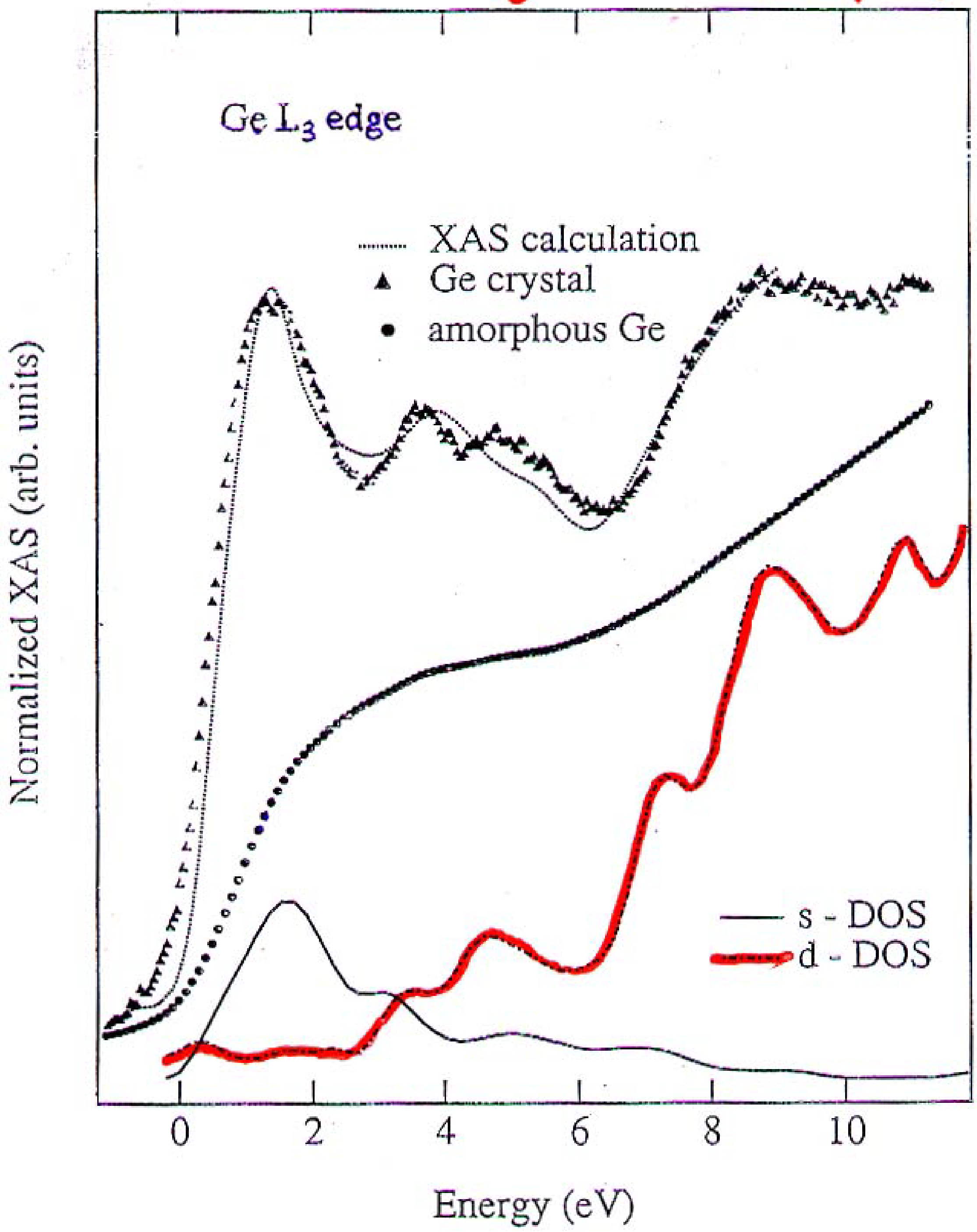

T=400 °C
[100]
Ge LMM
(c)
Si 2p
(b)
theory
exp
Ge LMM
3ML Ge/Sb/Si (100)
(a)
XPD(AED) Intensity (arb. units)
0
20
40
60
polar angle (deg)
T=400°C
[110]
Ge LMM
(c)
theory
exp
Si 2p
(b)
3ML Ge/Sb/Si (100)
Ge LMM
(a)
XPD(AED) Intensity (arb. units)
0
20
40
60
polar angle (deg)
Si/Ge/Sb/Si(001)
Si
Ge
substrato
a⊥ = (5.82 ± 0.02) Å
Ge/Sb/Si(001)
Ge
substrato
a⊥ = (5.82 ± 0.06) Å

