

Crystal Growth: Physics, Technology and Modeling

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Lecture 14. Not solved problems

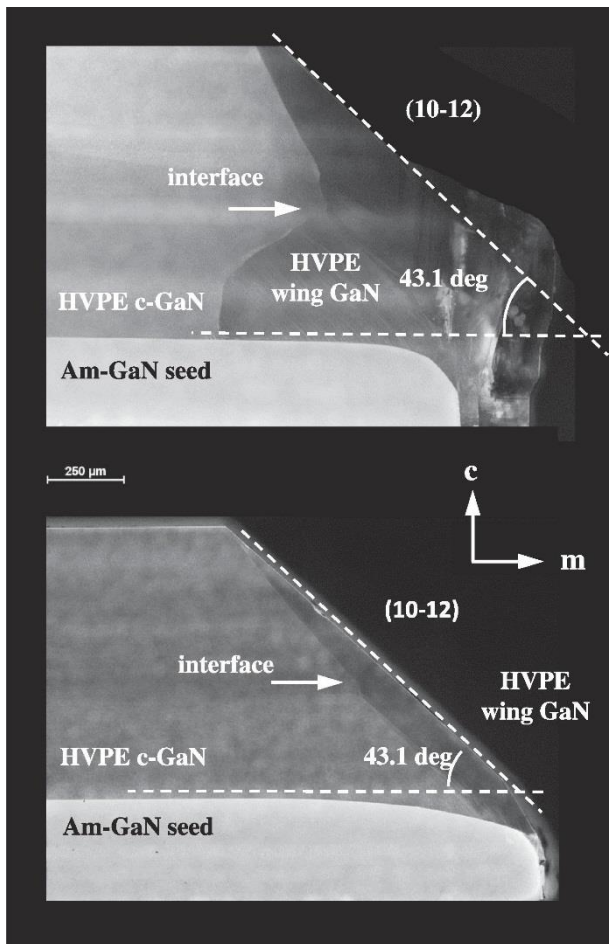
<http://w3.unipress.waw.pl/~stach/cg-2022-23/>

List of the problems

- **Incorporation of point defects during growth**
- **Shape selection during growth**
- **Strain influence on growth**

Incorporation of point defects during growth

- **Growth of GaN by HVPE method**



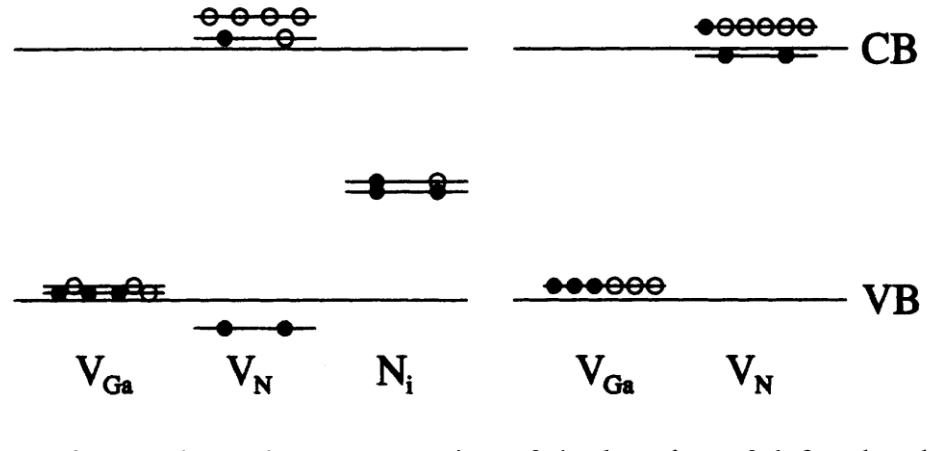
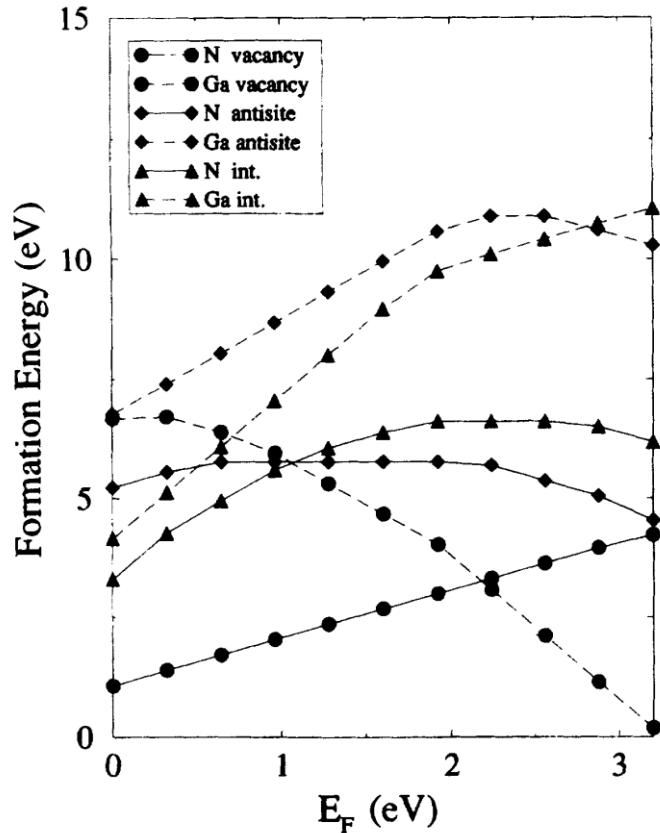
*T. Sochacki, et al.,
J. Cryst. Growth 556(2021) 125986*

