Strain and Surface Morphology in $ZnSe/In_{0.04}Ga_{0.96}As/GaAs(001)$ Heterostructures

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Motivation:

Most II-VI blue-green lasers grown on GaAs (lattice mismatch ZnSe / GaAs: 0.27%)

Active layers: strained ZnSe or ZnCdSe QW

Early degradation is assisted by strain in the lasing medium

Solution: $In_xGa_{1-x}As$ lattice matched substrates

Today: ZnSe / $In_{0.04}Ga_{0.96}As$ / GaAs(001)

II-VI	gap	λ [1]	a_0	$In_xGa_{1-x}As$
ZnSe	2.68 eV		5.668 Å	x = 0.04
$Zn_{0.85}Cd_{0.15}Se$	2.49 eV	478 nm	5.726 Å	x = 0.18
$Zn_{0.75}Cd_{0.25}Se$	2.37 eV	505 nm	5.764 Å	x = 0.27

[1] Hervé et al.: Appl. Phys. Lett. **67** (1995) 2144

EPI

Periodic Table of the Elements

Groups: IA, IIA, IIIB, IVB, VB, VIB, VIIB, VIII, IB, IIB, IIIA, IVA, VA, VIA, VIIA, NOBLE ELEMENTS

Atomic Number	Symbol	Element	Group	Density (gm cm⁻³)	Mass Number	Lattice Constant, a (Å)	Crystal Type
1	H	HYDROGEN	IA	0.089	1.0079	3.75	HEX
2	He	HELIUM	NOBLE ELEMENTS	0.179	4.0026	3.57	HEX
3	Li	LITHIUM	IA	0.53	6.941	3.49	BCC
4	Be	BERYLLIUM	IIA	1.85	9.0122	2.29	HEX
5	B	BORON	IIIA	2.34	10.81	8.73	TET
6	C	CARBON	IVA	2.26	12.01	3.57	DIA
7	N	NITROGEN	VA	1.03	14.007	4.038	HEX
8	O	OXYGEN	VIA	1.43	15.999	6.83	CUB
9	F	FLUORINE	VIIA	1.97 (a)	18.998		MCL
10	Ne	NEON	NOBLE ELEMENTS	1.56	20.18	4.43	FCC
11	Na	SODIUM	IA	0.97	22.9898	4.23	BCC
12	Mg	MAGNESIUM	IIA	1.74	24.305	3.21	HEX
13	Al	ALUMINUM	IIIA	2.70	26.982	4.05	FCC
14	Si	SILICON	IVA	2.23	28.086	5.43	DIA
15	P	PHOSPHORUS	VA	1.82	30.974	7.17	CUB
16	S	SULFUR	VIA	2.07	32.064	10.47	ORC
17	Cl	CHLORINE	VIIA	2.09	35.453	6.24	ORC
18	Ar	ARGON	NOBLE ELEMENTS	1.78	39.948	5.26	FCC
19	K	POTASSIUM	IA	0.86	39.09	5.23	BCC
20	Ca	CALCIUM	IIA	1.54	40.08	5.58	FCC
21	Sc	SCANDIUM	IIIB	2.99	44.956	3.31	HEX
22	Ti	TITANIUM	IVB	4.51	47.90	2.95	HEX
23	V	VANADIUM	VB	6.1	50.942	3.02	BCC
24	Cr	CHROMIUM	VIB	7.19	52.00	2.88	BCC
25	Mn	MANGANESE	VIIB	7.43	54.938	8.89	CUB
26	Fe	IRON	VIII	7.86	55.85	2.87	BCC
27	Co	COBALT	VIII	8.9	58.93	2.51	HEX
28	Ni	NICKEL	VIII	8.9	58.71	3.52	FCC
29	Cu	COPPER	IB	8.96	63.55	3.61	FCC
30	Zn	ZINC	IIB	7.14	65.38	2.86	HEX
31	Ga	GALLIUM	IIIA	5.91	69.72	4.51	ORC
32	Ge	GERMANIUM	IVA	5.32	72.59	5.66	DIA
33	As	ARSENIC	VA	5.72	74.922	4.13	RHL
34	Se	SELENIUM	VIA	4.79	78.96	4.36	HEX
35	Br	BROMINE	VIIA	4.10	79.91	6.67	ORC
36	Kr	KRYPTON	NOBLE ELEMENTS	3.07	83.80	5.72	FCC
37	Rb	RUBIDIUM	IA	1.53	85.47	5.59	BCC
38	Sr	STRONTIUM	IIA	2.60	87.62	6.08	FCC
39	Y	YTTRIUM	IIIB	4.46	88.91	3.65	HEX
40	Zr	ZIRCONIUM	IVB	6.49	91.22	3.23	HEX
41	Nb	NIOBIUM	VB	8.4	92.91	3.30	BCC
42	Mo	MOLYBDENUM	VIB	10.2	95.94	3.15	BCC
43	Tc	TECHNETIUM	VIIB	11.5	98.91	2.74	HEX
44	Ru	RUTHENIUM	VIII	12.2	101.07	2.70	HEX
45	Rh	RHODIUM	VIII	12.4	102.90	3.80	FCC
46	Pd	PALLADIUM	VIII	12.0	106.40	3.89	FCC
47	Ag	SILVER	IB	10.5	107.87	4.09	FCC
48	Cd	CADMIUM	IIB	8.65	112.40	2.98	HEX
49	In	INDIUM	IIIA	7.31	114.82	4.59	TET
50	Sn	TIN	IVA	7.30	118.69	5.82	TET
51	Sb	ANTIMONY	VA	6.62	121.75	4.51	RHL
52	Te	TELLURIUM	VIA	6.24	127.60	4.45	HEX
53	I	IODINE	VIIA	4.94	126.90	7.27	ORC
54	Xe	XENON	NOBLE ELEMENTS	3.77	131.30	6.20	FCC
55	Cs	CESIUM	IA	1.90	132.91	6.05	BCC
56	Ba	BARIUM	IIA	3.5	137.34	5.02	BCC
57	La	LANTHANUM	IIIB	6.17	138.91	3.75	HEX
72	Hf	HAFNIUM	IVB	13.1	178.49	3.20	HEX
73	Ta	TANTALUM	VB	16.6	180.95	3.31	BCC
74	W	TUNGSTEN	VIB	19.3	183.85	3.16	BCC
75	Re	RHENIUM	VIIB	21.0	186.2	2.76	HEX
76	Os	OSMIUM	VIII	22.6	190.2	2.74	HEX
77	Ir	IRIDIUM	VIII	22.5	192.22	3.84	FCC
78	Pt	PLATINUM	VIII	21.4	195.09	3.92	FCC
79	Au	GOLD	IB	19.3	196.97	4.05	FCC
80	Hg	MERCURY	IIB	13.6	200.59	2.99	RHL
81	Tl	THALLIUM	IIIA	11.85	204.37	3.46	HEX
82	Pb	LEAD	IVA	11.4	207.19	4.95	FCC
83	Bi	BISMUTH	VA	9.8	208.98	4.75	RHL
84	Po	POLONIUM	VIA	9.4	210	3.35	SC
85	At	ASTATINE	VIIA		210		
86	Rn	RADON	NOBLE ELEMENTS	4.4	222		(FCC)
87	Fr	FRANCIUM	IA		223		(BCC)
88	Ra	RADIUM	IIA	(5.0)	226		
89	Ac	ACTINIUM	IIIB	10.1	227	5.31	FCC