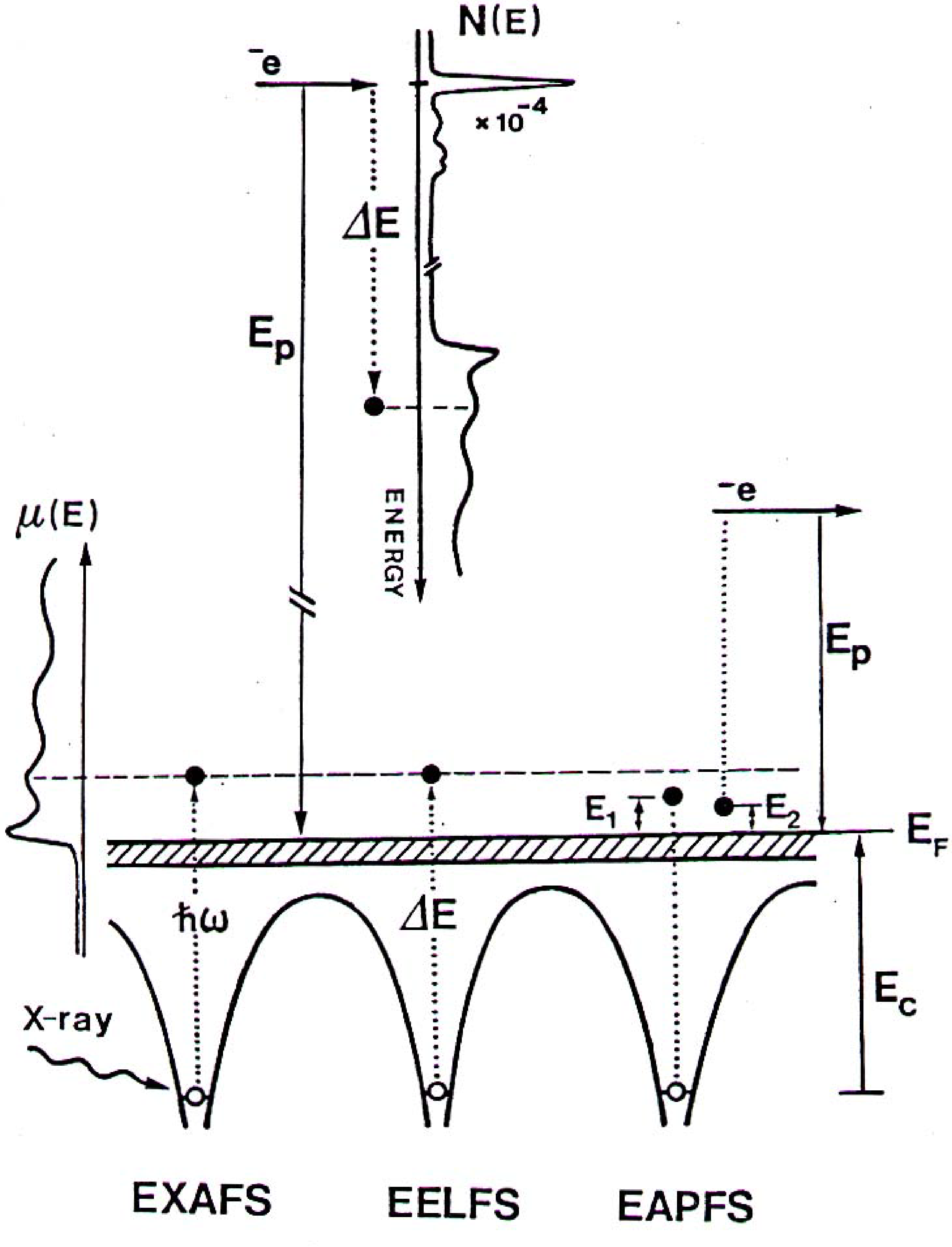


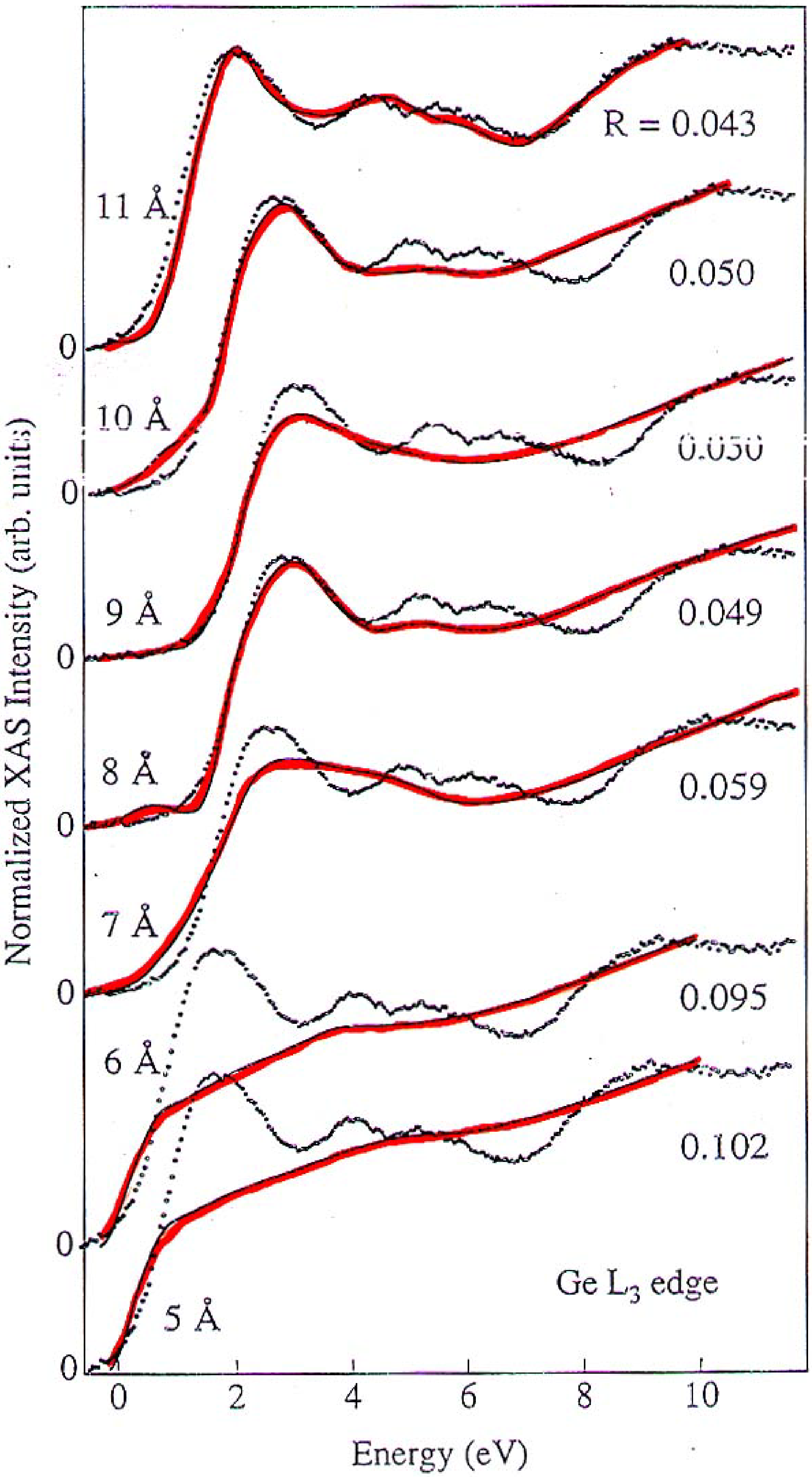
R. Gunnella et al. Fig. 14


RT 3ML Ge/Sb/Si(001)
[110]
Ge LMM
annealing 600°C
RT growth
Ge LMM
[100]
AED Intensity (arb. units)
polar angle (deg)
0.8
0.7
0.6
0.5
0.4
0.8
0.7
0.6
0.5
0.4
0
20
40
60