Incorporation of point defects during growth – *ab initio*

- Defect formation energy (native - GaN)

$$E^f(q) = E^{tot}(q) - n_{Ga}\mu_{Ga} - n_N\mu_N - qE_F$$

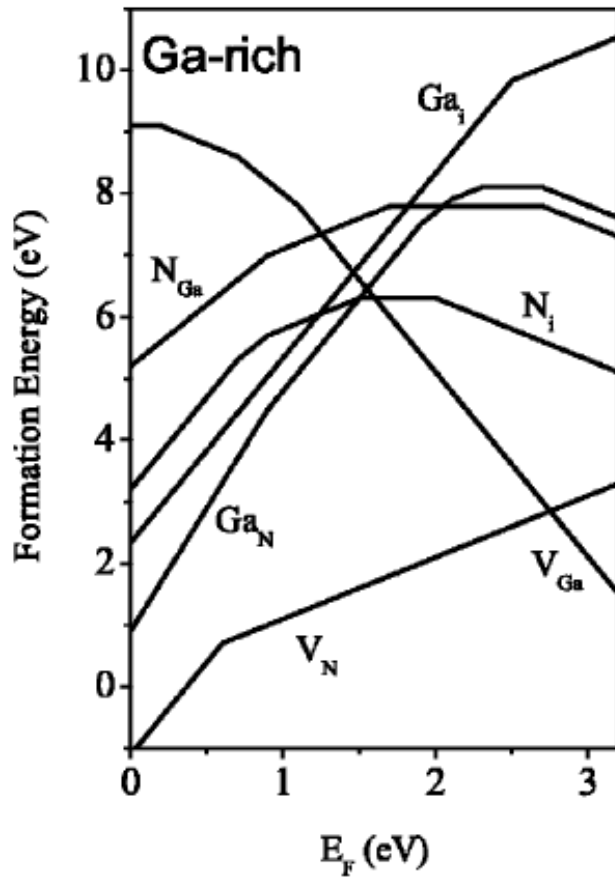
$$\mu_{Ga} + \mu_N = \mu_{GaN}$$



*J. Neugebauer & C Van de Walle,
Phys. Rev. B 50 (1994) 8067*

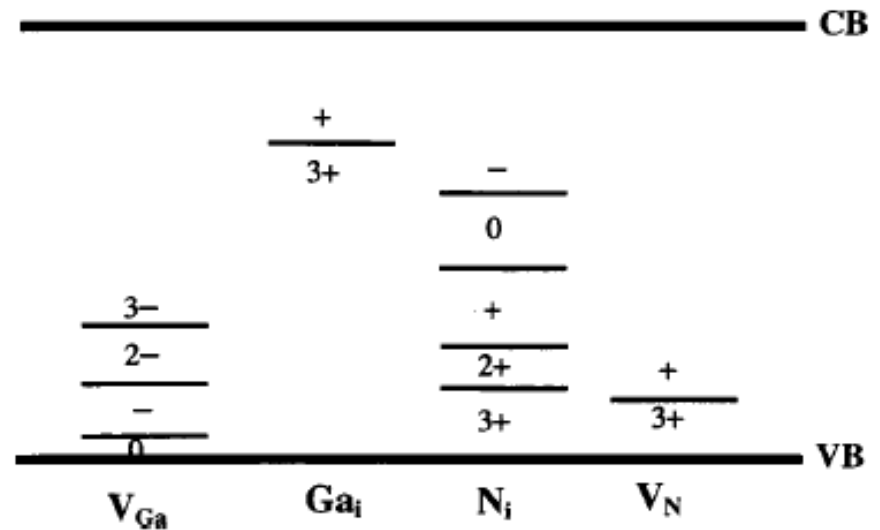
Incorporation of point defects during growth – *ab initio*

- Defect formation energy (native - GaN)



$$E^f(q) = E^{tot}(q) - n_{Ga}\mu_{Ga} - n_N\mu_N - qE_F$$

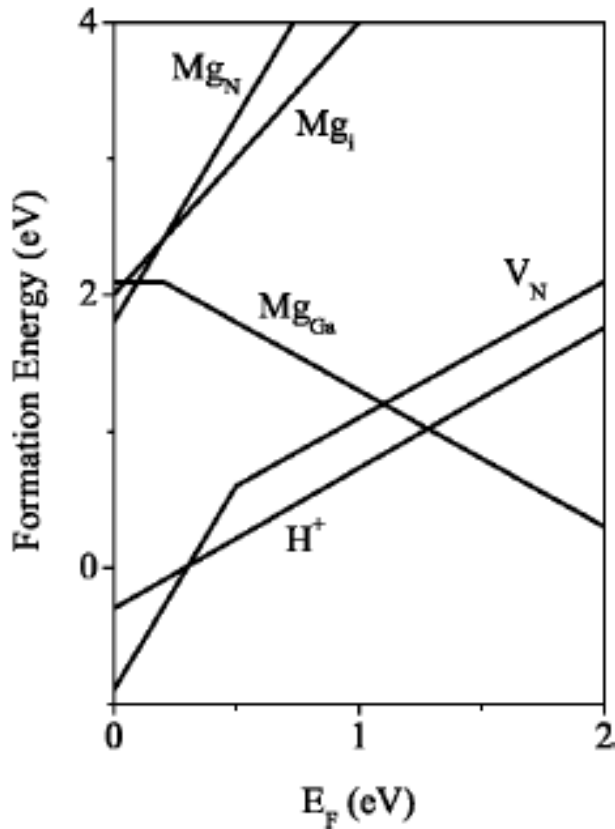
$$\mu_{Ga} + \mu_N = \mu_{GaN}$$



C Van de Walle & J. Neugebauer, J. Appl. Phys. 95 (2004) 3865

Incorporation of point defects during growth – *ab initio*

- Defect formation energy (Mg - GaN)