RARE EARTHS

Atomic Number	Symbol	Element	Series	Density (gm cm⁻³)	Mass Number	Lattice Constant, a (Å)	Crystal Type
58	Ce	CERIUM	LANTHANIDES 6	6.77	140.12	5.16	FCC
59	Pr	PRASEODYMIUM	LANTHANIDES 6	6.77	140.91	3.67	HEX
60	Nd	NEODYMIUM	LANTHANIDES 6	7.00	144.24	3.66	HEX
61	Pm	PROMETHIUM	LANTHANIDES 6		145		
62	Sm	SAMARIUM	LANTHANIDES 6	7.54	150.35	9.00	RHL
63	Eu	EUROPIUM	LANTHANIDES 6	7.90	151.96	4.61	BCC
64	Gd	GADOLINIUM	LANTHANIDES 6	8.23	157.25	3.64	HEX
65	Tb	TERBIUM	LANTHANIDES 6	8.54	158.92	3.60	HEX
66	Dy	DYSPROSIUM	LANTHANIDES 6	8.78	162.50	3.59	HEX
67	Ho	HOLMIUM	LANTHANIDES 6	9.05	164.93	3.58	HEX
68	Er	ERBIUM	LANTHANIDES 6	9.37	167.26	3.56	HEX
69	Tm	THULIUM	LANTHANIDES 6	9.31	168.93	3.54	HEX
70	Yb	YTTERBIUM	LANTHANIDES 6	6.97	173.04	5.49	FCC
71	Lu	LUTETIUM	LANTHANIDES 6	9.84	174.97	3.51	HEX
90	Th	THORIUM	ACTINIDES 7	11.7	232.04	5.08	FCC
91	Pa	PROTACTINIUM	ACTINIDES 7	15.4	231	3.92	TET
92	U	URANIUM	ACTINIDES 7	19.07	238.03	2.65	ORC
93	Np	NEPTUNIUM	ACTINIDES 7	20.3	237.05	4.72	ORC
94	Pu	PLUTONIUM	ACTINIDES 7	19.8	244		MCL
95	Am	AMERICIUM	ACTINIDES 7	11.8	243		
96	Cm	CURIUM	ACTINIDES 7		247		
97	Bk	BERKELIUM	ACTINIDES 7		247		
98	Cf	CALIFORNIUM	ACTINIDES 7		251		
99	Es	EINSTEINIUM	ACTINIDES 7		254		
100	Fm	FERMIUM	ACTINIDES 7		257		
101	Md	MENDELEVIUM	ACTINIDES 7		256		
102	No	NOBELIUM	ACTINIDES 7		254		
103	Lw	LAWRENCIUM	ACTINIDES 7		257		

Source: N. W. Ashcroft and N. D. Mermin, *Solid State Physics*, Holt, Rinebart and Winston, USA (1992).

LEGEND

MOLYBDENUM: Density (gm cm⁻³) → 10.2; Mass Number → 95.94; Mo; Lattice Constant, a (Å) → 3.15; Crystal Type (Common Crystal Phase) → BCC; Atomic Number → 42

- FCC - Face - Centered Cubic
- BCC - Body - Centered Cubic
- SC - Simple Cubic
- CUB - Cubic
- TET - Tetragonal
- ORC - Orthorhombic
- HEX - Hexagonal
- DIA - Diamond
- RHL - Rhombohedral
- MCL - Monoclinic

Recommended Sources

See Page 12 for a complete Selection Guide

- EPI Low Temperature Cell
- EPI High Temperature Cell
- EPI Standard or Modified Filament Cell
- EPI Special Source Available
- EPI Valved or Standard Cracker
- EPI Dual Filament Cell
- EPI Dopant Cell

Beamline ID3 @ ESRF

Surface diffraction

undulator

monochromator: Si (111) double crystal

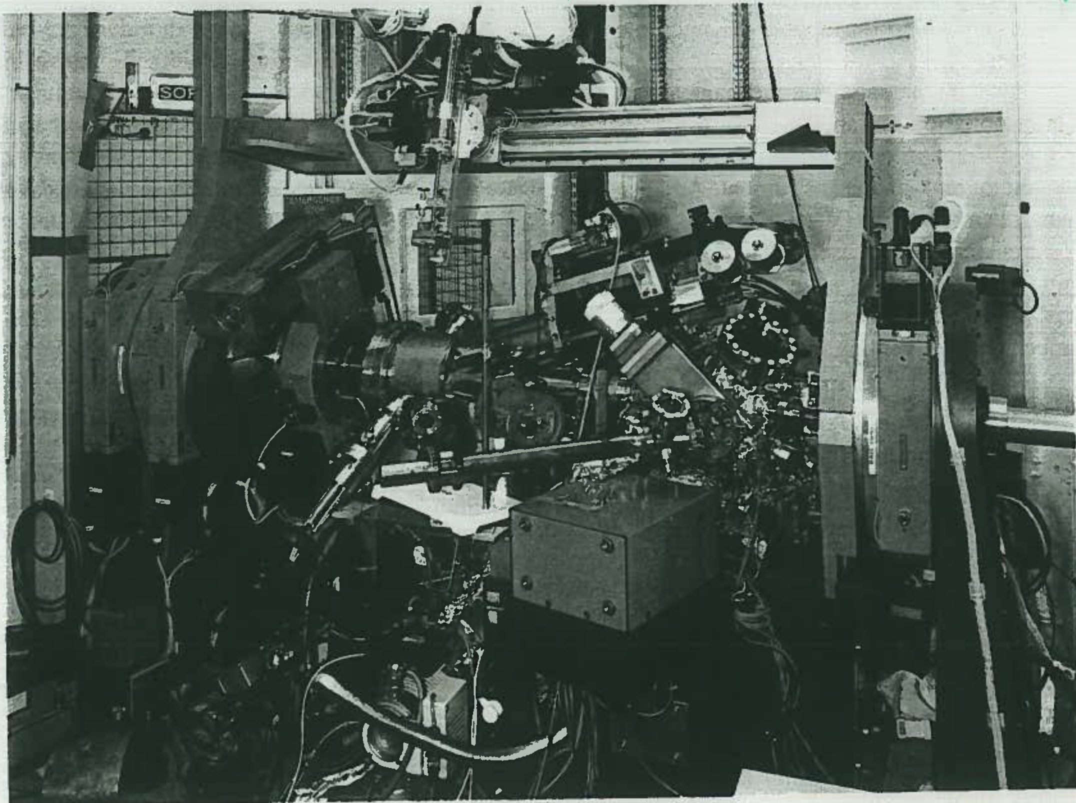
1st: cryo cooled

2nd: horizontal focusing

5-30 keV

$\Delta E/E \approx 3 \times 10^{-4}$

flux at sample: $10^{12} \sim 10^{13}$ ph s^{-1}



ID 3 SURFACE DIFFRACTION • *Beamline 7*

at the ESRF

Operational

scientist in charge	Salvador Ferrer, tel. +33 76 88 20 68, fax: +33 76 88 21 60 e-mail: ferrer@esrf.fr beamline tel. +33 76 88 25 99
scientific applications	Surface and interface studies

