Crescimento Epitaxial

Ciência e Tecnologia de Filmes Finos – POSMAT/2
Prof. José Humberto Dias da Silva

Epitaxia

Crescimento de uma camada de uma substância sobre um cristal de outra, de maneira que a estrutura da camada seja similar à do substrato.

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1 – Explic Basica
2 - Motivação

Motivação

- Relembrando nossos circuitos de alta integração...

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... m u u u i i i itas camadas !

- \+ baixa densidade de defeitos entre camadas...

  para não "espalhar" os elétrons

5

- Por que é importante crescer multiplas camadas / junções de diferentes materiais (heteroestruturas) ?

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Idéias que se tornaram práticas...

- Prêmios Nobel
  - 1973
  - 2000
  - 2007

entre outras importantes...

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Nobel - 1973

http://nobelprize.org/mediaplayer/index.php?id=712&player=2

Entrevista_Esaki_Editada_DVD.wmv

Leo Esaki

"for his experimental discoveries regarding tunneling phenomena in semiconductors"

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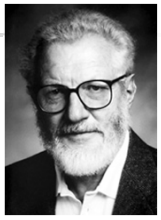
Nobel 2000

Zhores Alferof

Herbert Kroemer



"for developing semiconductor heterostructures used in high-speed- and opto-electronics"

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Nobel - 2007

Magneto-resistência gigante

Albert Fert

Peter Grünberg

3 – Tipos de Heteroestrut

Hetero-estruturas (super-redes)

Esquema de bandas de energia

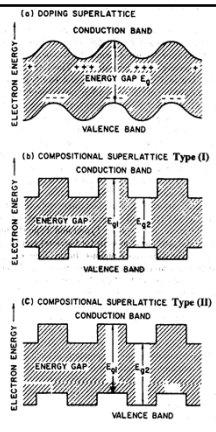
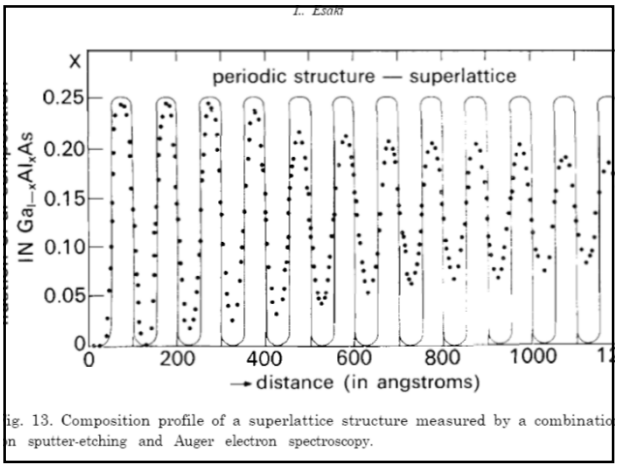


Figure 541.1: Spatial variations of the conduction and valence bandedges in (a) doping (n-i-p-i) superlattice (b) compositional superlattice (Type I) (c) compositional superlattices



ig. 13. Composition profile of a superlattice structure measured by a combinatio
n sputter-etching and Auger electron spectroscopy.

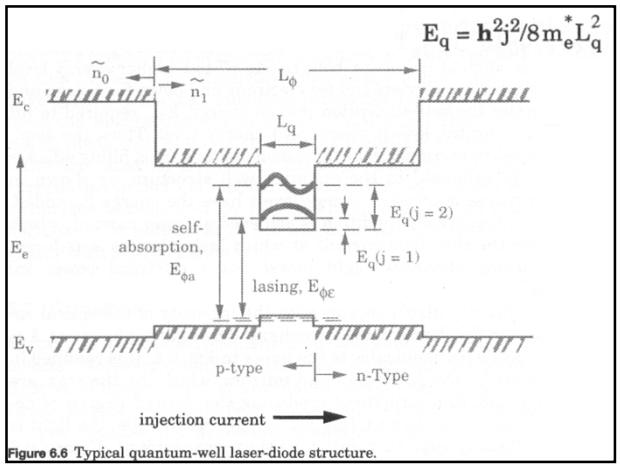


Figure 6.6 Typical quantum-well laser-diode structure.