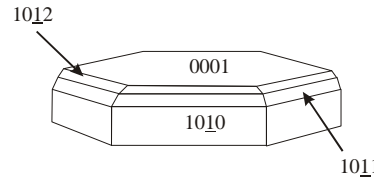
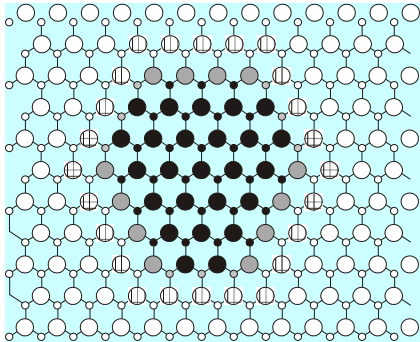
$$E_i^f(q) = E^{tot}(q) - n_{Mg}\mu_{Mg} - qE_F$$

$$E_{MgN}^f(q) = E^{tot}(q) - n_{Mg}\mu_{Mg} + n_N\mu_N - qE_F$$

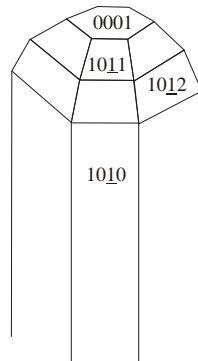
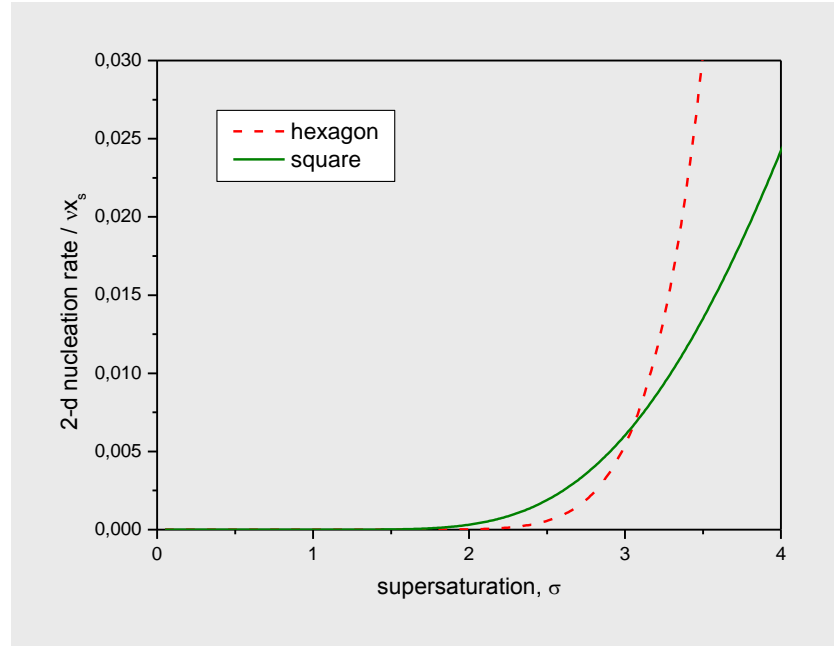
$$E_{MgGa}^f(q) = E^{tot}(q) - n_{Mg}\mu_{Mg} + n_{Ga}\mu_{Ga} - qE_F$$

**C Van de Walle & J. Neugebauer,
J. Appl. Phys. 95 (2004) 3865**

Shape selection during growth - GaN wurtzite lattice



$$I = \nu x_s \left(\frac{6\phi}{\Delta\mu} + 6 \right) \exp \left[-\frac{1}{kT} \left(\frac{3\phi^2}{\Delta\mu} - \frac{\Delta\mu}{4} \right) \right]$$

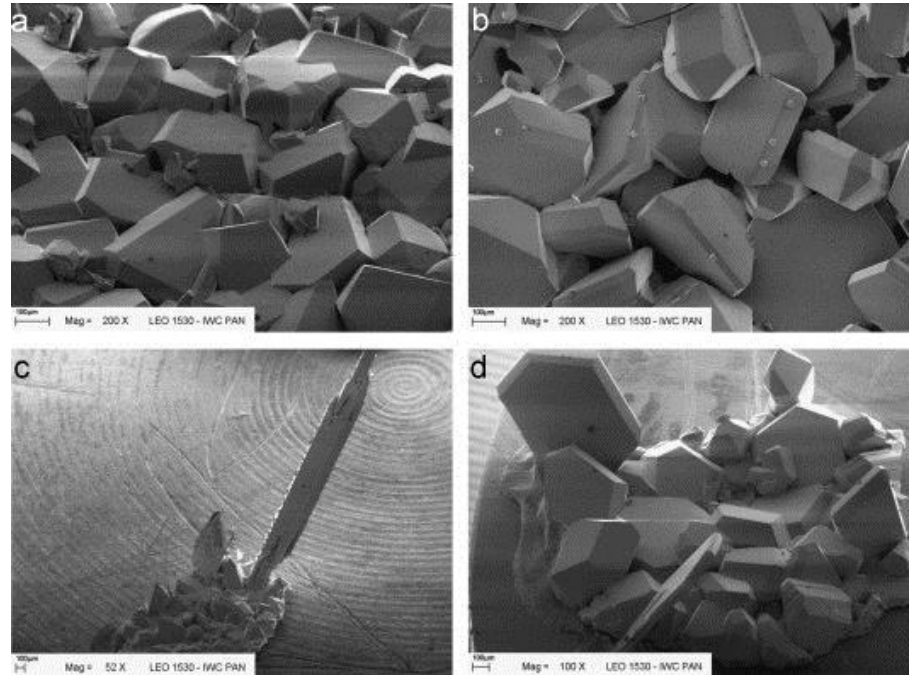
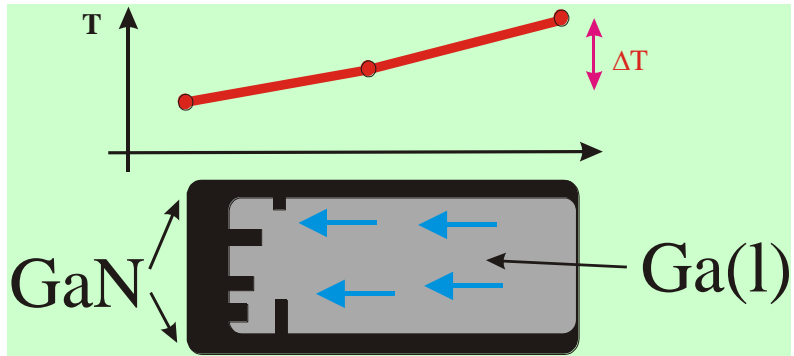


