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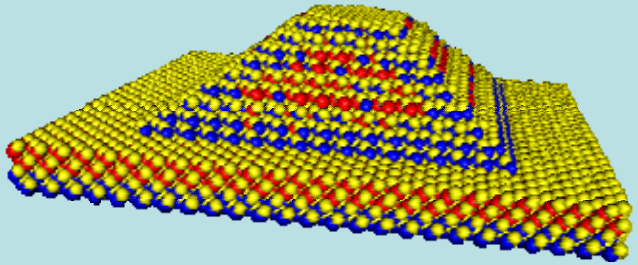
Microelectronics and Nanostructures group

The use of Abel-Tersoff potentials in atomistic simulations of InGaAsSb/GaAs

V. Haxha, M.A. Migliorato, R. Garg, I.W. Drouzas, J. M. Ulloa, P. M. Koenraad, M. J. Steer, H. Y. Liu, M. Hopkinson, D. J. Mowbray



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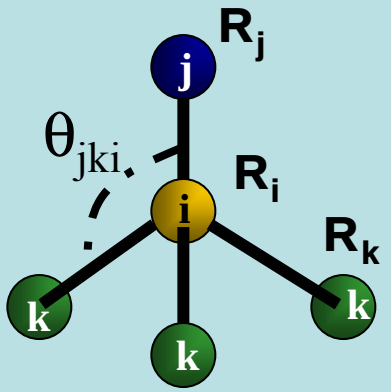
Overview

- Introduction: Empirical Potential Methods
- Abel-Tersoff Potential
  - parameterization of InSb, GaSb, GaAs, InAs
- Modelling of low dimensional Semiconductors
  - Modelling strain energy of Quantum Wells
  - Modelling Quantum Dots
- Segregation
  - Kinetic model of segregation for coupled group III and V exchange processes
- Conclusions & Acknowledgements

Valence Force Field

"force field" represented as a 3 body potential.

$$V_{VFF} = \sum_{ij} V_2(R_i - R_j) + \sum_{ij} V_3(\hat{\theta}_{ijk})$$



$$V_2 = \frac{1}{2}\sum_{i}^{nn}\sum_{j}\frac{3\alpha_{ij}}{8\cdot(d_{ij}^0)^2}\left[(R_i - R_j)^2 - (d_{ij}^0)^2\right]^2$$

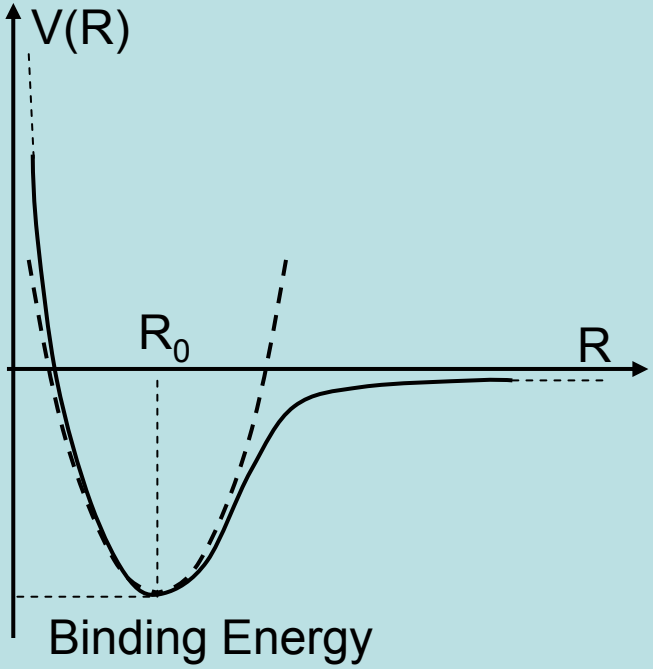
$$V_3 = \frac{1}{2}\sum_{i}^{nn}\sum_{j,k>i}\frac{3\beta_{i,jk}}{8\cdot(d_{ij}^0)^2}\left[(R_j - R_i)\times(R_k - R_i) - (d_{ij}^0)^2\cos\theta_0\right]^2$$

d_{ij}^0 : unstrained bond length between *i* and *j*
θ_0 is the unstrained bond angle
θ_{ijk} is the angle between *i*, *j* and *k*.
two parameters α and β are fitted to the elastic constants

P.N. Keating, Phys. Rev. 145, 637 (1966)

Valence Force Field

Parabolic approximation to the potential of solids

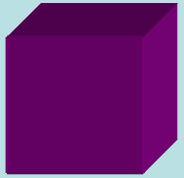


Ω : volume occupied by one atom

The main limitation is that there are only 2 parameters (α and β) but 3 elastic constants even for Zincblende!!!