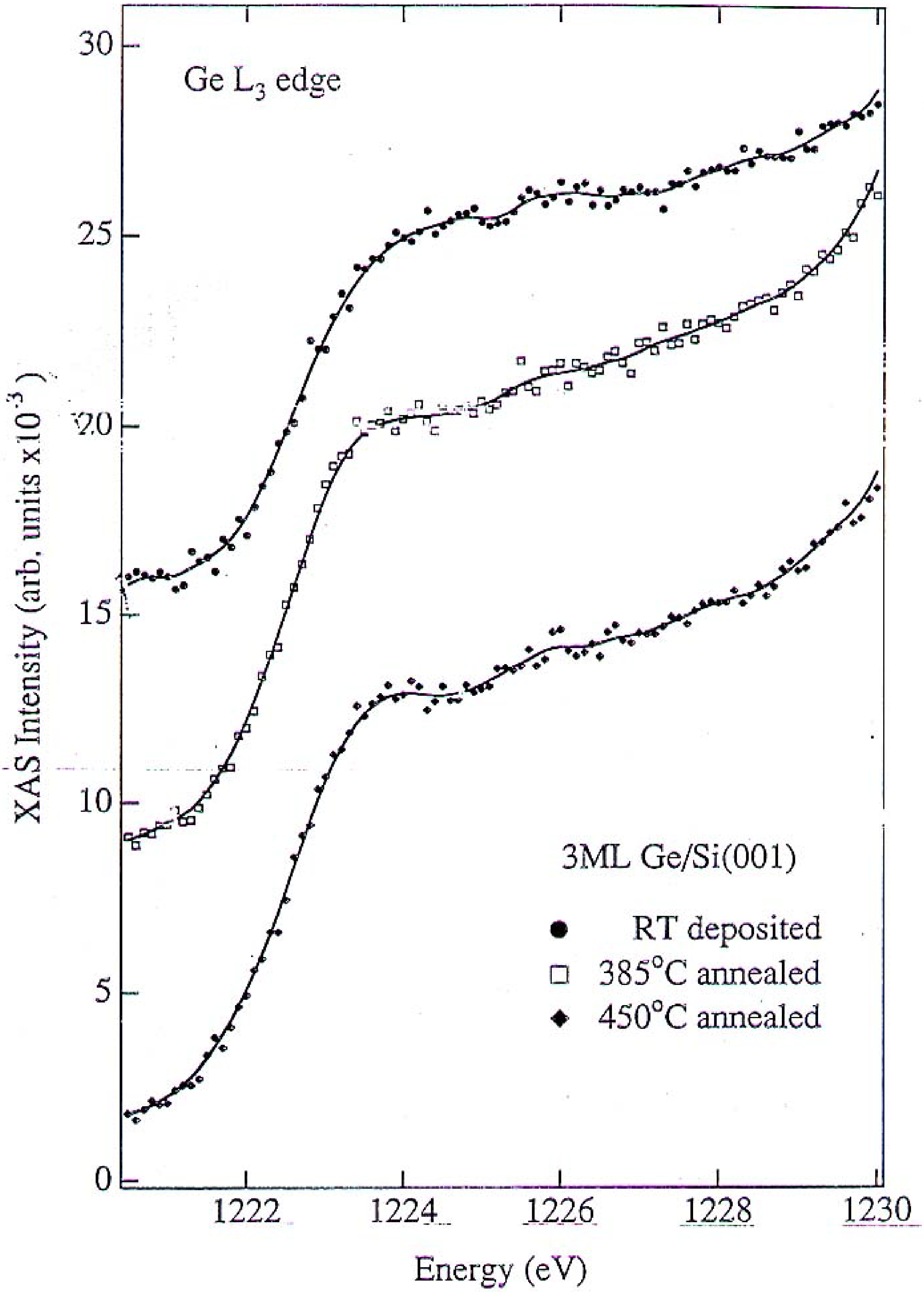
P. Castrucci et al. - Surf. Sci. 416 (1998) 466
- Phys. Rev. B 58 (98) 4095
- Phys. Rev. B 60 (99) 5759