$$I = \nu x_s \left(\frac{4\phi}{\Delta\mu} - 1 \right) \exp \left[-\frac{1}{kT} \left(\frac{2\phi^2}{\Delta\mu} - \frac{\Delta\mu}{8} \right) \right]$$

Diagram recovers:
-Growth anisotropy
-Acceleration of the growth along (0001) direction for high supersaturation

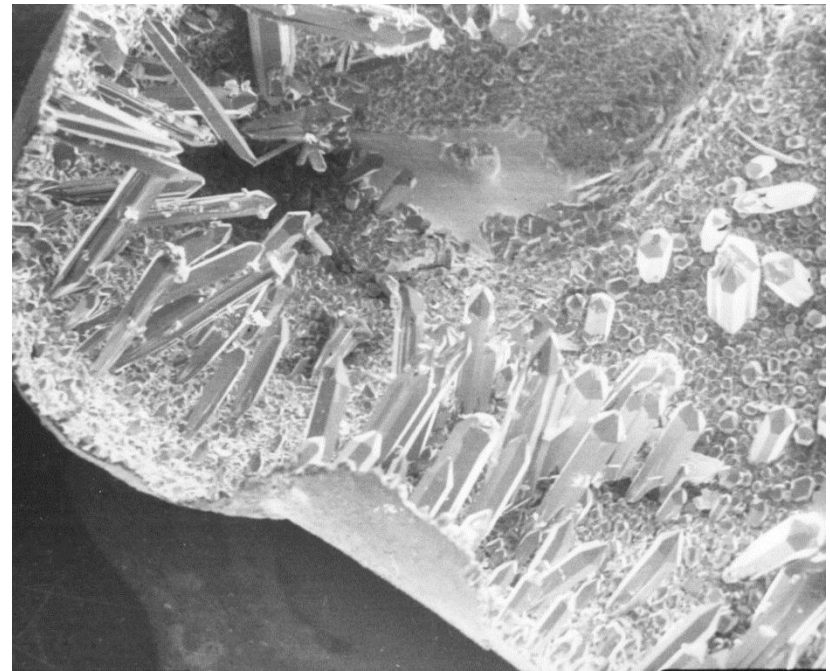
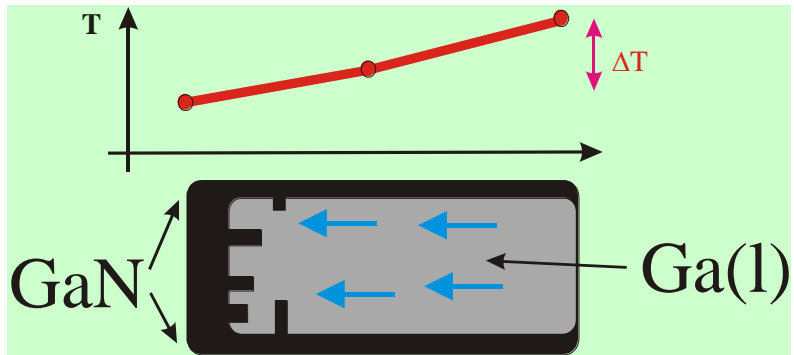
*I. Grzegory et al. ,
 J. Cryst. Growth 246 (2002) 177*

Shape selection during growth



***M. Boćkowski et al. ,
J. Cryst. Growth 305 (2007) 414***

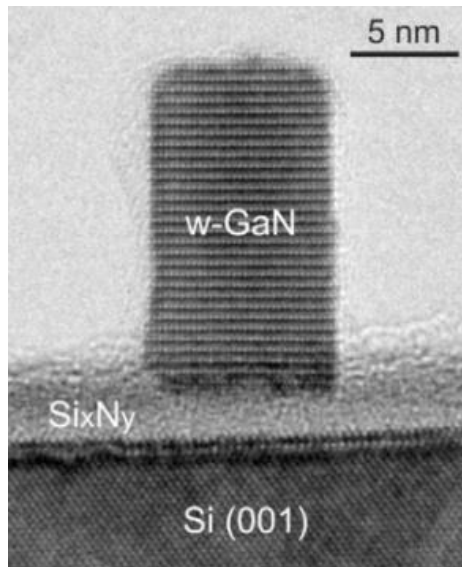
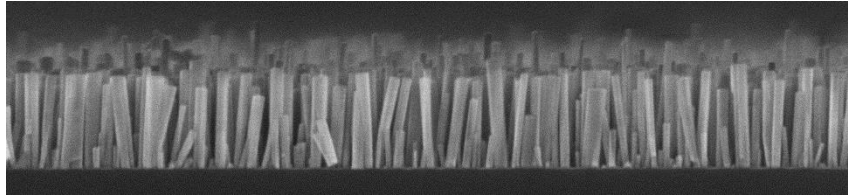
Shape selection during growth