source characteristics undulator on a low β section

magnet period:	44 mm
critical energy ε_c:	11.8 keV
K_{max}:	1.85
field B_{max}:	0.45 T
source size:	0.16 x 0.11 mm^2 (HxV) FWHM
source divergence:	210 x 38 μrad^2 (HxV)
peak brightness:	10^{16} ph s^{-1} $mrad^{-2}$, 0.1%bw, 0.1A (at min. gap)
total power:	0.74 kW
power density at 25 m:	17 Wmm^{-2}
beam size at 30 m:	6.5 x 1.2 mm^2 (HxV) FWHM

optics

optical elements:	1st monochr.	2nd monochr.
focusing type:	Si (111) cryocooled	horiz. focusing
demagnification:		2
ideal beam size at sample:	80 x 30 μm^2 (HxV) focused	
spectral range:	5 - 30 keV	
resolution in $\Delta E/E$:	~3.10^{-4}	
flux at sample:	~10^{13} ph s^{-1} at low energy (0.1%bw, 0.1A)	
	~10^{12} ph s^{-1} at high energy (0.1%bw, 0.1A)	

detectors	NaI scintillator
beamline control	SPEC
ancillary equipment	ultra-high vacuum He cryostat, Knudsen cells, electron bombardment evaporator

100nm/300nm ZnSe

BPR=1

0.27% lattice mismatch

critical thickness: 150nm

GaAs buffer

GaAs(100)

100nm/300nm ZnSe

BPR=1

2 µm $In_{0.04}Ga_{0.96}As$

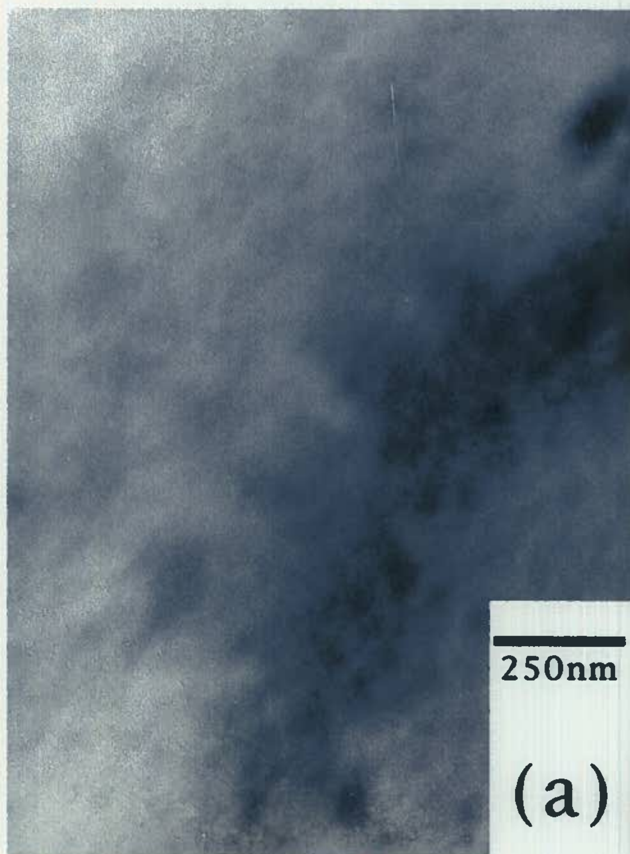
lattice matched to ZnSe

GaAs(100)