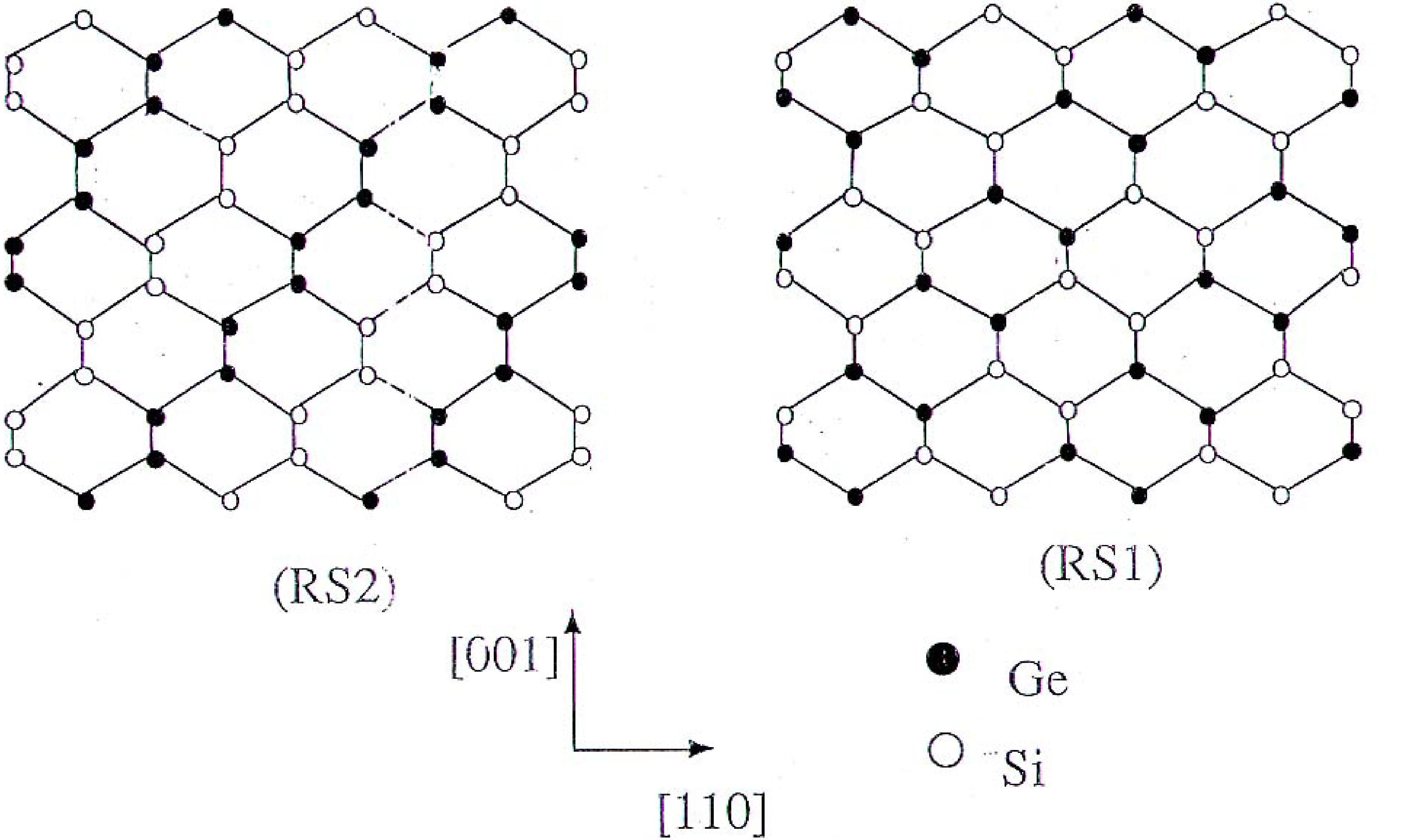

N(E)
⁻e
× 10⁻⁴
ΔE
Eₚ
ENERGY
μ(E)
⁻e
Eₚ
E₁
E₂
E_F
ħω
ΔE
E_c
X-ray
EXAFS
EELFS
EAPFS