***M. Boćkowski et al. ,
J. Cryst. Growth 305 (2007) 414***

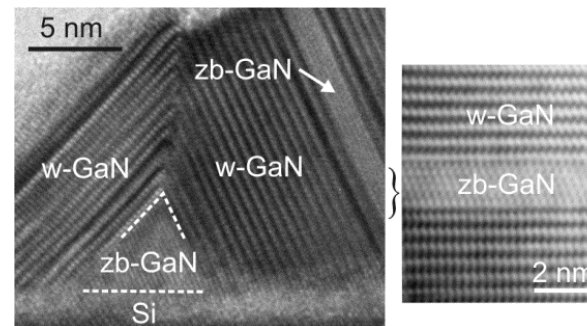
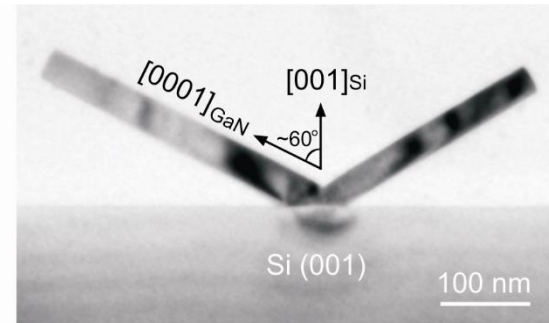
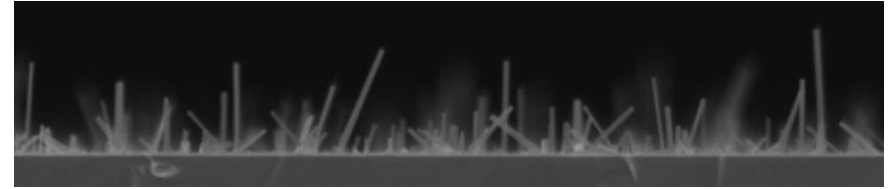
Shape selection during MBE growth (GaN on Si(001)) - rods