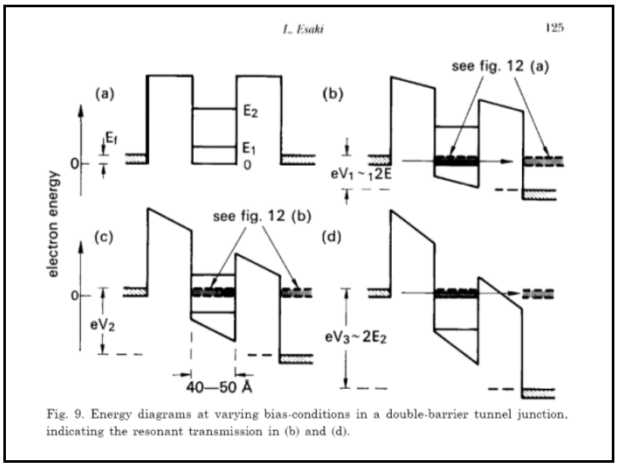


Fig. 9. Energy diagrams at varying bias-conditions in a double-barrier tunnel junction, indicating the resonant transmission in (b) and (d).

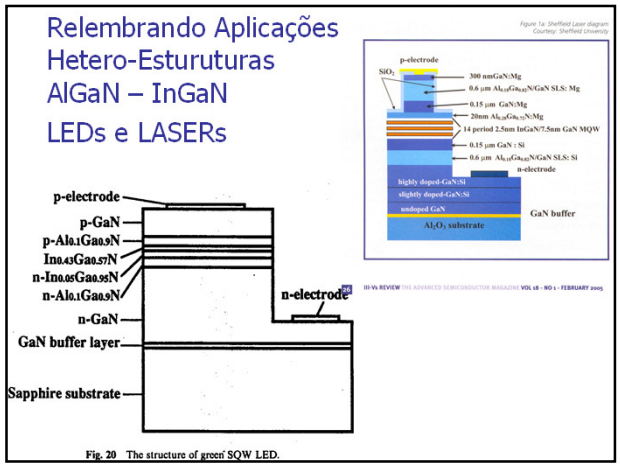
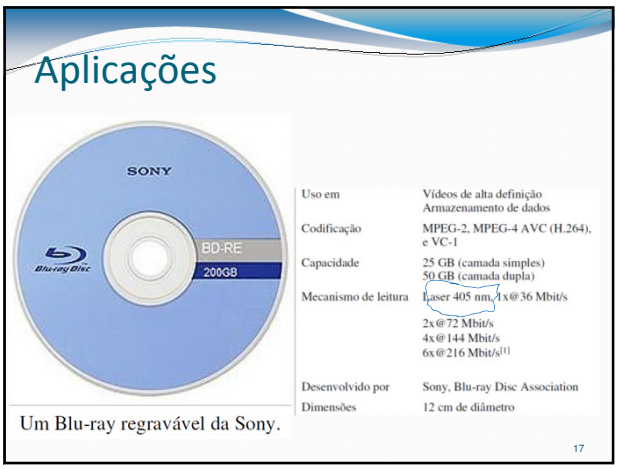
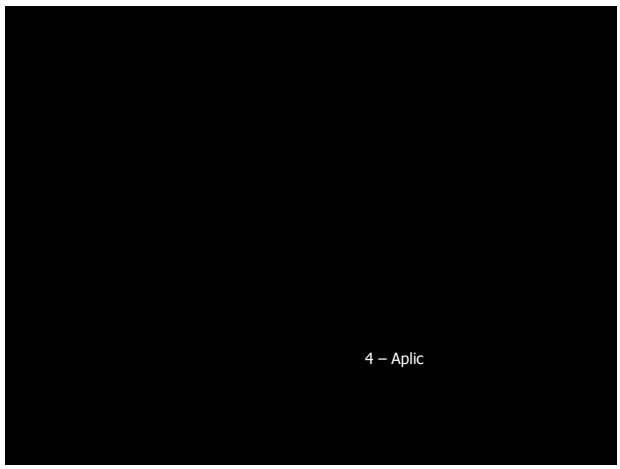


Fig. 20 The structure of green SQW LED.