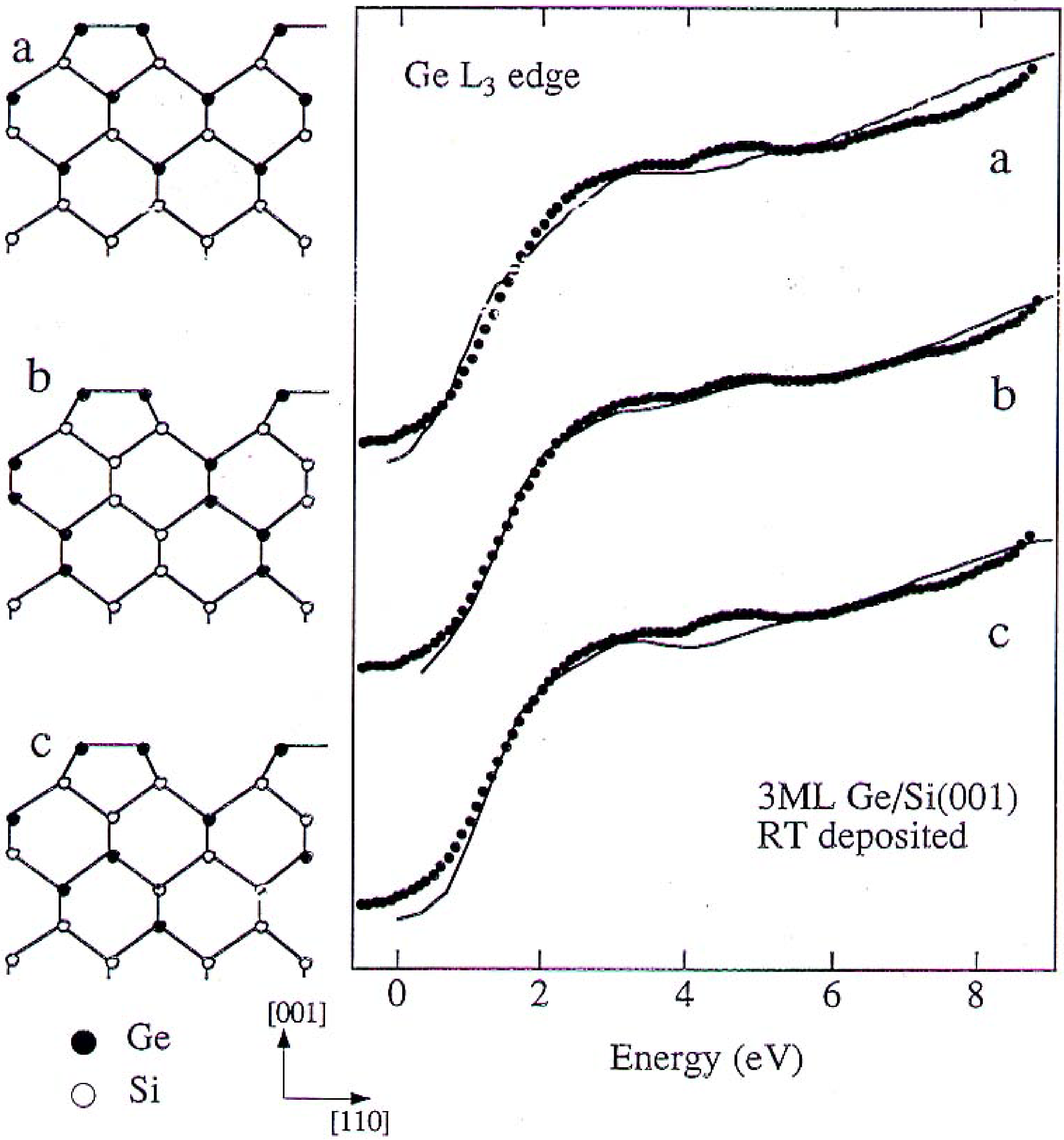


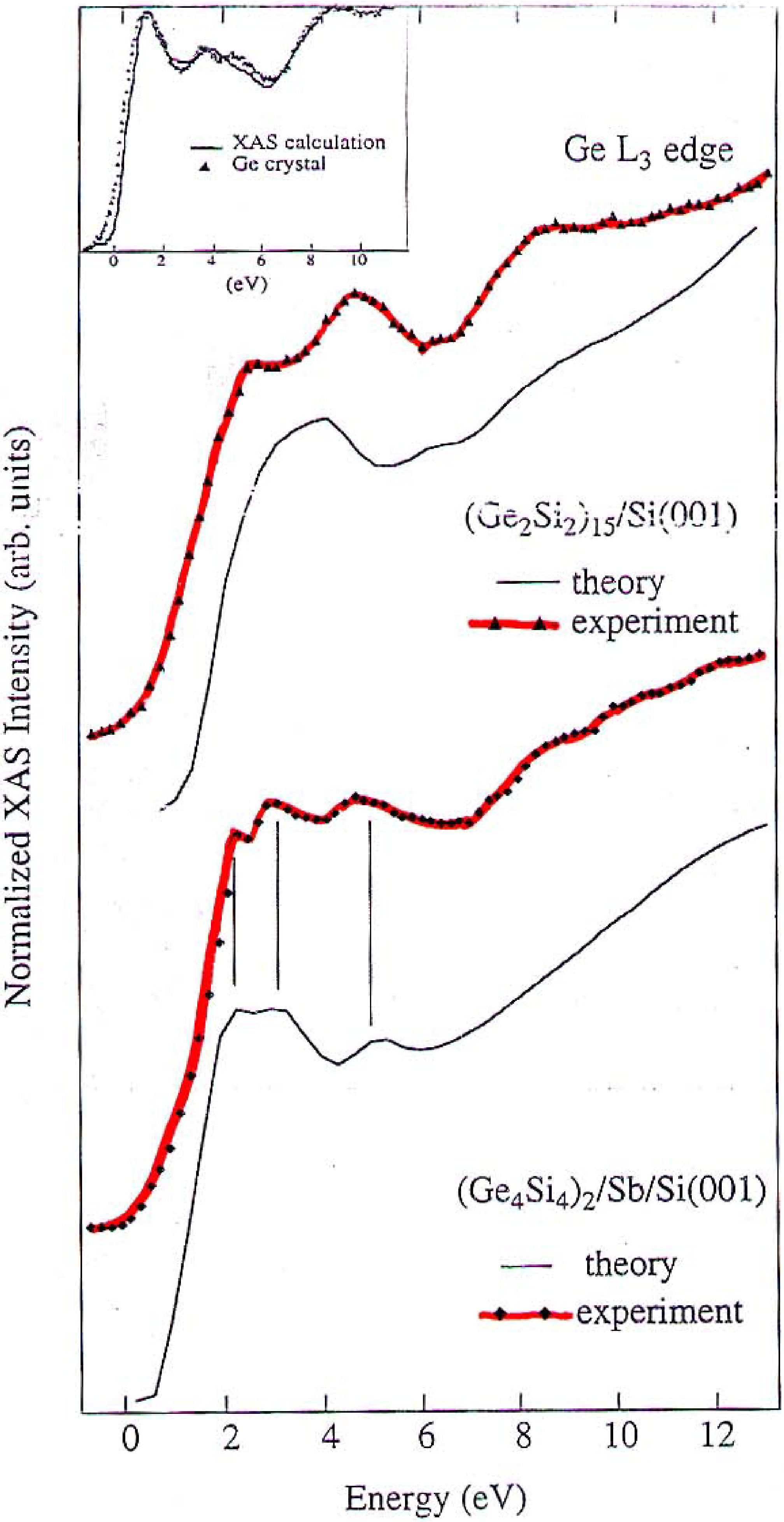
Normalized XAS Intensity (arb. units)
Energy (eV)
R = 0.043
0.050
0.050
0.049
0.059
0.095
0.102
11 Å
10 Å
9 Å
8 Å
7 Å
6 Å
5 Å
Ge L3 edge
0
2
4
6
8
10