- Non-epitaxial growth

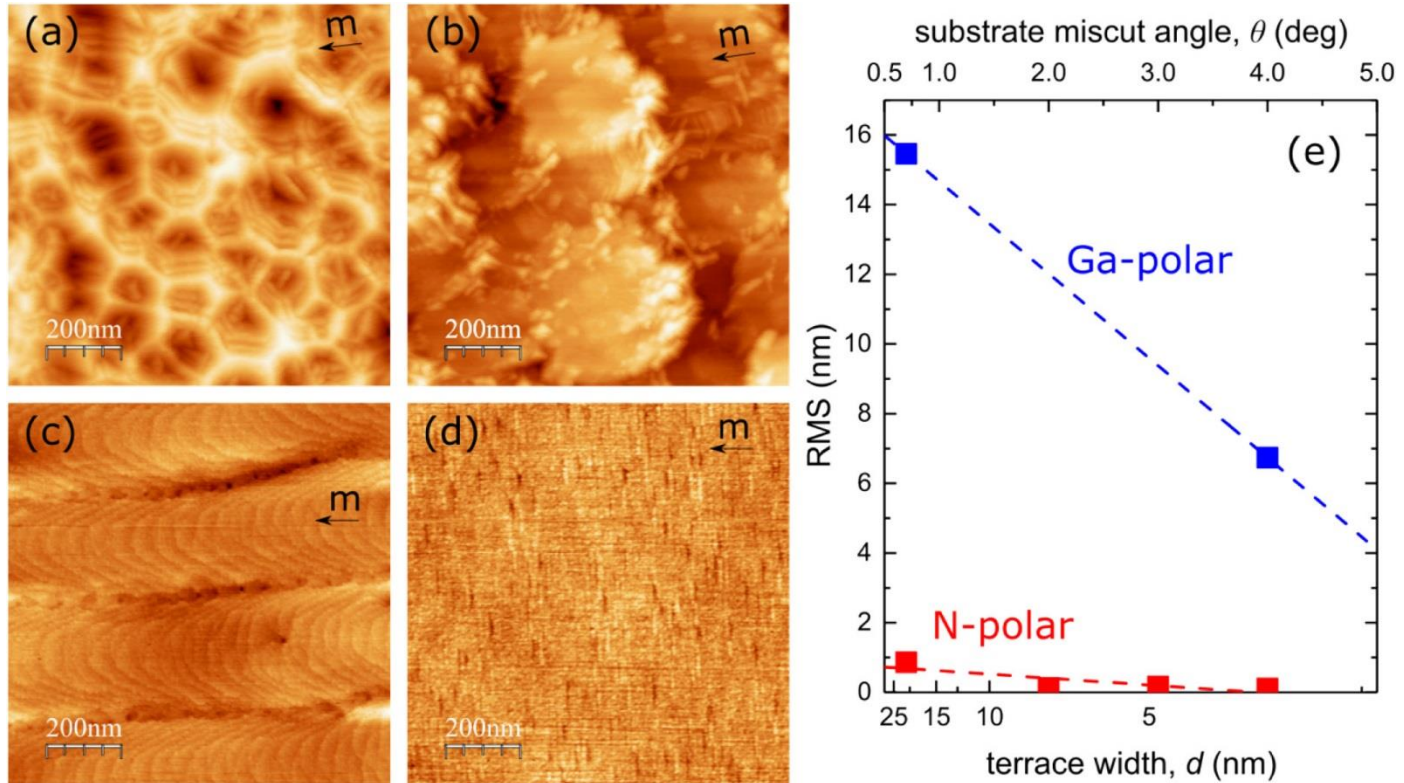


***A. Wierzbicka et al. ,
Nanotechnology 35 (2013) 035703***

- Epitaxial growth



Shape selection during MBE growth (GaN on Si(001)) - plates



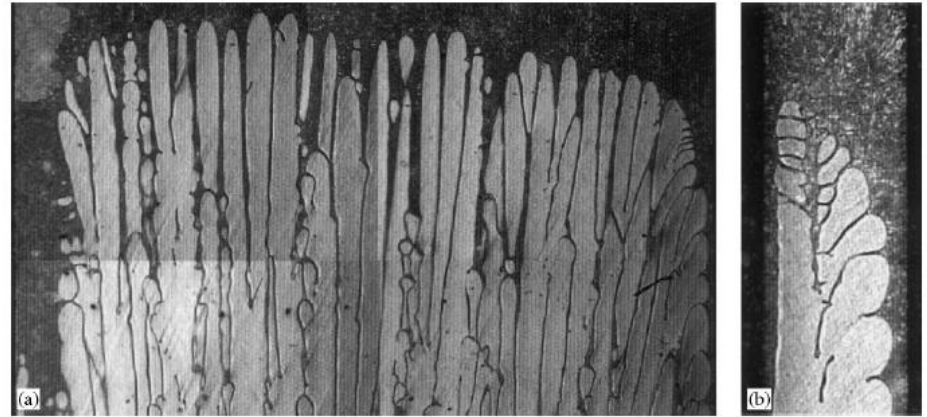
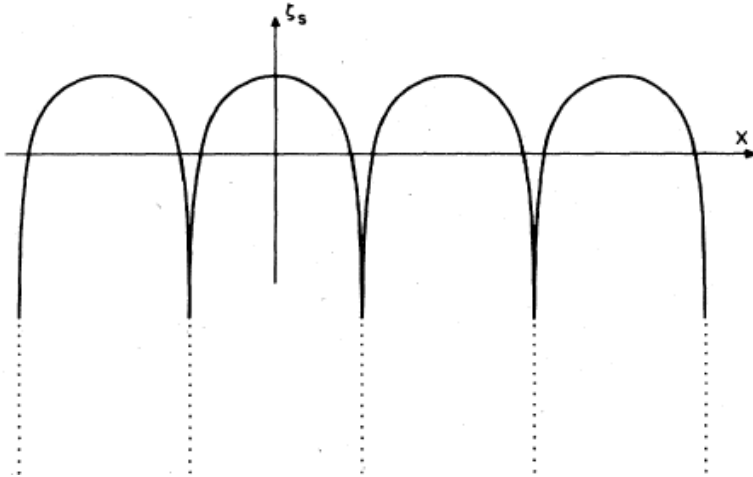
***H. Turski et al. ,
Appl. Surf. Sci. 484 (2019) 771***

Shape selection during growth of snow crystals - dendrites



<http://www.its.caltech.edu/~atomic/snowcrystals/photos/photos.htm>

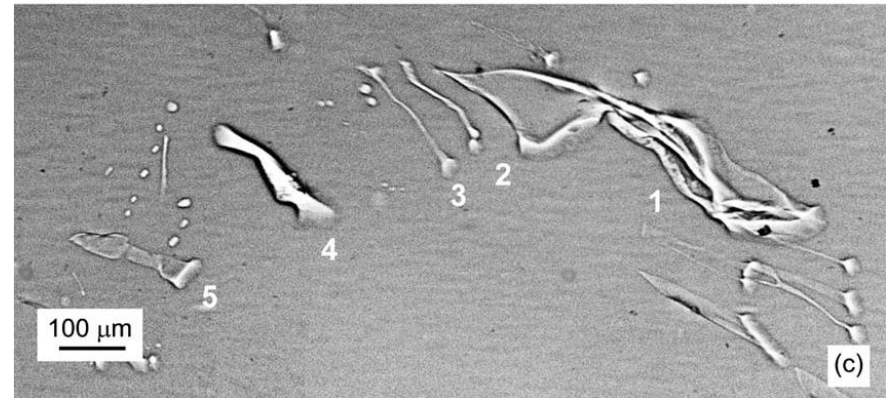
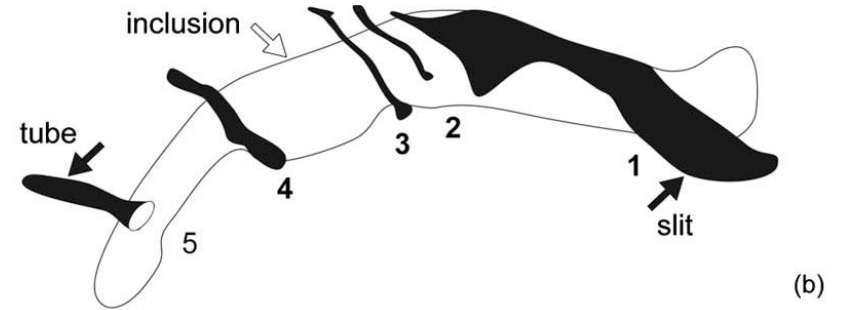
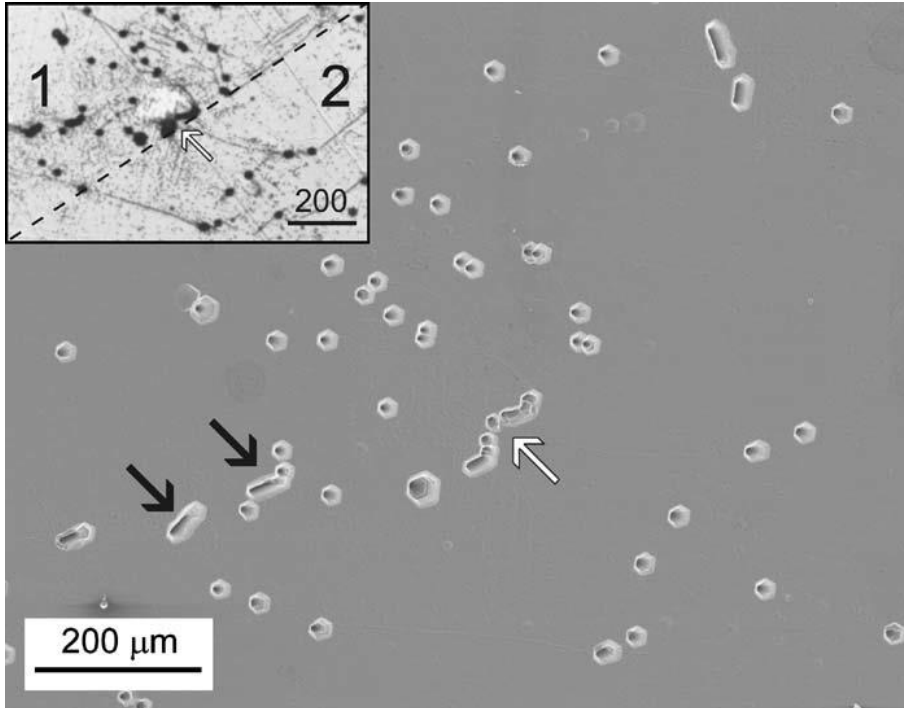
Shape selection – cellular growth