Uniform: same distortion in x,y and z

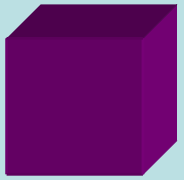
$$B = \frac{1}{\Omega}\frac{d^2E}{dv^2}\bigg|_{E=Ecoh}$$



$$R^1 = v^{\frac{1}{3}}R$$

Non Uniform: z stretch, x,y compress (by the same amount) and viceversa

$$C' = \frac{1}{\Omega}\frac{d^2E}{d\varepsilon^2}\bigg|_{E=Ecoh}$$

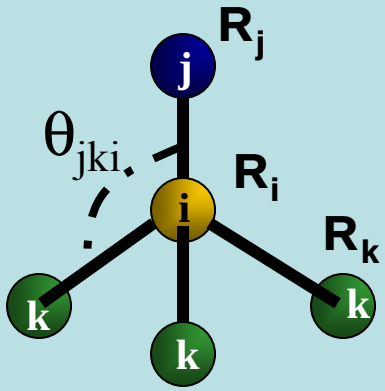


$$R_x^1 = R_x(1+\varepsilon)$$
$$R_y^1 = R_y/(1+\varepsilon)$$
$$R_z^1 = R_z$$

Stillinger-Weber

$$V_{SW} = \sum_{ij}^{nn} V_2(r_{ij}) + \sum_{ijk}^{nn} V_3(r_{ij}) \cdot \left(\cos\theta_{ijk} + \frac{1}{3} \right)^2$$

$$V_2 = \frac{1}{2} \sum_i \sum_j^{nn} A\left(B r_{ij}^{-p} - r_{ij}^{-q} \right) \cdot e^{\left(r_{ij} - a\right)^{-1}}$$



This in an adaptation of the well known Lennard-Jones potential used for liquefied noble gasses.

$$V_3 = \frac{1}{2} \sum_i \sum_{j,k>i}^{nn} \lambda e^{\left(\gamma\left(r_{ij} - a\right)^{-1} + \gamma\left(r_{ik} - a\right)^{-1} \right)} \cdot \left(\cos\theta_{ijk} + \frac{1}{3} \right)^2$$

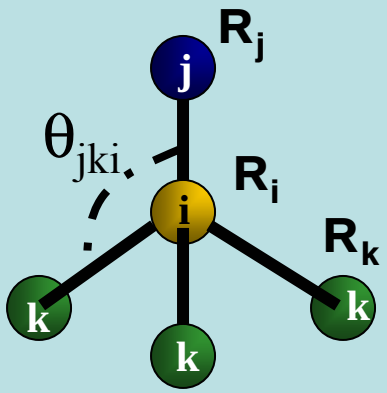
Works reasonably well for diamond-Si but not for other crystal structures.

F. Stillinger and T. A. Weber, Phys. Rev. B 31, 5262 (1985)

Tersoff Potential

$$V_{ij} = A_{ij}\, e^{\left(-\alpha_{ij}(r_{ij}-r_e)\right)} - b_{ij} B_{ij}\, e^{\left(-\beta_{ij}(r_{ij}-r_e)\right)}$$

$$b_{ij} = \left[1+\left(\gamma_{ij}\zeta_{ij}\right)^{n_i}\right]^{-1/2n_i}$$



The expression for b_{ij} (known as bond order) is written as to emulate the atomic coordination number Z. Hence ζ is sometimes called the pseudo-coordination.

$$\zeta_{ij} = \sum_{k\neq i,j} f_c(r_{ik})\, g(\theta_{ijk}) \cdot \omega_{ijk}$$

g(θ) and ω describe the angular and radial forces dependence.

$$g(\theta_{ijk}) = 1 + \left(\frac{c_i}{d_i}\right)^2 - \frac{c_i^2}{d_i^2 + (h_i - \cos\theta_{jki})^2} \qquad \omega_{ijk} = e^{\left[\lambda^3 (r_{ij}-r_{ik})^3\right]}$$

Tersoff Potential

$$g(\theta_{ijk}) = 1 + \left(\frac{c_i}{d_i}\right)^2 - \frac{c_i^2}{d_i^2 + (h_i - \cos\theta_{jki})^2}$$