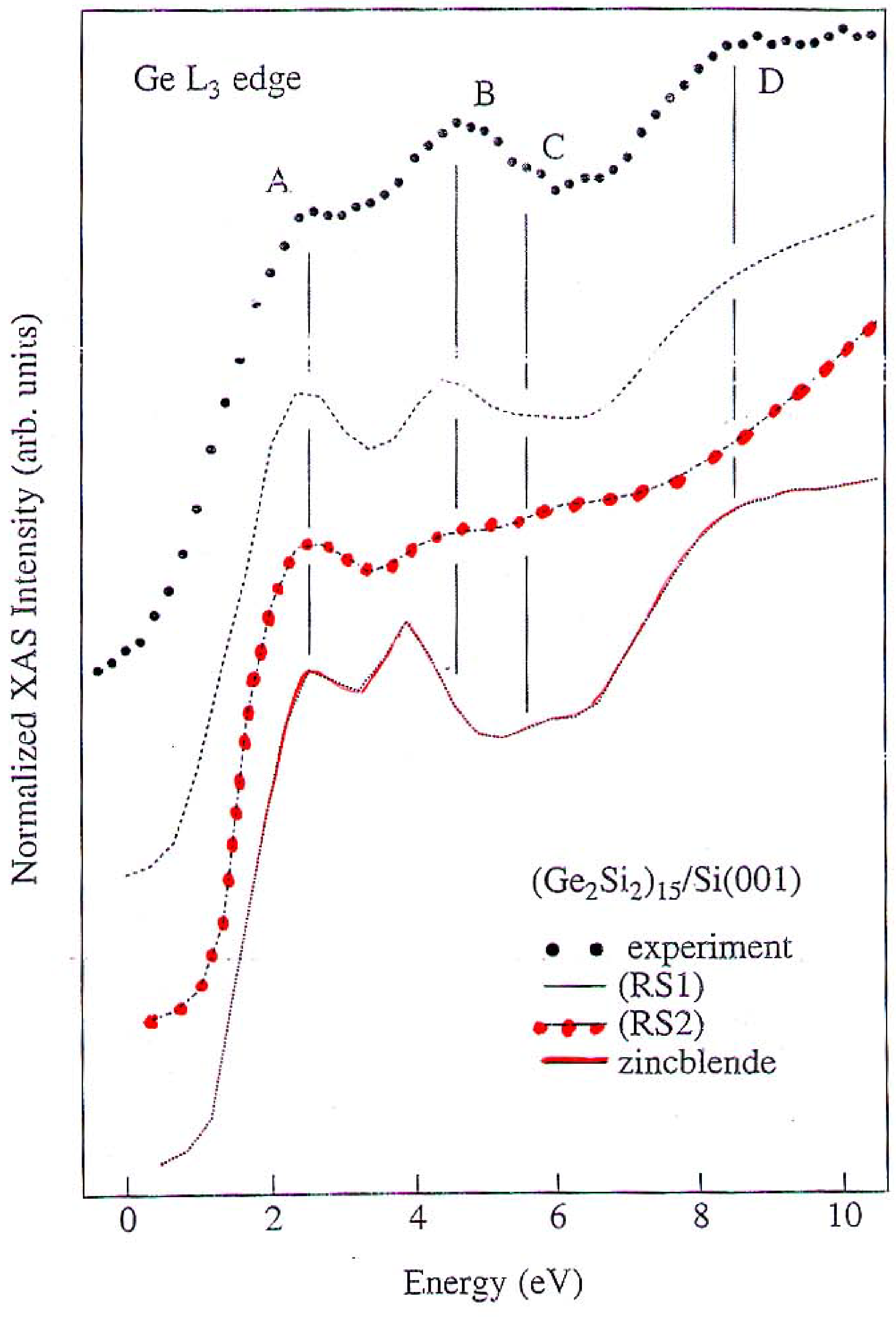
30
25
20
15
10
5
0
Ge L3 edge
XAS Intensity (arb. units x10^-3)
3ML Ge/Si(001)
RT deposited
385°C annealed
450°C annealed
1222
1224
1226
1228
1230
Energy (eV)