pseudomorphic

relaxed

lattice-matched

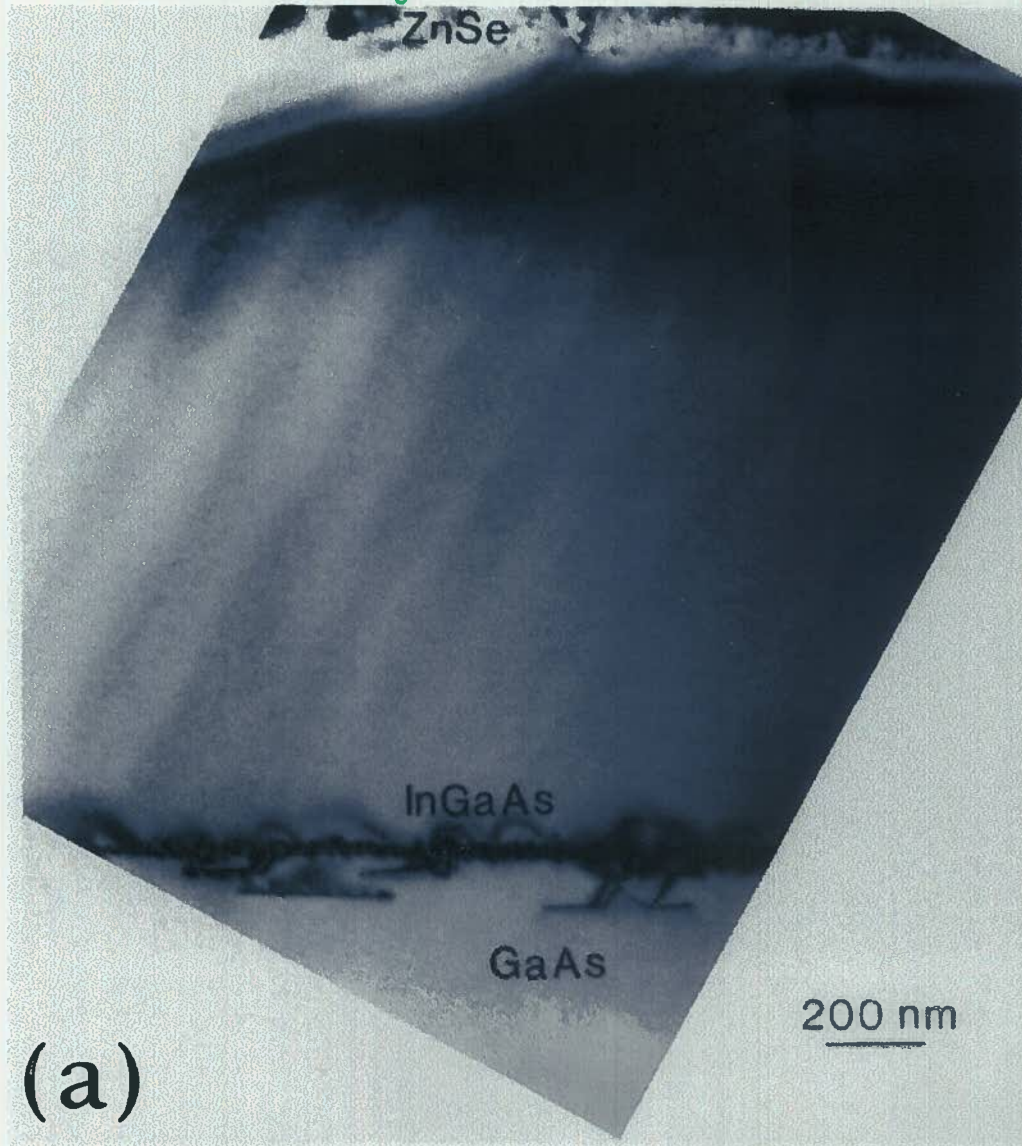


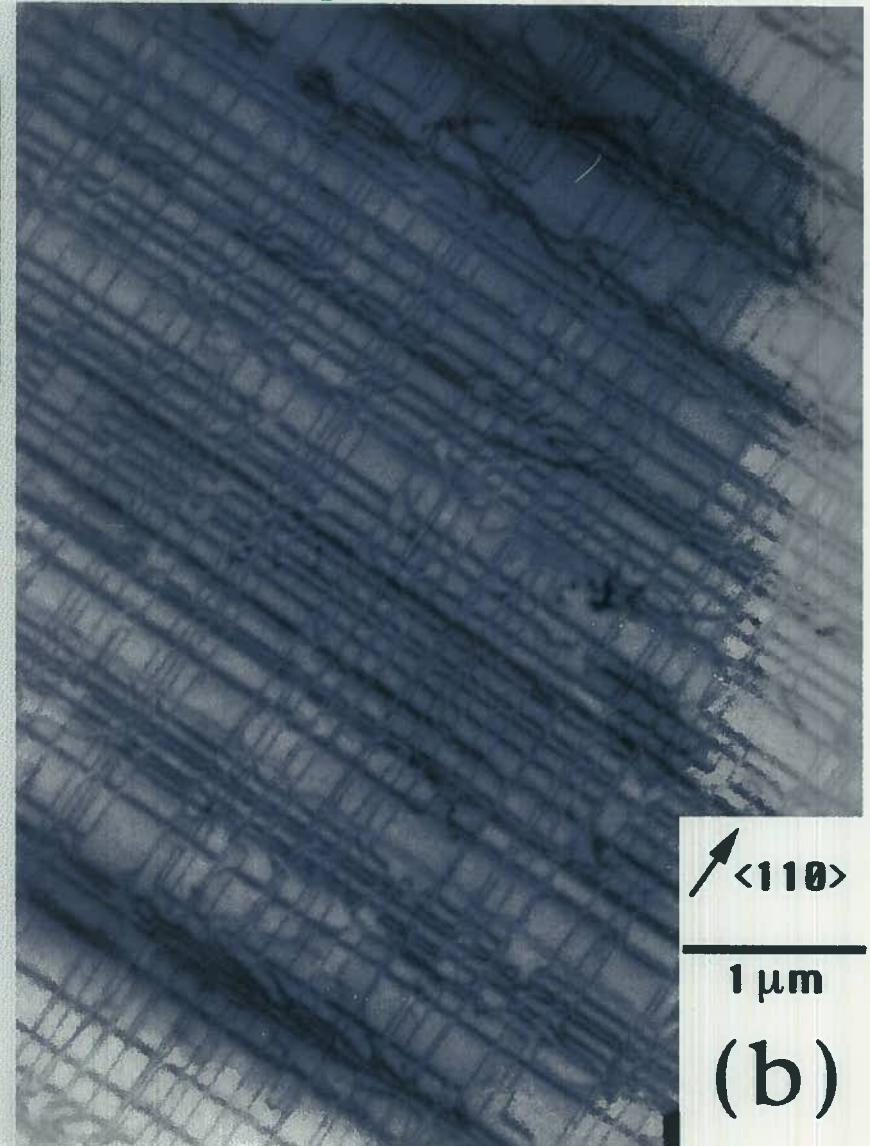
100 nm ZnSe / GaAs

300nm ZnSe / GaAs

300 nm ZnSe / $In_{0.04}Ga_{0.96}As$

No threading dislocations ($< 2 \times 10^4 cm^{-2}$) $In_{0.04}Ga_{0.96}As$ – buffer relaxed!





100 nm ZnSe / 2 µm $In_{0.04}Ga_{0.96}As$ / GaAs (001)

XRD results

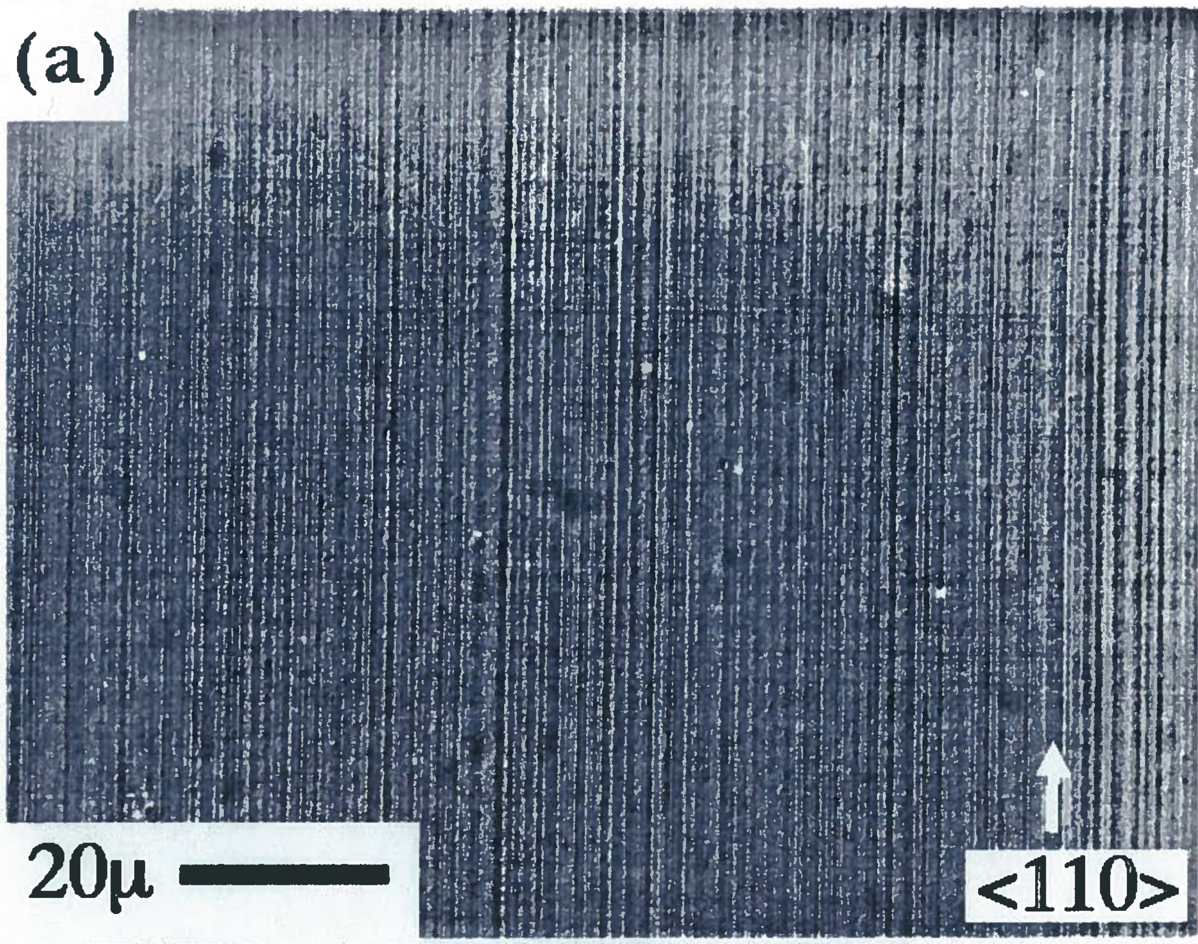
300 nm ZnSe / 2 μm $In_{0.04}Ga_{0.96}As$ / GaAs (001)