Um Blu-ray regravável da Sony.



Epitaxia

ordem cristalográfica do filme

ordem cristalográfica do substrato.

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- **Homoepitaxia** = filme e substrato de mesmo material.
  Exemplos: Si/Si; GaAs/GaAs
- **Heteroepitaxia** = filme e substrato de material diferente.
  Exemplos: GaN/Al_2O_3 (Safira)

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Epitaxia

- Como crescer um cristal sobre outro?
  - Quais as condições ?
  - Para que ?

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GaAs (001)/Fe(001)

FCC 0,565nm/BCC 0,573x0,5

Cu – FCC, $\sqrt{2}a_o = 0{,}512nm$

Cu [100]

Si [110]

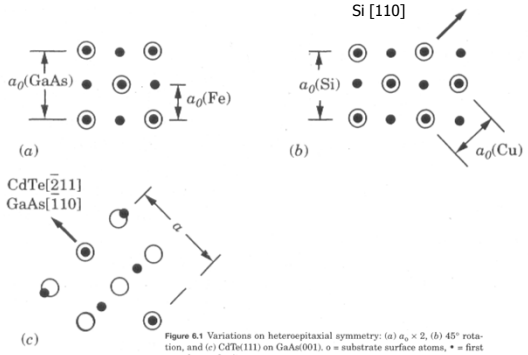

Figure 6.1 Variations on heteroepitaxial symmetry: (a) $a_o \times 2$, (b) 45° rotation, and (c) CdTe(111) on GaAs(001). o = substrate surface atoms, • = first monolayer of epitaxy.

Hetero-Estruturas

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Hetero-estruturas

Tensões e Defeitos

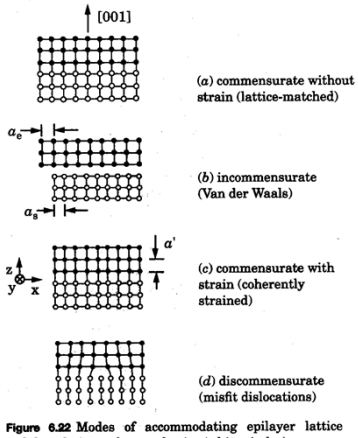

Figure 6.22 Modes of accommodating epilayer lattice (solid circles) to substrate lattice (white circles).

Fator de discordância de uma hetero-junção

$$f = \frac{(a_e - a_s)}{(a_e + a_s)/2} \approx (a_e - a_s)/a_s$$

Smith Eq.6.1

Epitaxia possível quando:

$$f \approx (a_e - a_s)/a_s < 0{,}15$$

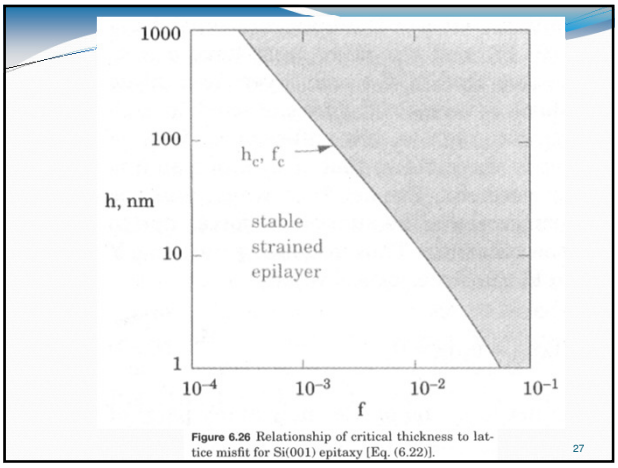

Figure 6.26 Relationship of critical thickness to lattice misfit for Si(001) epitaxy [Eq. (6.22)].