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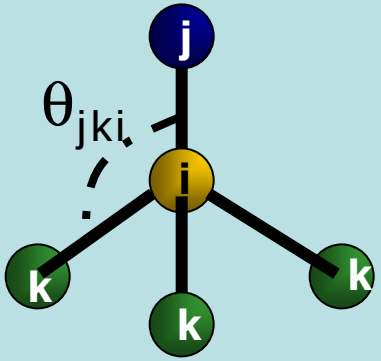
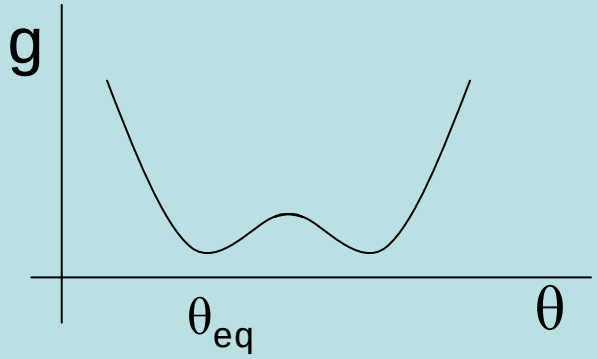
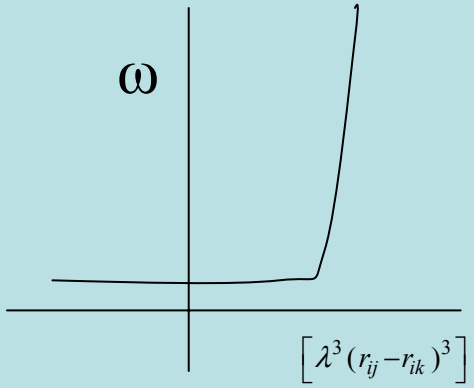






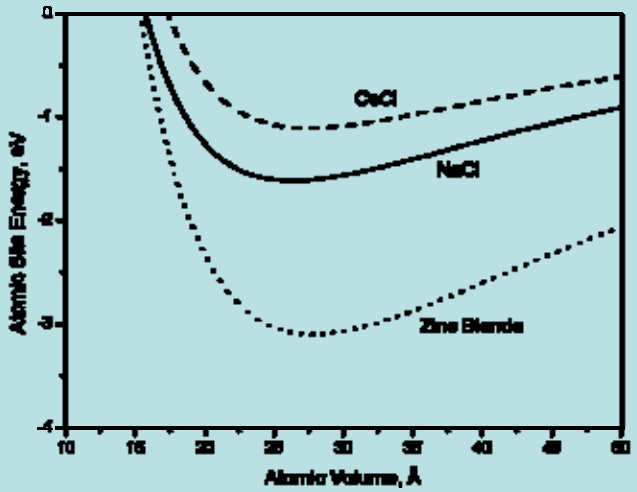
angular forces: resistance to bend
radial forces: resistance to stretch

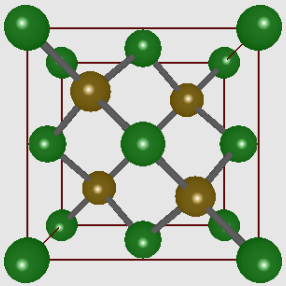
- This potential describes covalent bonding
- Works very well for different crystal structures for group IV
- Despite the partial ionicity of the bond also very good for group III-V.
- Many parameters to fit.

J. Tersoff, Phys Rev Lett 56, 632 (1986) & Phys Rev B 39, 5566 (1989)

Tersoff Potential

Better than VFF as it is not a parabolic approximation
Many parameters but also many properties correctly reproduced like the phase diagram, C44 and the Kleinman deformation