(RS2)
(RS1)
[001]
[110]
Ge
Si

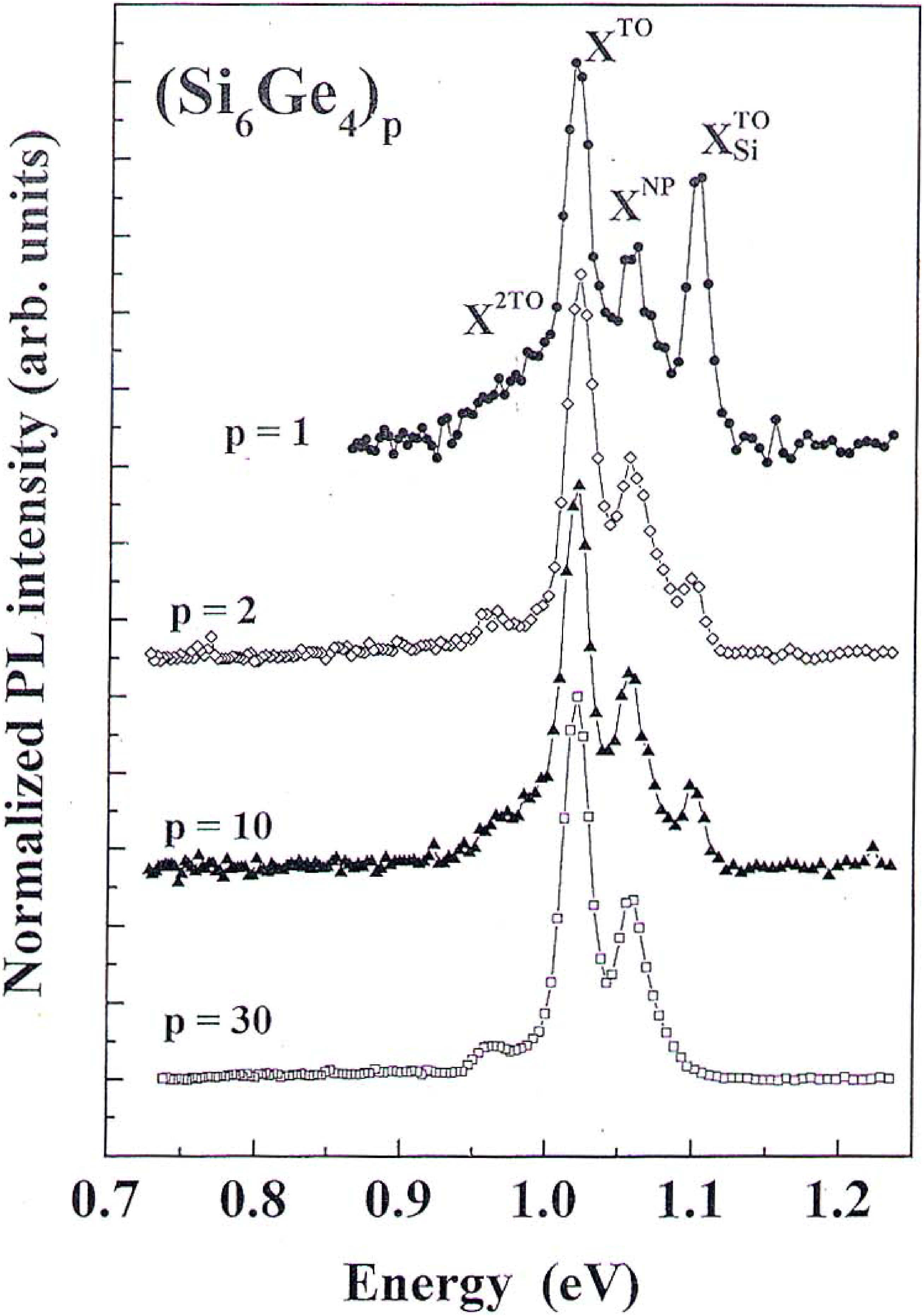

a
b
c
Ge
Si
[001]
[110]
Ge L_3 edge
a
b
c
3ML Ge/Si(001)
RT deposited
0
2
4
6
8
Energy (eV)



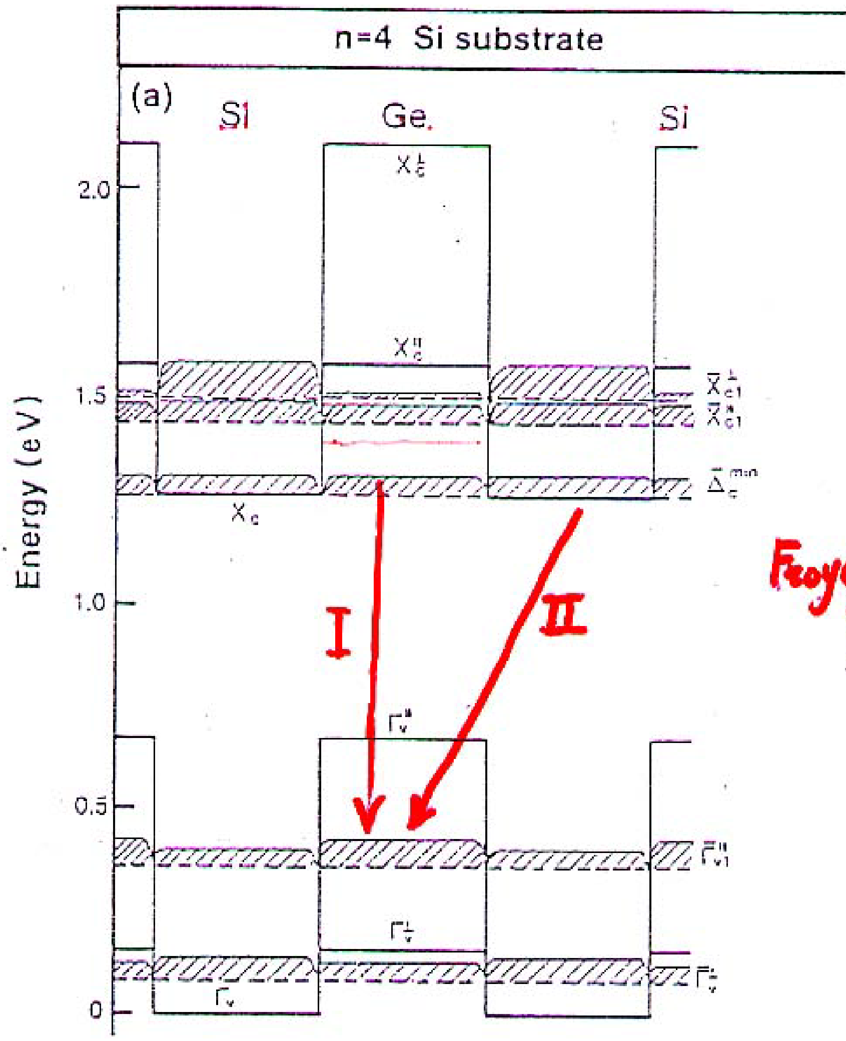
XAS calculation
Ge crystal
(eV)
Ge L3 edge
(Ge2Si2)15/Si(001)
theory
experiment
(Ge4Si4)2/Sb/Si(001)
theory
experiment
Normalized XAS Intensity (arb. units)
0
2
4
6
8
10
12
Energy (eV)



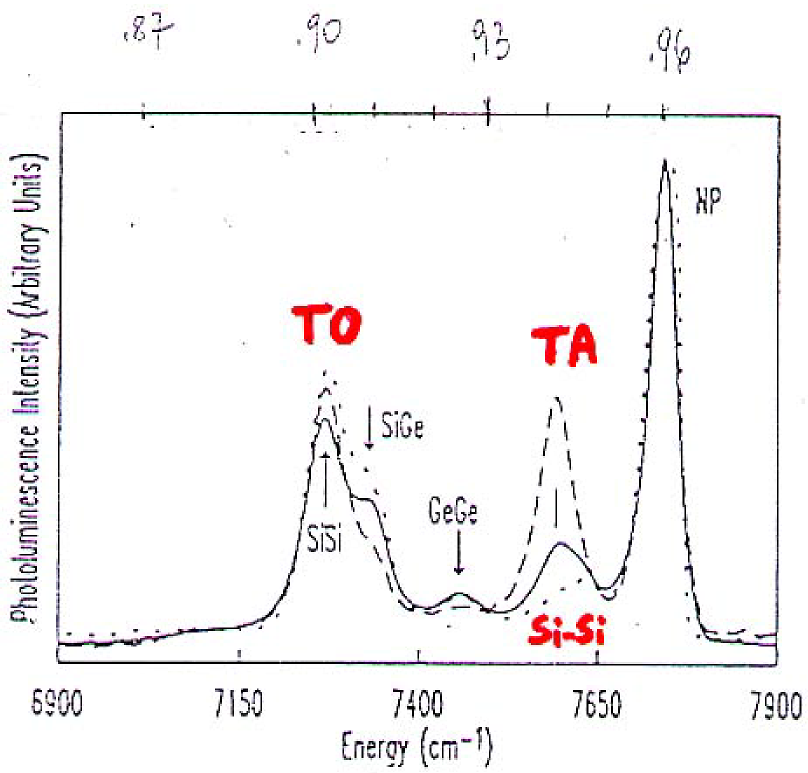
Ge L_3 edge
A
B
C
D
Normalized XAS Intensity (arb. units)
$(Ge_2Si_2)_{15}/Si(001)$
experiment
(RS1)
(RS2)
zincblende
0
2
4
6
8
10
Energy (eV)