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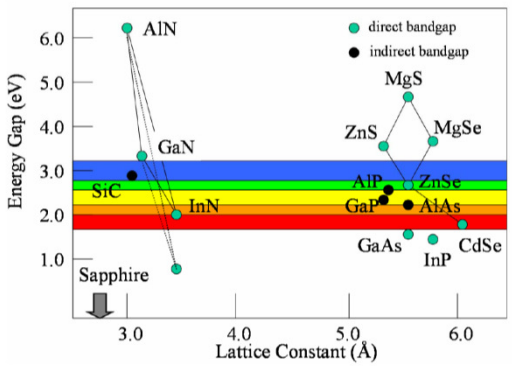
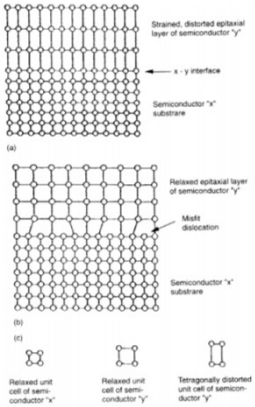
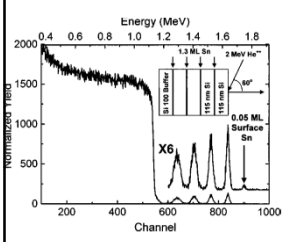
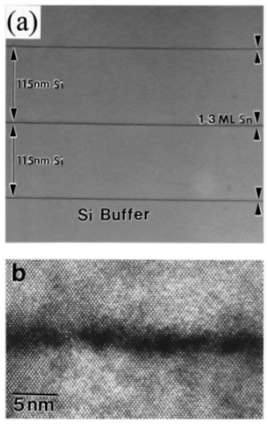
- Parâmetro de Rede vs. Bandgap









K. S. Min and H. A. Atwater
Appl. Phys. Lett., Vol. 72, No. 15, 13 April 1998

Estudo de caso – GaN em Safira

Estudo de Caso

- GaN / Safira

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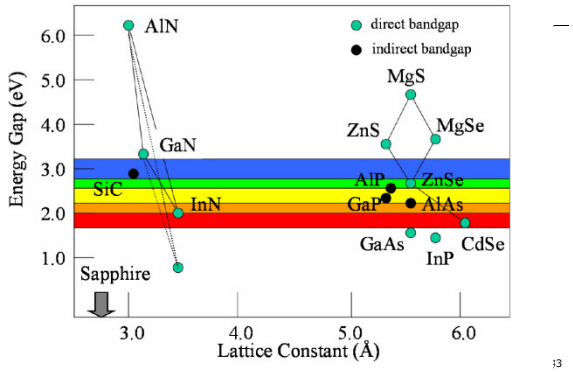
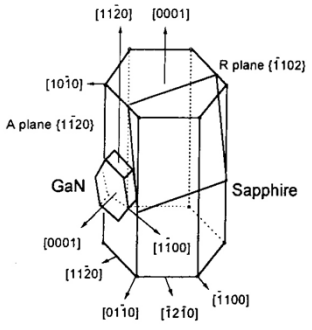
- Parâmetro de Rede vs. Bandgap





Relative orientations of the crystallographic axes of GaN in case of heteroepitaxy sapphire. Note that the (0001) plane of sapphire is parallel to the (11-20) plane of pilayer.