$$c_{44} = \frac{1}{\Omega}\frac{d^2 E_{coh}}{d\gamma^2}\bigg|_{E=E_{coh}}$$

$$R_x' = R_x + \gamma R_y$$
$$R_y' = R_y$$
$$R_z' = R_z$$

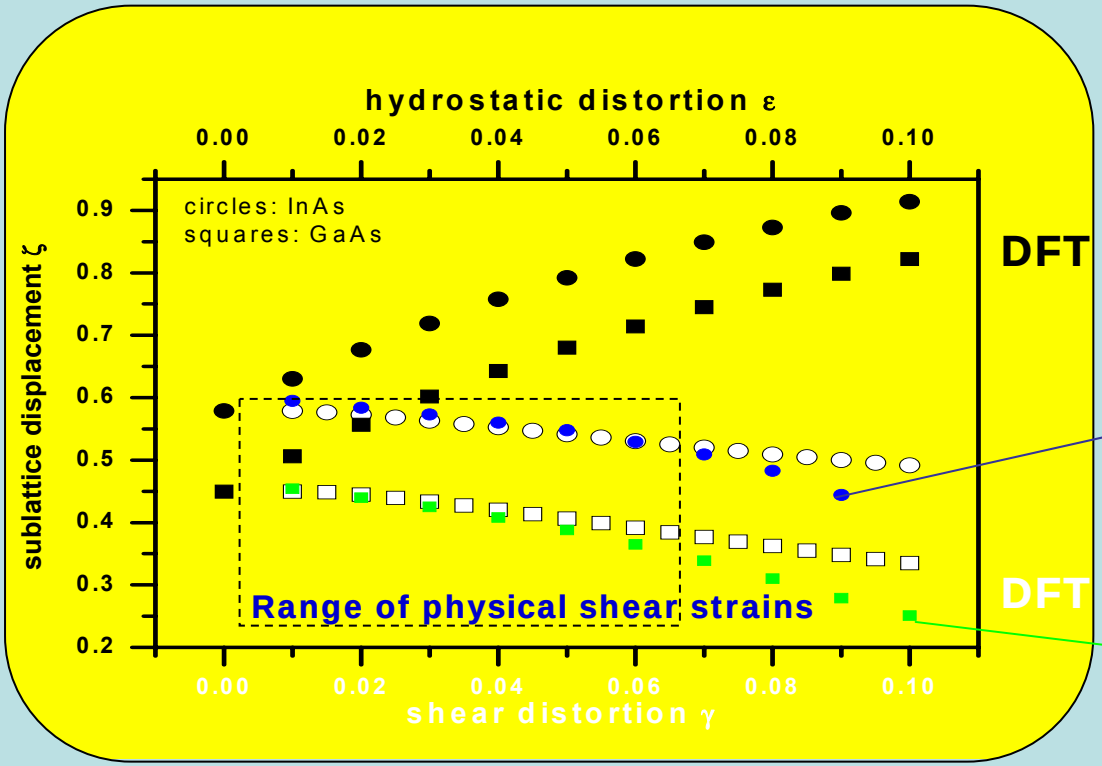
Works rather well for zincblende and diamond group IV and III-V but it is not yet optimized for thermodynamic and vibrational properties.

D. Powell, M.A. Migliorato and A.G. Cullis, Phys. Rev. B 75, 115202 (2007)

Potential Energy Function (PEF)

Parameterisation are now available for all III-Vs.

	Ga-As	In-As	Ga-Sb	In-Sb
D_e	1.7804	1.7684	2.1042	1.8929
S	6.9602	1.3275	1.4339	3.0262
β	1.5665	1.4987	1.4777	1.4378
r_e	2.4324	2.5693	2.4991	2.7203
R	3.6	3.8	3.6	3.6
R_{cut}	3.4	3.6	3.4	3.4
c	2.1634	2.1003	1.2087	5.3212
d	0.7501	0.8276	0.8397	1.3991
h	-0.4488	-0.4421	-0.4277	-0.4895
n	3.5558	2.3507	4.6022	1.8926
γ	0.2571	0.1396	0.3630	0.3043
λ	0.2443	0.1408	0.9686	2.4767