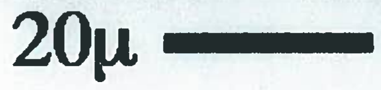
	$In_xGa_{1-x}As$	ZnSe
a_n [Å]	5.6789 +- 0.0009	5.6701 +- 0.0004
a_p [Å]	5.6683 +- 0.0005	5.6683 +- 0.0008
a_0 [Å]	5.6738 +- 0.0007	5.6691 +- 0.0006
x (XRD)	0.051 +- 0.002	-----
x (PL)	0.050 +- 0.002	-----
ε_n	0.90×10^{-3}	1.76×10^{-4}
ε_p	-0.97×10^{-3}	-1.41×10^{-4}

GaAs: $a_0 = 5.6533$ Å

ZnSe / GaAs: $\varepsilon = 2.72 \times 10^{-3}$

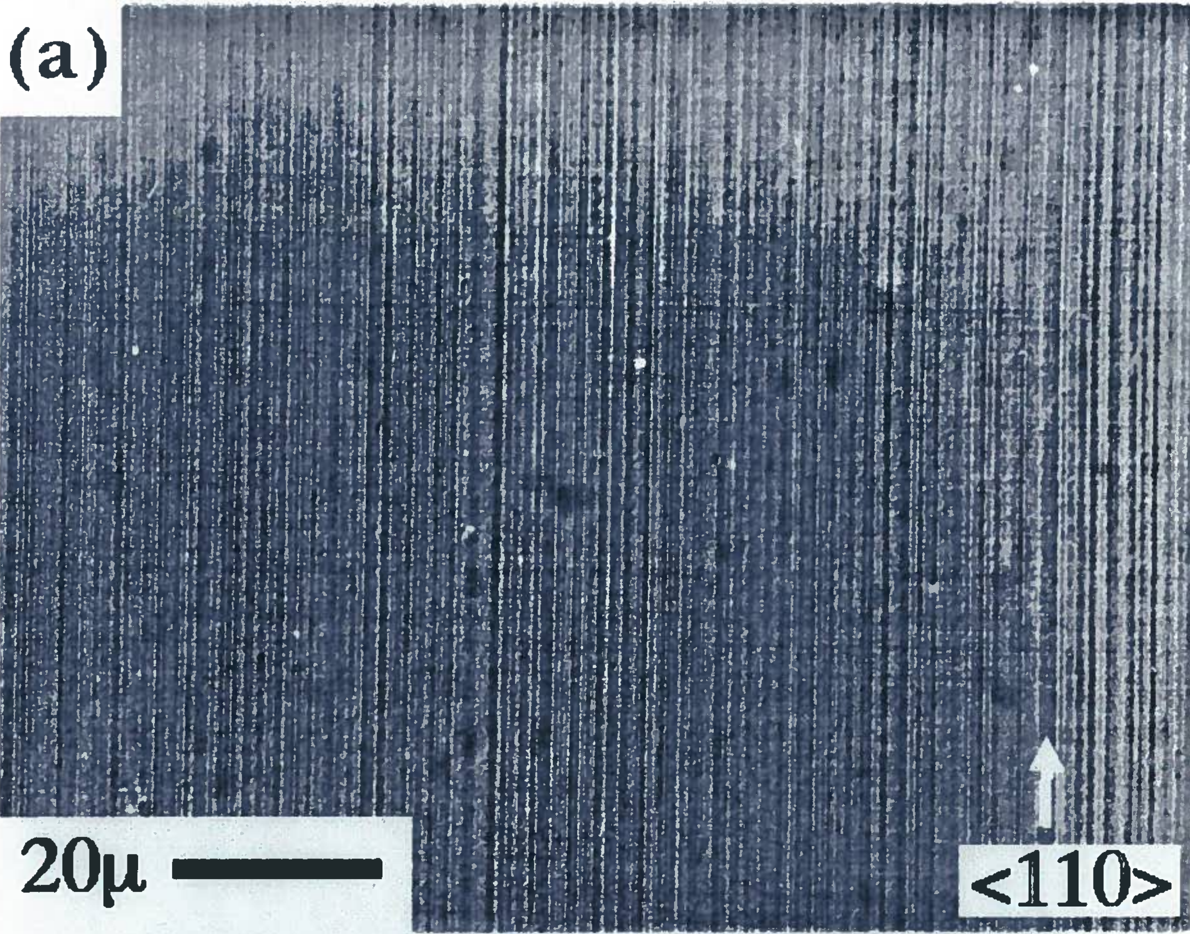
Nomarski Optical Microscopy



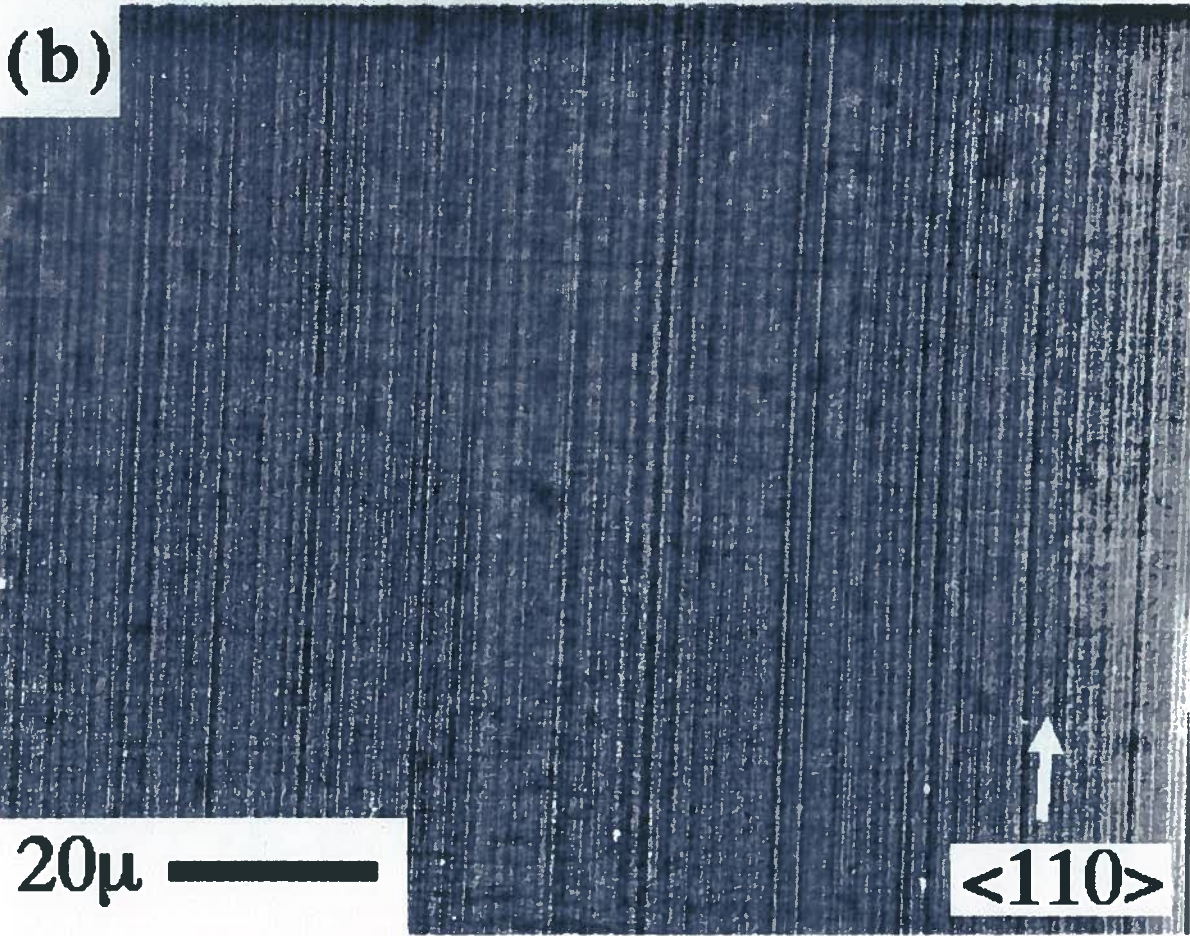


2μm $In_{0.04}Ga_{0.96}As$ / GaAs (001)

Nomarski Optical Microscopy



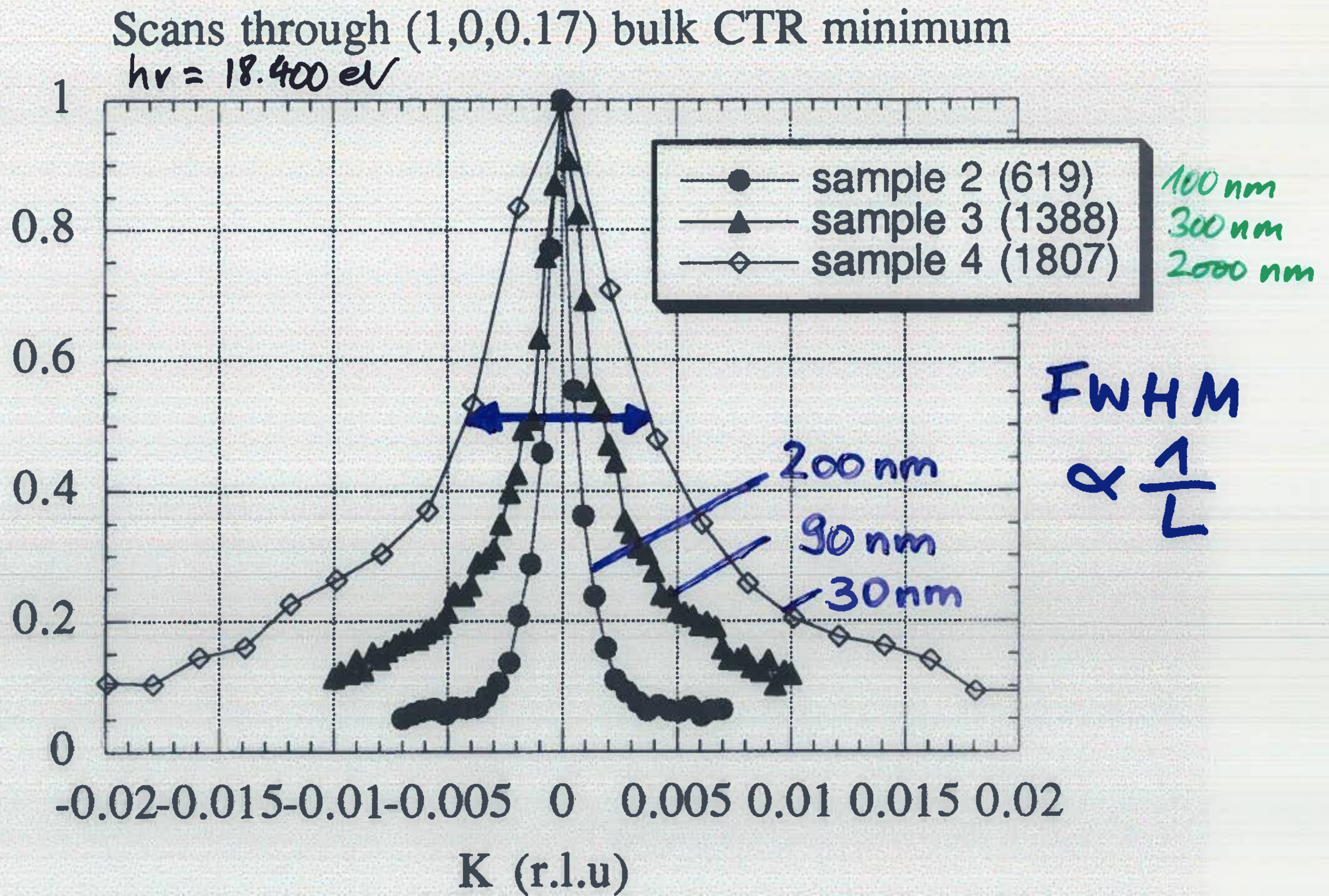
2μm $In_{0.04}Ga_{0.96}As$ / GaAs (001)