B. Gil (in: (eds) Pankove / Moustakas (GaN II) – Beer Willardson Vol. 57).

perature θ_D for some group-IV, III–V and II–VI semiconductors. C_p and θ_D are at 300 K

System	Material	T_m (K)	C_p (J/g K)	θ_D (K)
IV	Diamond	4100[a]	0.5148	1870
	Si	1687	0.713	643
	Ge	1210.4	0.3295[b]	348[b]
	α-Sn		0.278[c]	238[c]
	3C-SiC	2810	0.677[d]	1122
	6H-SiC	2810	0.58	1126
	15R-SiC	2810		
III–V	*c*-BN	>3246	0.643	1613
	h-BN		0.805	323
	BP	>3300	0.75	1025[e]
	BAs	2300	0.408	800
	w-AlN	3487	0.728	988
	AlP	2823	0.727	687
	AlAs	1740	0.424	450
	AlSb	1338	0.326[b]	370[b]
	α-GaN	2791	0.42	821
	GaP	1730	0.313	493[e]
	GaAs	1513	0.327	370
	GaSb	991	0.344[b]	240[b]

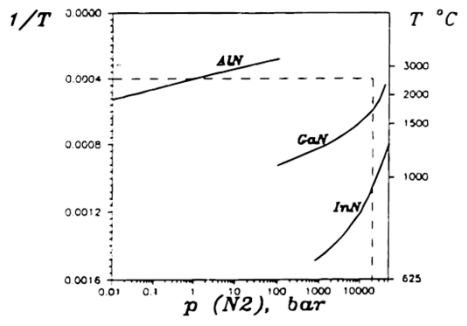


Figure 3. Stability limits for AlN, GaN, and InN. Reprinted with permisson from ref 20. Copyright 1993 Elsevier Science.

- Parâmetro de Rede vs. Bandgap

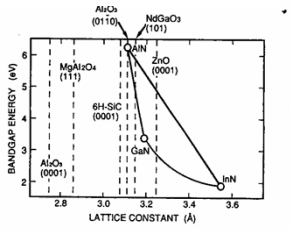


Fig. 19 Relationship between bandgap energy and lattice constant. Dotted lines atomic spaces in-plane corresponding to GaN.

TABLE I
Mismatch of lattice constant and thermal expansion coefficient between GaN and substrates.

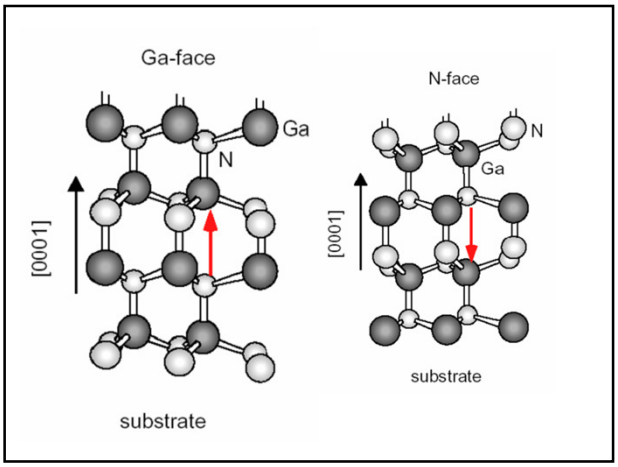
Substrate	Lattice Mismatch (%)	Thermal Expansion Mismatch (%)
(0001) Sapphire	13.8	−25.5
(01$\bar{1}$0) Sapphire	−1.9,2.6	9,62
(0001) 6H-SiC	3.4	25
(101) $NdGaO_3$	1.2	20.6
(111) $MgAl_2O_4$	9.5	—

Mismatch = (GaN − Substrate)/GaN.

TABLE II
Relationships of orientation, lattice mismatch and crystallographic symmetry between GaN epitaxial film and sapphire substrate (after Ref. [4]).