Tersoff

Tersoff

D. Powell, M.A. Migliorato and A.G. Cullis, Phys. Rev. B 75, 115202 (2007)

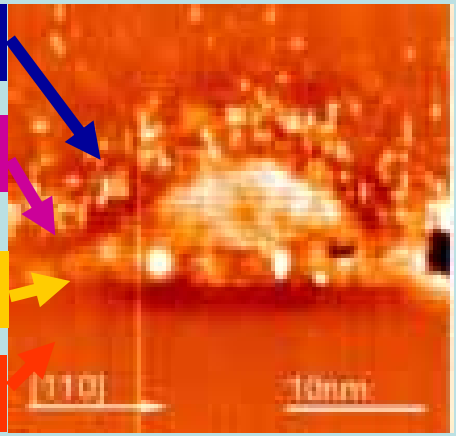
Decomposition into InGaAs and GaSbAs

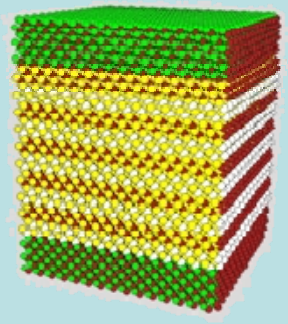
GaSbAs

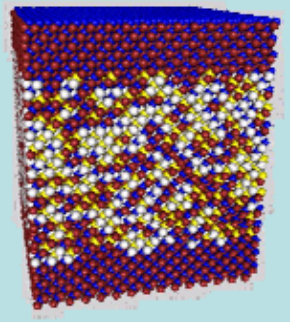
In & Sb depleted

In rich InGaAs

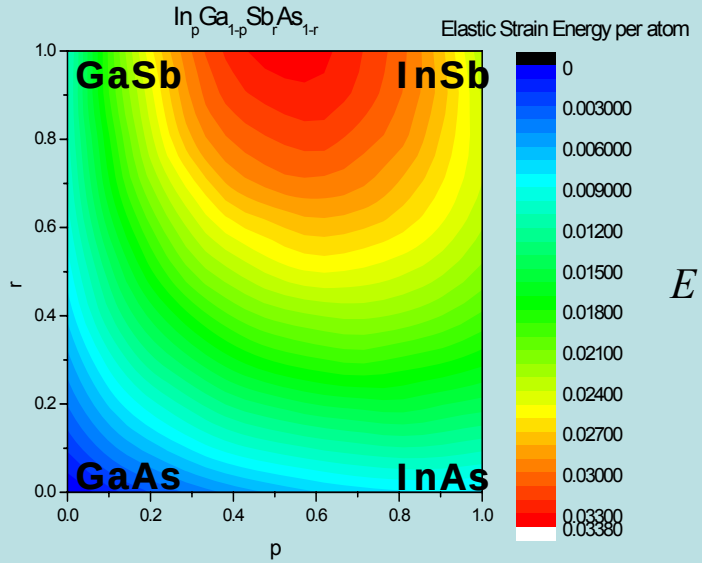
GaAs Buffer



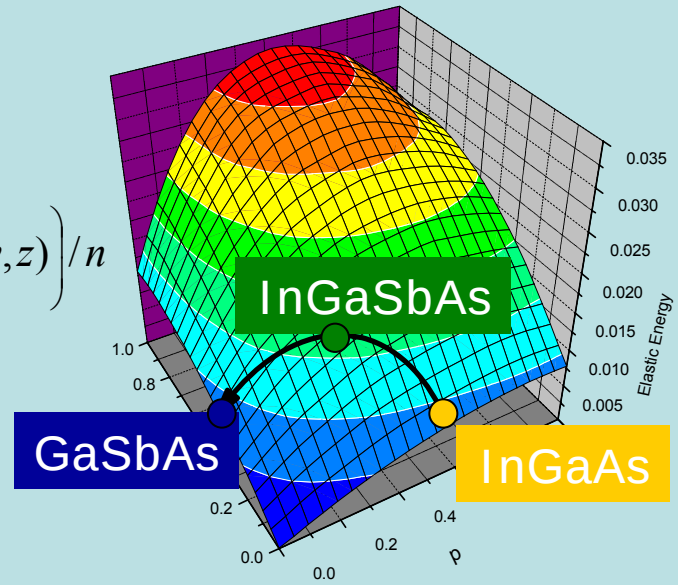




*** The structures have been relaxed using mpi IMD™ software**

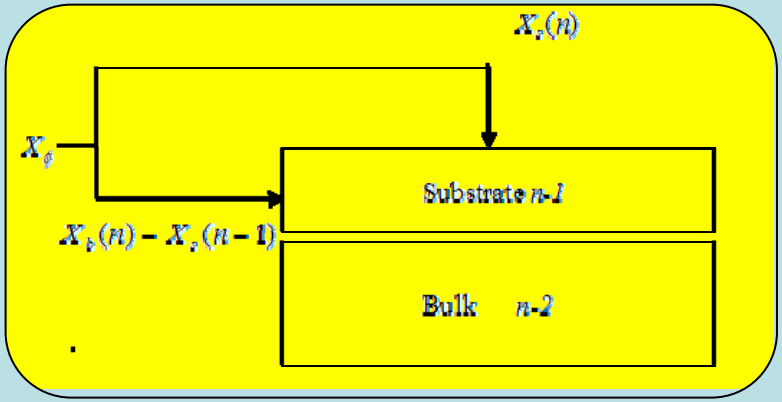


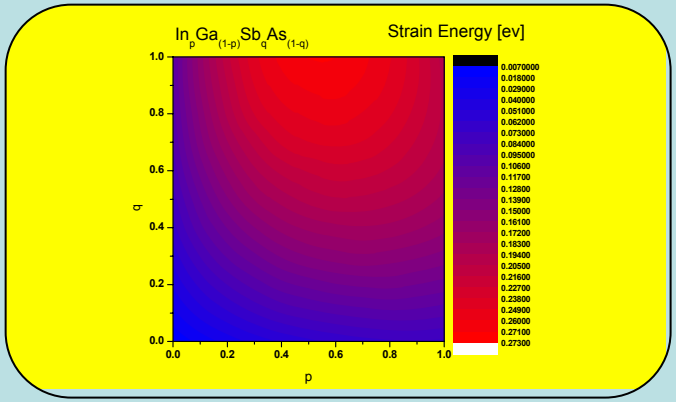