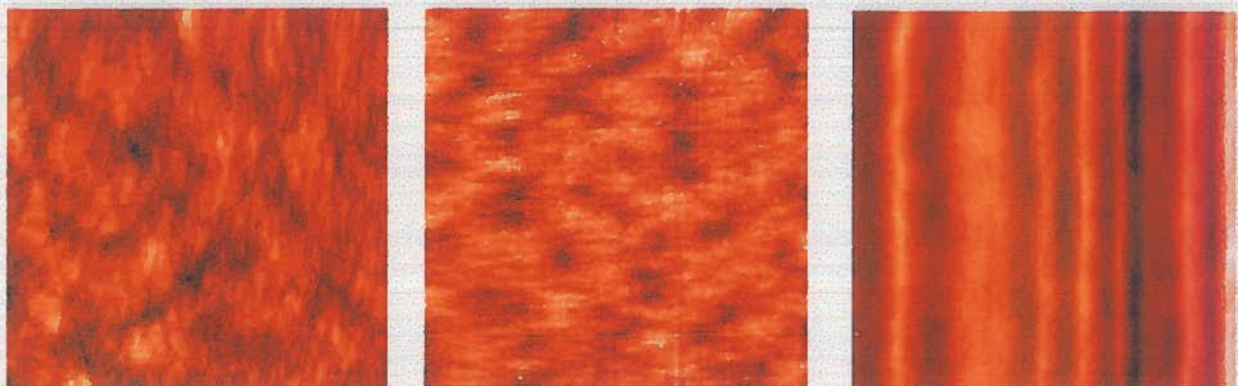
300nm ZnSe / $In_{0.04}Ga_{0.96}As$

No such cross-hatch for ZnSe / GaAs (001)

Surface XRD @ ESRF



Atomic Force Microscopy

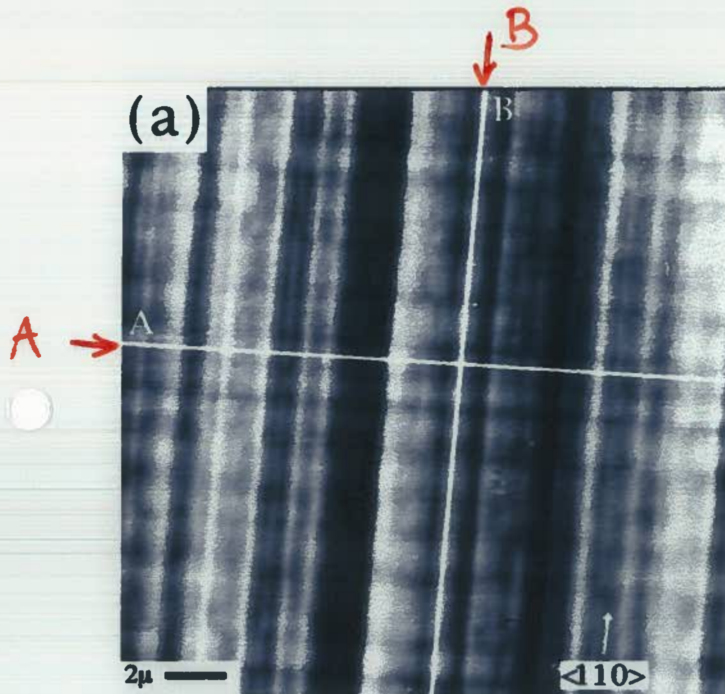


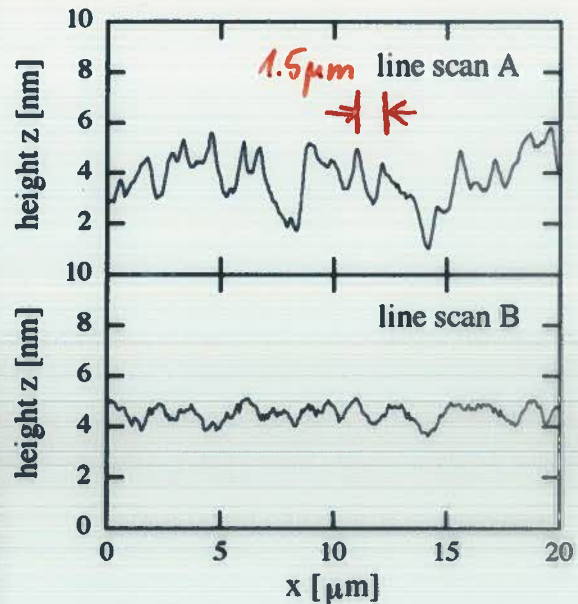
#2: 100 nm #3: 300 nm #4: 2000 nm

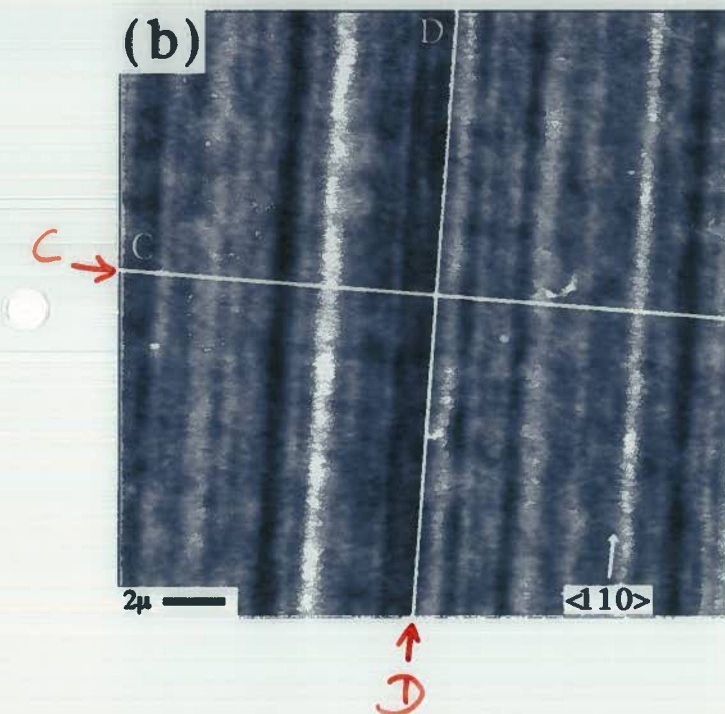
$In_{0.04}Ga_{0.96}As$ on GaAs

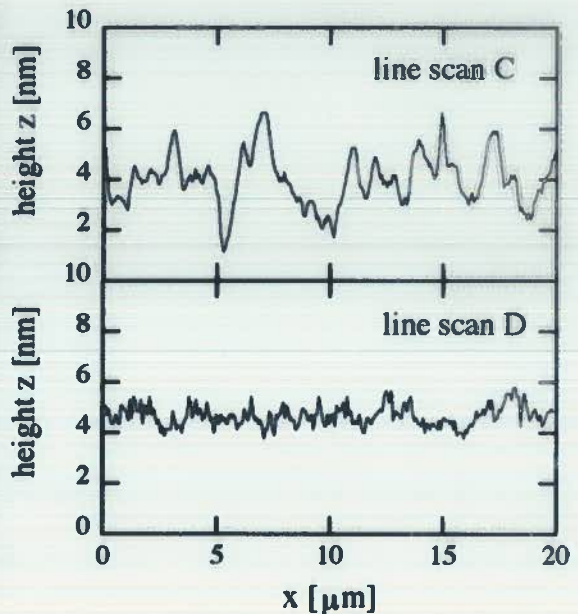
RMS-Δ: 2~3 Å 3~4 Å 8 Å

Atomic Force Microscopy









(a) 2µ $In_{0.04}Ga_{0.96}As$ on GaAs (001)