$(Si_6Ge_4)_p$
X^{TO}
X^{NP}
X_{Si}^{TO}
X^{2TO}
p = 1
p = 2
p = 10
p = 30
Normalized PL intensity (arb. units)
0.7
0.8
0.9
1.0
1.1
1.2
Energy (eV)



Froyen, Wood, Zunger
PRB 37, 6893 (1988)



PL from the $Si_{0.75}Ge_{0.25}/Si$ QW at two different excitation densities without external strain.

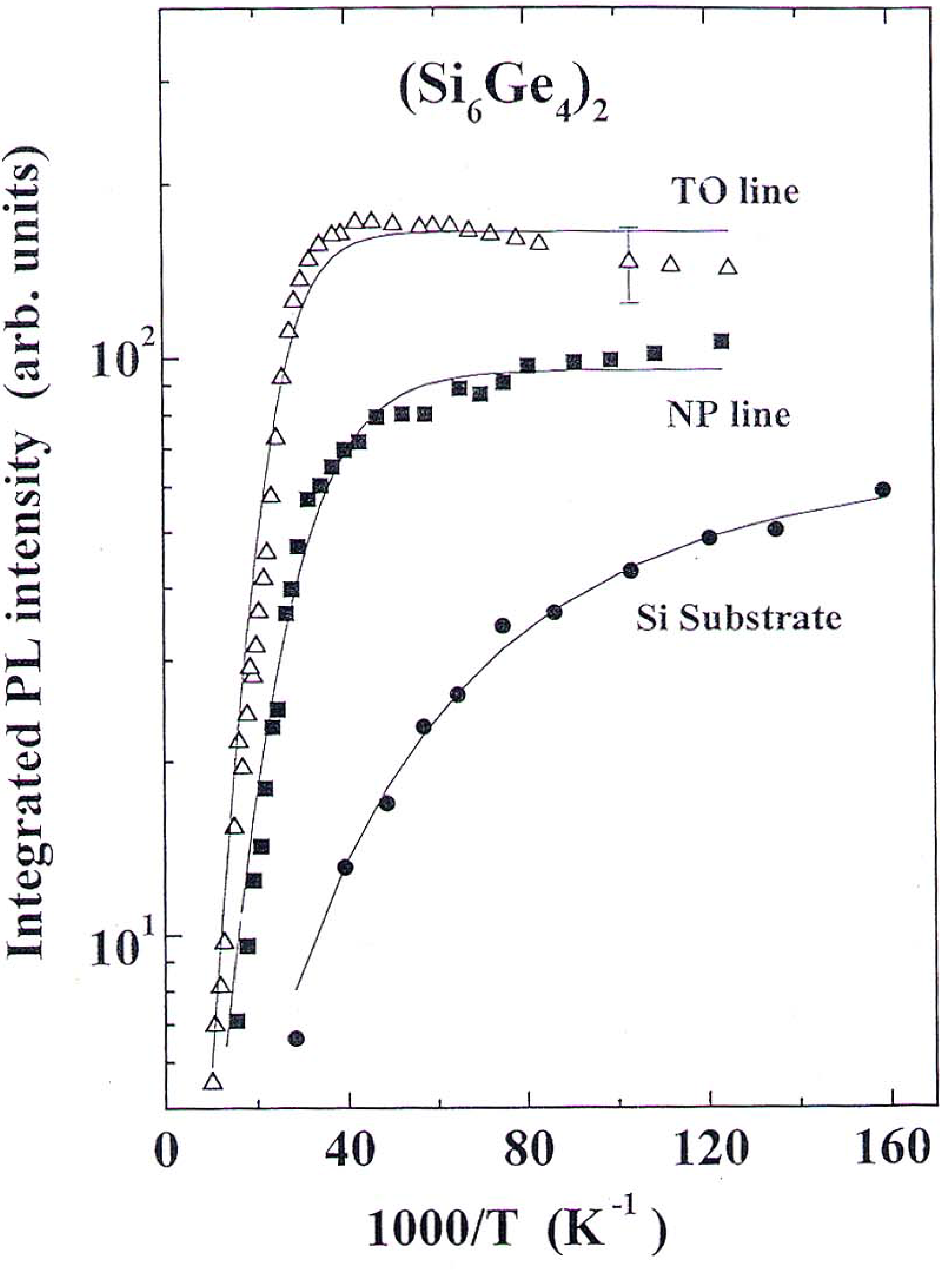


Figure 3, N. Pinto et al.

Conclusions

- Intermixing in Ge/Si(001) system has been recently observed and has emerged as a crucial and controversial topic in the study of the first stage of interface formation.

- We have discussed the structure of Ge overlayers epitaxially grown on Si(001) substrates. We have used the XPD spectroscopy from Ge core levels to check the film tetragonal distortion and the pseudomorphic growth morphology.

- Evidence for an interfacial intermixing has been found by means of the observation of the angular behaviour of the intensity of the emitted electrons. We have also investigated the effects of Sb as a surfactant on such an interface obtaining a reduced intermixing and a laminar growth of strained Ge overlayer.

- XAS spectra recorded at the Ge L3 edge at LURE have been directly compared to several Ge near edge features calculated for different Ge/Si(001) growth models making use of a multiple-scattering approach.

- Also this analysis clearly excludes a layer-by-layer Ge laminar growth and confirms the occurrence of intermixing processes. Information on the interface structure has been evidenced and the occurrence of a preferential double-layer ordering mechanism along the <111> crystallographic direction has been singled out.