$$E = \left(\sum_{i=0}^{n} F(x,y,z) \right) / n$$



Segregation

Surface segregation is the physical effect which can happen during the epitaxial growth of different materials, resulting in one or more atomic species not being incorporated in the crystal but rather segregate on the growing surfaces.





Un-coupled In/Sb :

$$P_1 = v_1 e^{-\frac{E_1}{kT}} \qquad P_2 = v_2 e^{-\frac{E_2}{kT}} \qquad E_2 = E_1 + E_s$$

$$\frac{dX_{In}^{(s)}(t)}{dt} = \phi_{Iin} + P_1 X_{In}^{(b)}(t) X_{Ga}^{(s)}(t) - P_2 X_{In}^{(s)}(t) X_{Ga}^{(b)}(t)$$

$$X_{In}^{(s)}(t) + X_{In}^{(b)}(t) = X_{In}^{(s)}(0) + X_{In}^{(b)}(t) + \phi_{In} t$$

$$X_{In}^{(s)}(t) + X_{Ga}^{(s)}(t) = X_{In}^{(s)}(0) + X_{Ga}^{(s)}(0) + (\phi_{In} + \phi_{Ga}) t$$

Coupled In/Sb :

$$P_1 = v_1 e^{-\left(\frac{E_1}{kT} - \frac{E_{SE}}{kT}\right)}$$

$$P_2 = v_2 e^{-\left(\frac{E_2}{kT} + \frac{E_{SE}}{kT}\right)}$$

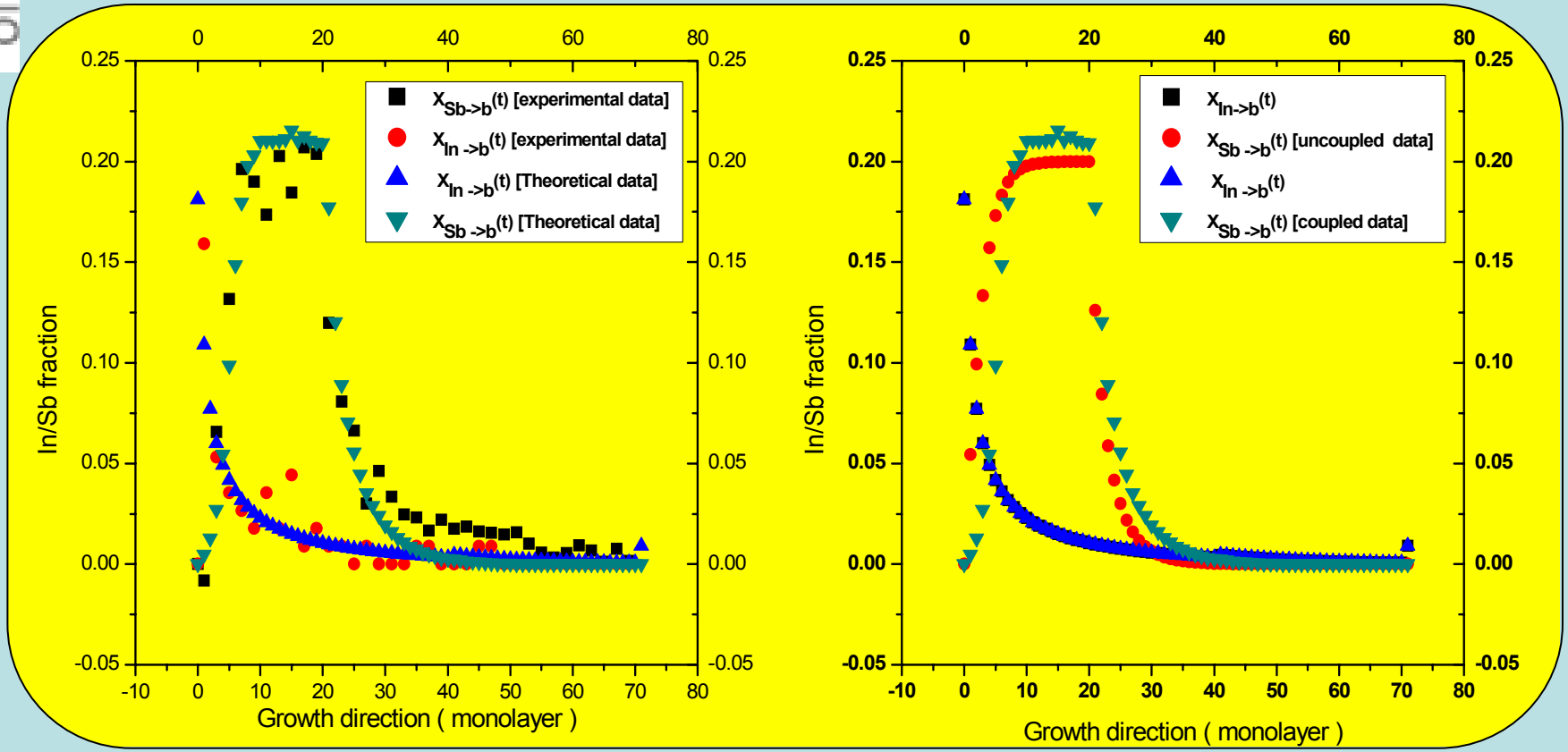
$$E_{SE} = E_{StrainEnergy}\left(X_{In \to S}(t), \phi_{Sb}\right) - E_{StrainEnergy}\left(0.0, \phi_{Sb}\right)$$