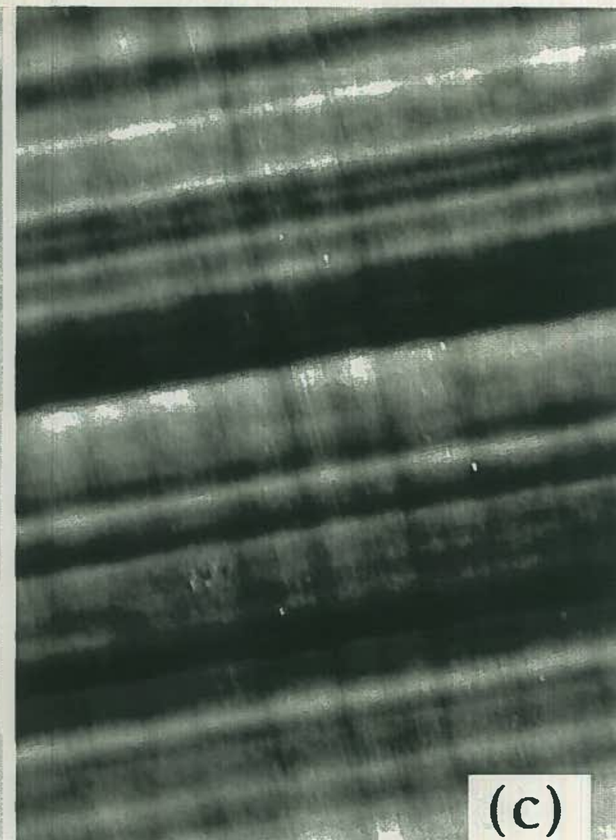
(b) 300 nm ZnSe on (a)

$\Delta_{RMS} \simeq 1$ nm

TEM

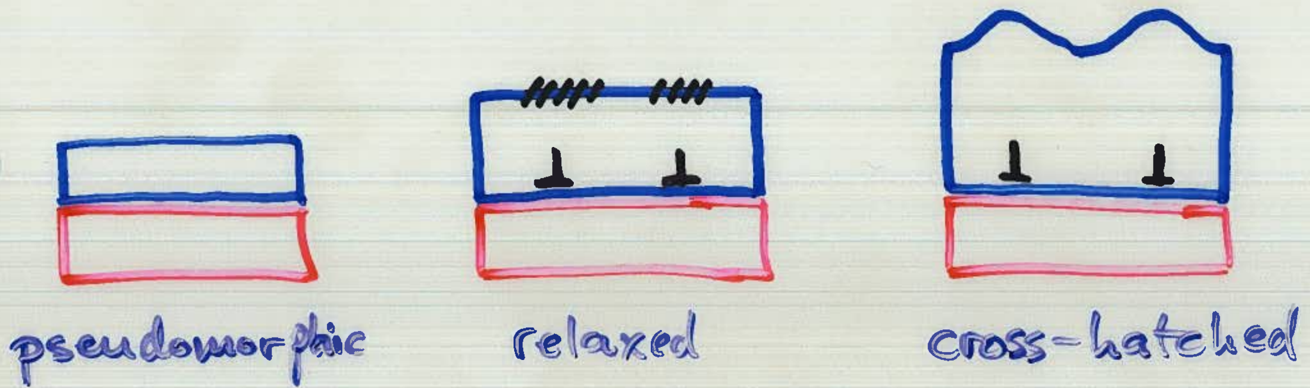
TEM * Tip

AFM

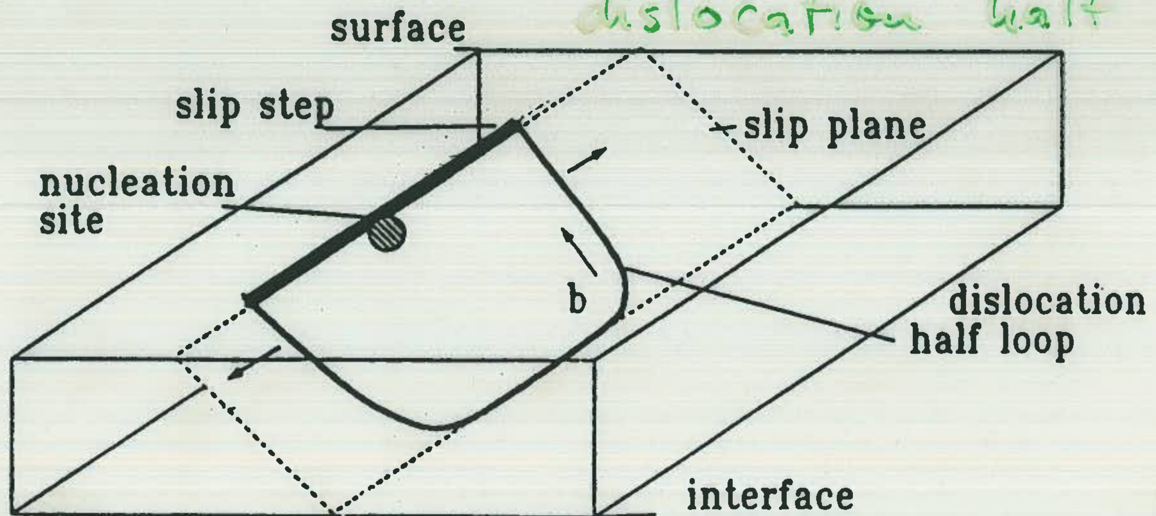


MODELS

ⓐ local growth rate differences due to dislocations



ⓑ slip-related surface steps caused by dislocation half loops



TEM: average spacing between dislocations: 100nm

AFM: spacing of surface corrugations: 1.5μm

⤳ 15 steps / period ⤳ height modulation: 2.1nm

AFM: 3nm

Results:

$In_{0.04}Ga_{0.96}As$ - buffer:

dislocation network at the interface to the GaAs

surface corrugation along <110>

corrugations are related to distribution of dislocations

ZnSe / $In_{0.04}Ga_{0.96}As$:

No misfit and threading dislocations (< 2×10^4 cm^{-2})

High bulk structural quality of the II-VI epilayer

surface morphology affected

cross-hatch amplitude 3 nm

period 1 - 2 μm

replicates $In_{0.04}Ga_{0.96}As$ buffer surface