Interface Plane GaN/Al_2O_3	In-Plane GaN//Al_2O_3	Lattice Mismatch (%)	Crystallographic Symmetry
(01$\bar{1}$3)//(01$\bar{1}$0)	[0$\bar{3}$32]//[2$\bar{1}$$\bar{1}$0]	−2.6	Coincidence
	[2$\bar{1}$$\bar{1}$0]//[0001]	1.9	
(0001)//(0001)	[2$\bar{1}$$\bar{1}$0]//[01$\bar{1}$0]	13.8	Coincidence
	[01$\bar{1}$0]//[2$\bar{1}$$\bar{1}$0]	13.8	
(0001)//(2$\bar{1}$$\bar{1}$0)	[01$\bar{1}$0]//[01$\bar{1}$0]	−0.4	Non Coincidence
	[2$\bar{1}$$\bar{1}$0]//[0001]	1.9	
(2$\bar{1}$$\bar{1}$0)//(01$\bar{1}$2)	[01$\bar{1}$0]//[2$\bar{1}$$\bar{1}$0]	13.8	Coincidence
	[0001]//[0$\bar{1}$11]	1.1	

(01$\bar{1}$0) – M-Plane, (0001) – C-Plane, (2$\bar{1}$$\bar{1}$0) – A-Plane, (01$\bar{1}$2) – R-Plane.



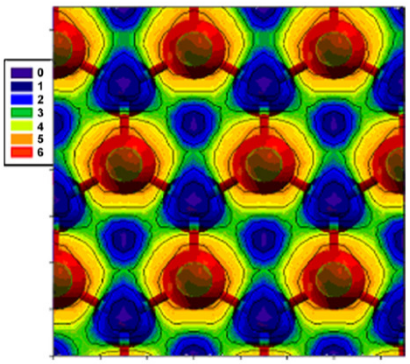


Fig. 1. PES of a Ga adatom on the N terminated (0 0 0 1) GaN surface. The *Y*-axis corresponds to the (1 −2 1 0) direction while the *X*-axis corresponds to the (0 1 −1 0) direction. The color scale corresponds to the relative binding energy of the adatom at each spot on the surface.

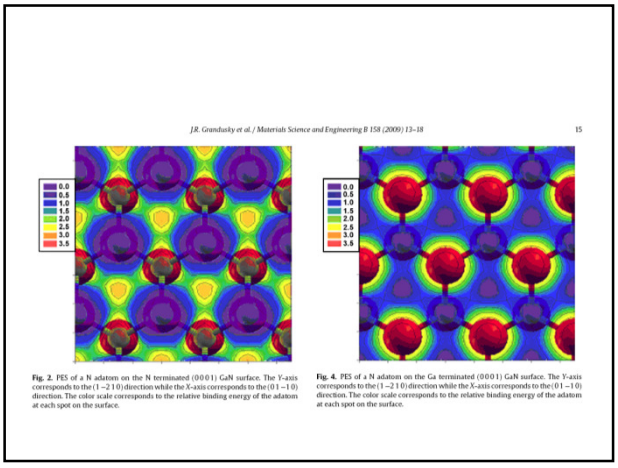


Fig. 2. PES of a N adatom on the N terminated (0 0 0 1) GaN surface. The *Y*-axis corresponds to the (1 −2 1 0) direction while the *X*-axis corresponds to the (0 1 −1 0) direction. The color scale corresponds to the relative binding energy of the adatom at each spot on the surface.

Fig. 4. PES of a N adatom on the Ga terminated (0 0 0 1) GaN surface. The *Y*-axis corresponds to the (1 −2 1 0) direction while the *X*-axis corresponds to the (0 1 −1 0) direction. The color scale corresponds to the relative binding energy of the adatom at each spot on the surface.

Conclusão

Conclusão

- Epitaxia

- Camadas de alta qualidade
- Junções / Hetero-estruturas
- Depende da concordância entre parâmetros de rede e bandgaps

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Como faço para crescer camadas epitaxiais de alta qualidade ?

Resposta: MBE