- Al-4% Cu alloy

R. Trvedi et al. J. Cryst. Growth 222 (2001) 365

SiC- polytypes, micropipes & inclusions



**M. Yu. Gutkin et al. J. Appl. Phys. 106 (2009)
123515**

Strain influence on the growth – dislocations

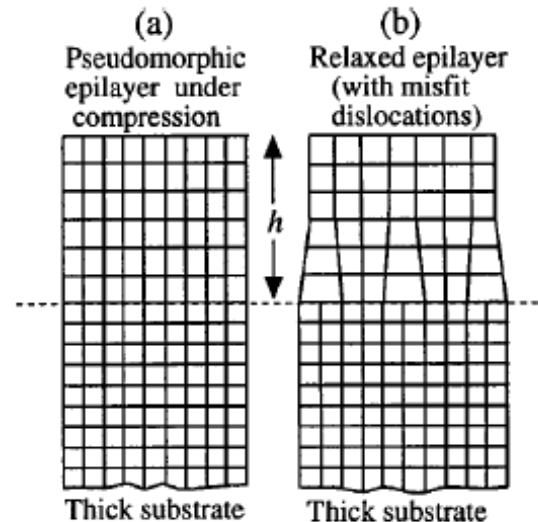
- Lattice misfit

$$f_m = \frac{a_{lay} - a_{sub}}{a_{sub}}$$

- Critical thickness - h_c

$$h_c = \frac{b(1 - \nu \cos^2 \beta)}{8\pi f_m (1 + \nu) \cos \beta} \ln \left(\frac{\rho_c h_c}{q} \right)$$

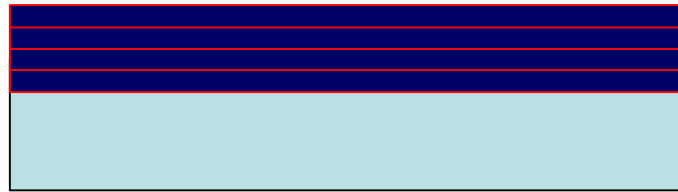
- Core cutoff parameter - $q \approx b$
- Burgers vector – b , angle - β



*S.C. Jain, M. Wilander, J. Narayan, R Van Overstaeten,
J. Appl. Phys. 87 (2000) 965*