O.Dehaese, X. Wallart, and F. Mollot, Appl. Phys. Lett. 66, 52 (1995)

Segregation

The coupled In/Sb concentration profile, compared with experimental data

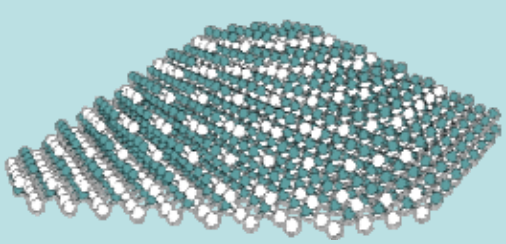
- Substrate 7Å Temp: 500°C,
- DWELL: 60Å, Temp : 475°C
- Covered with 100Å, Temp: 475°C
- And Than 500Å, 590°C
- QD growth rate: 0.094ML/s

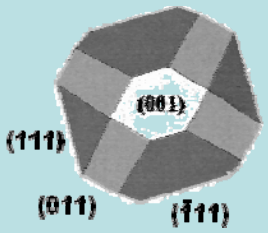


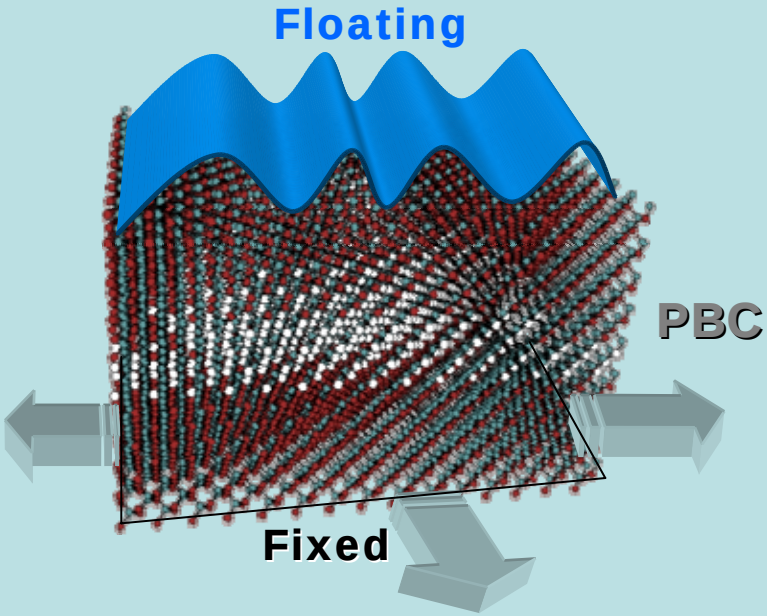
Molecular Dynamics of Quantum Dots

* unrelaxed $e_{xx} = e_{yy}$ -0.667, e_{zz} = 0.7 as expected

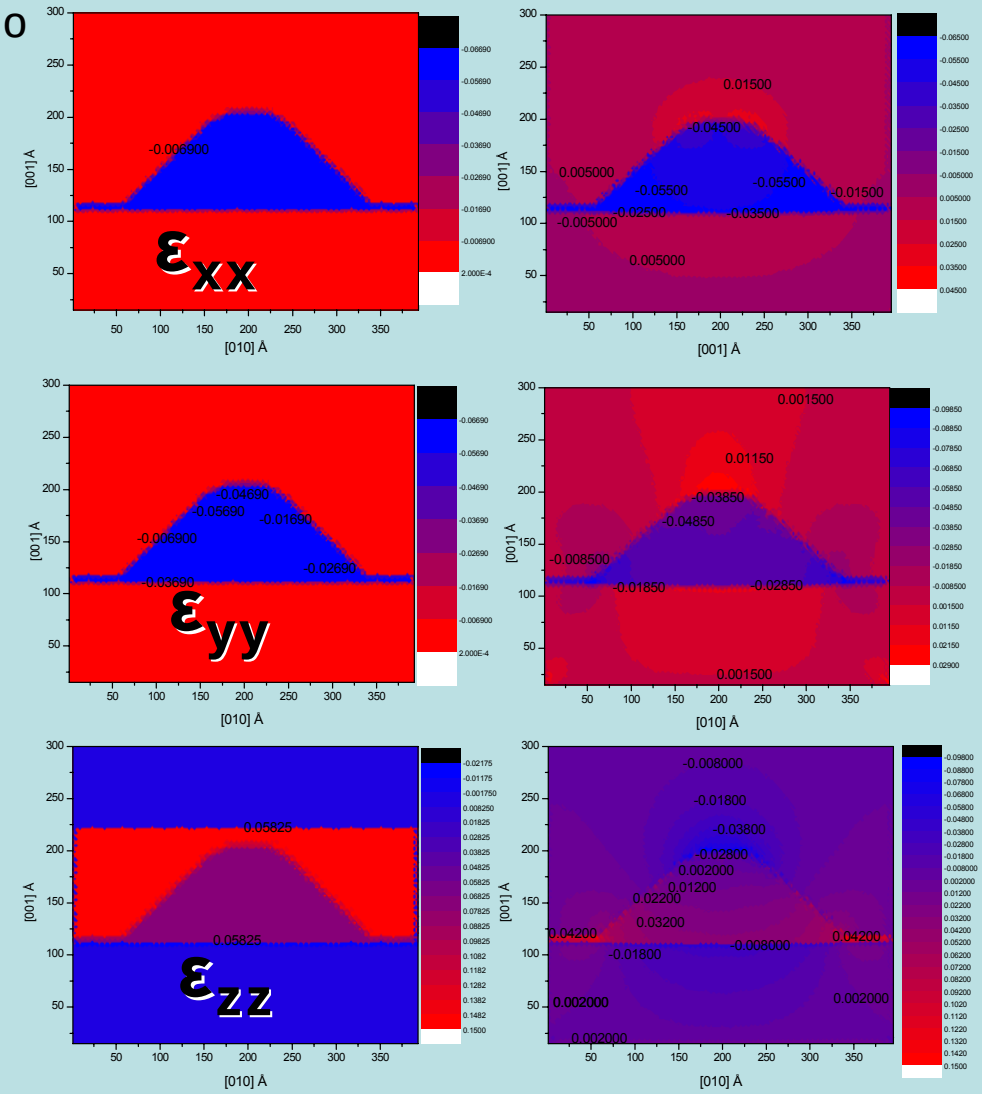
* Relaxed e_{xx} and e_{yy} and e_{zz} vary
* Strain component e_{zz} is almost zero at the top of the island







Before MD ⇒ **After MD**



G. Costantini, C. Manzano, R. Songmuang, O.K. Schmidt, and K. Kern, Appl. Phys. Lett. 82, 3194 (2003)

Conclusions & Acknowledgements

- It is now possible to implement 3 Million Atom simulations using the Tersoff potential, which is available for all III-V semiconductors and their alloys
- We have modelled the elastic strain Energy of InGaAsSb and explained the experimental observations of decomposition into ternary alloys
- We have used the results in conjunction with a new improved model of segregation showing very good agreement with the experimental data.
- We have also simulated very large Quantum Dots.

Many thanks and gratitude go to:
- **M.A. Migliorato, R. Garg (Manchester)**
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- **J. M. Ulloa, P. M. Koenraad (Eindhoven)**
- **H. Y. Liu (University College London)**
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