Strain influence on the growth – epitaxial growth modes

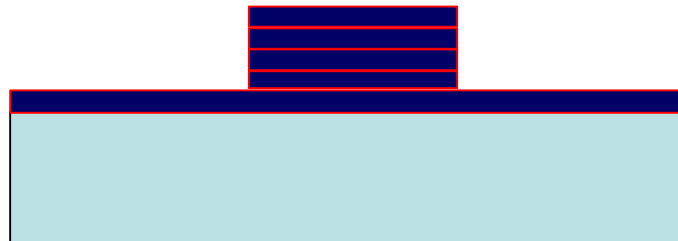
- **Frank-van der Merve**



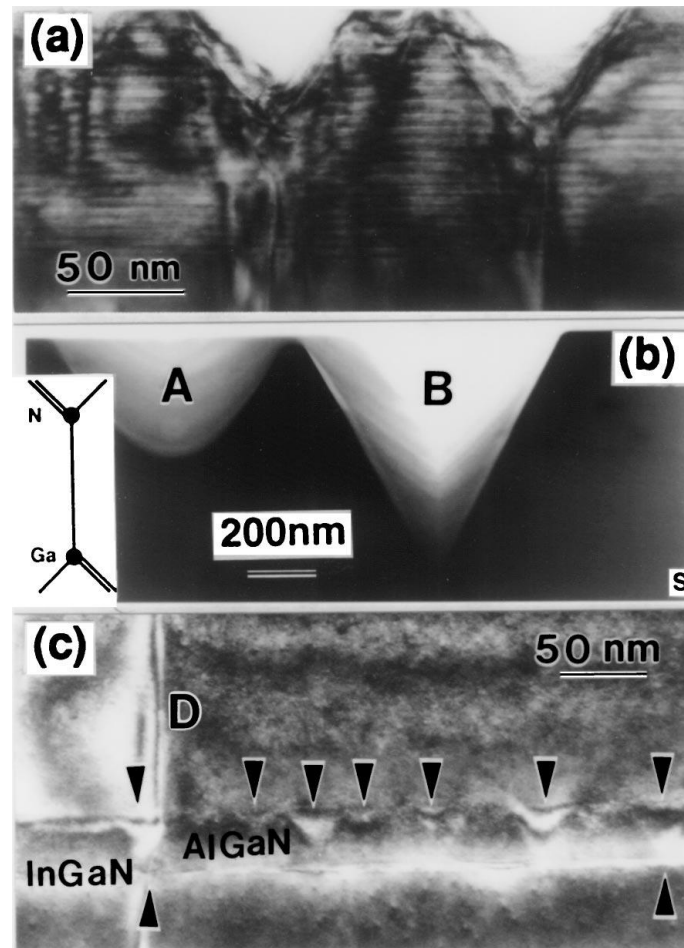
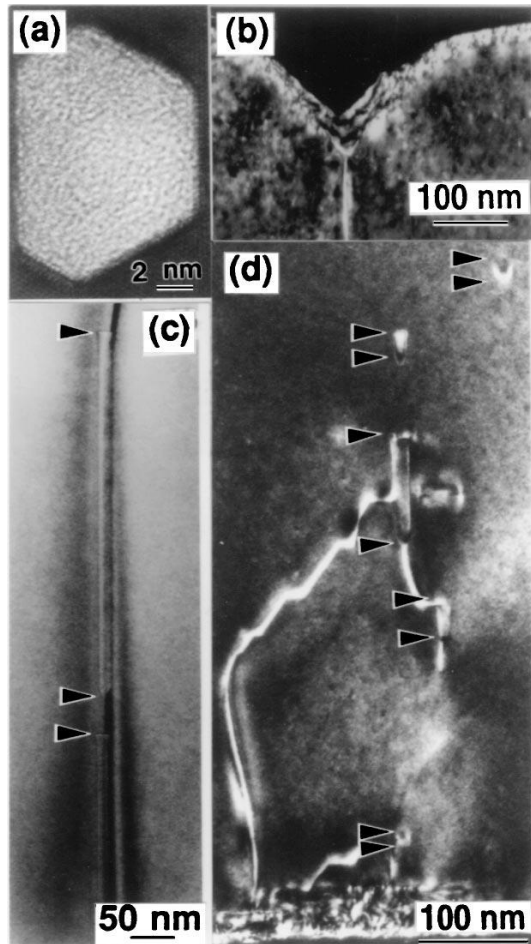
- **Volmer-Weber - wetting**



- **Stranski-Krastanov - strain**

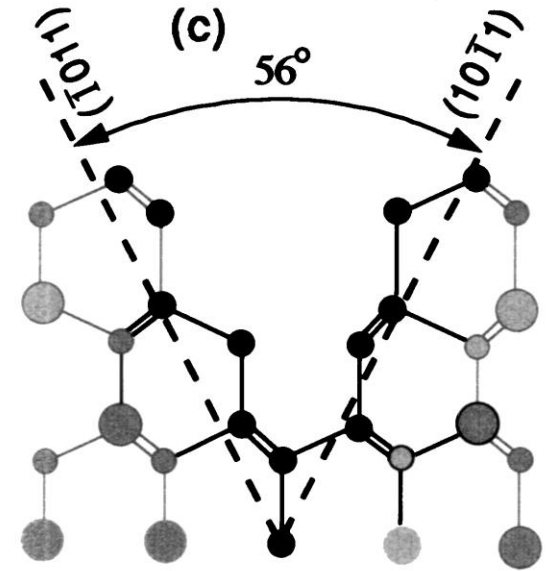
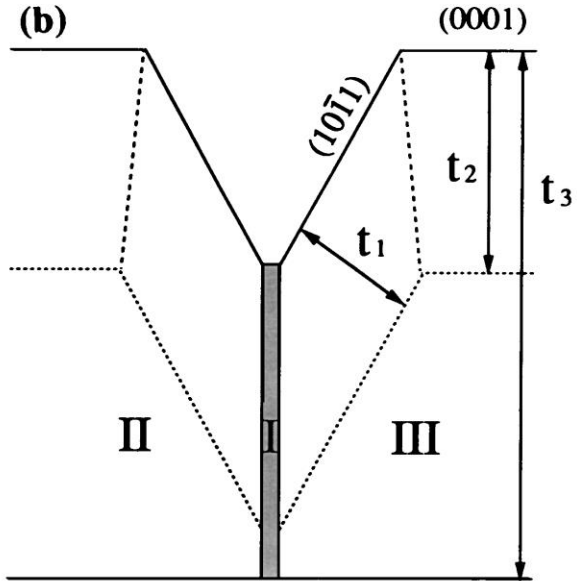
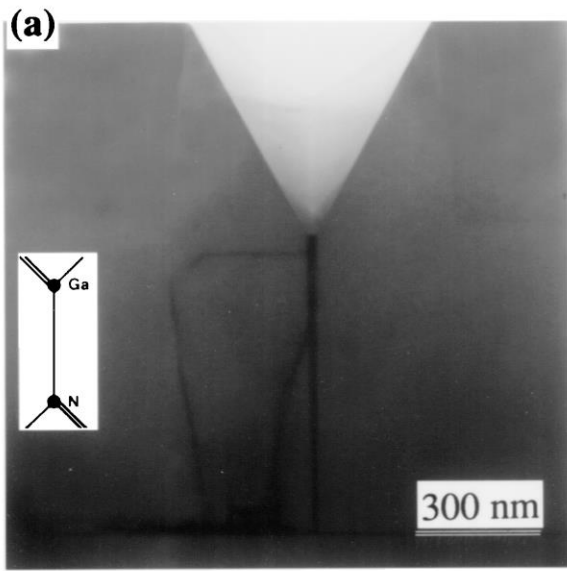


Strain influence on the growth – nanotubes & pinholes



*Z. Lilental-Weber et al. ,
Phys. Rev. Lett. 79 (1997) 2835*

Strain influence on the growth – pinholes



*Z. Lilental-Weber et al. ,
Phys. Rev. Lett. 79 (1997) 2835*