Workshop "Intensive Discussion on Crystal Growth of Nitride Semiconductors , Sendai, Japan, 22-23 October, 2012

Phase separation in III-nitride alloys

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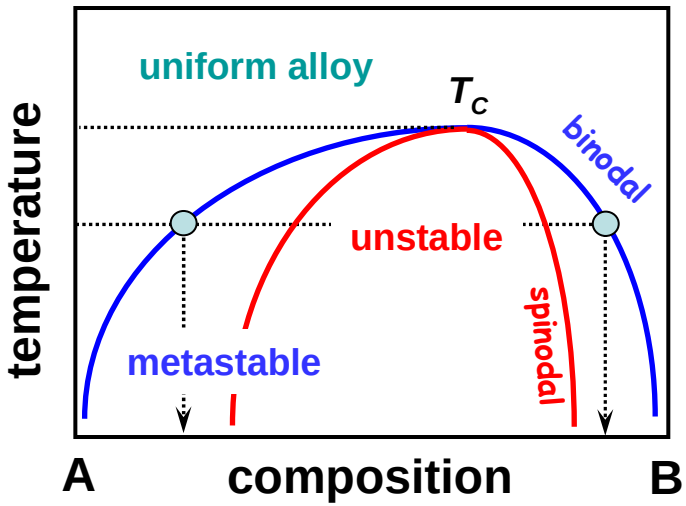
Origin of tendency to phase separation

huge lattice constant mismatches between binary III-nitride compounds

Lattice constant (nm)	AlN	GaN	InN	wz- BN
a	0.31106	0.31890	0.35371	0.22502
c	0.49795	0.51864	0.57052	0.42131
Mismatch with GaN (%)	2.5 / 4.0	0 / 0	10.9 / 10.0	29.4 / 18.8

large lattice constant mismatch between binary constituents along with the high elastic stiffness of III-nitride semiconductors is the main reason for the tendency of III-nitride alloys to phase separation



Factor affecting immiscibility gap in III-nitride alloys

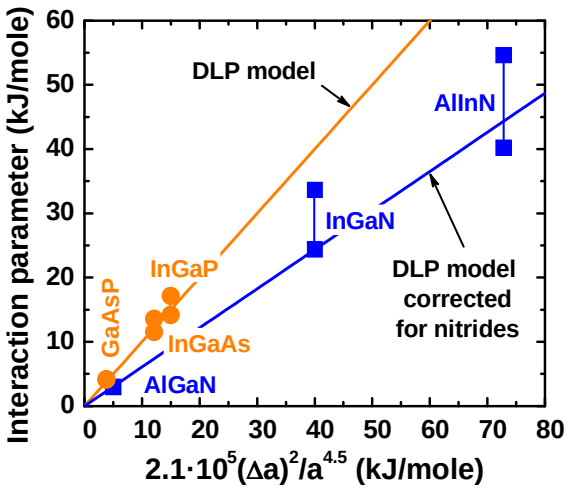
free energy of binary constituents mixing in an alloy

$$G_{mix}(x) = \underbrace{H(x,T)}_{\text{enthalpy of mixing}} - RT\left[x\ln x + (1-x)\ln(1-x)\right]$$

regular solution approximation

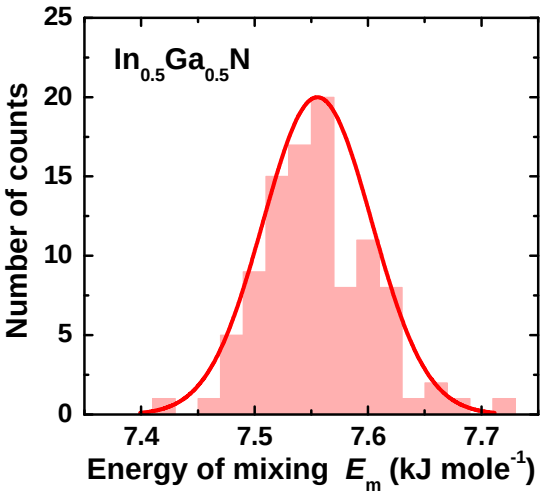
$$H(x,T) \approx E_{mix}(x) \approx Wx(1-x)$$

DLP model $W = K(\Delta a)^2 / \bar{a}^{4.5}$

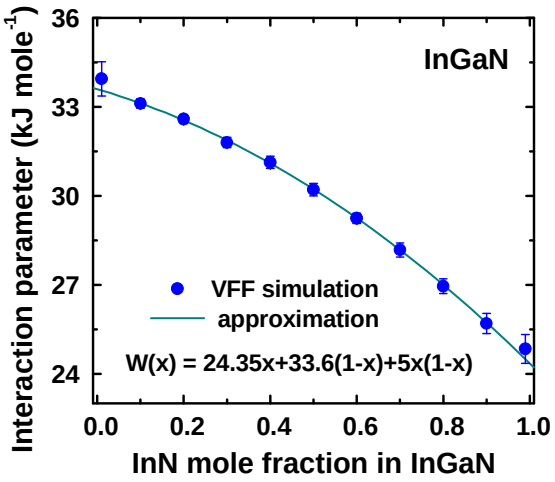


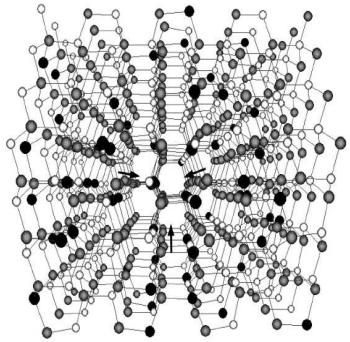
valence force field (VFF) simulation

E_{mix} exibit statistical scatter



W depends on composition



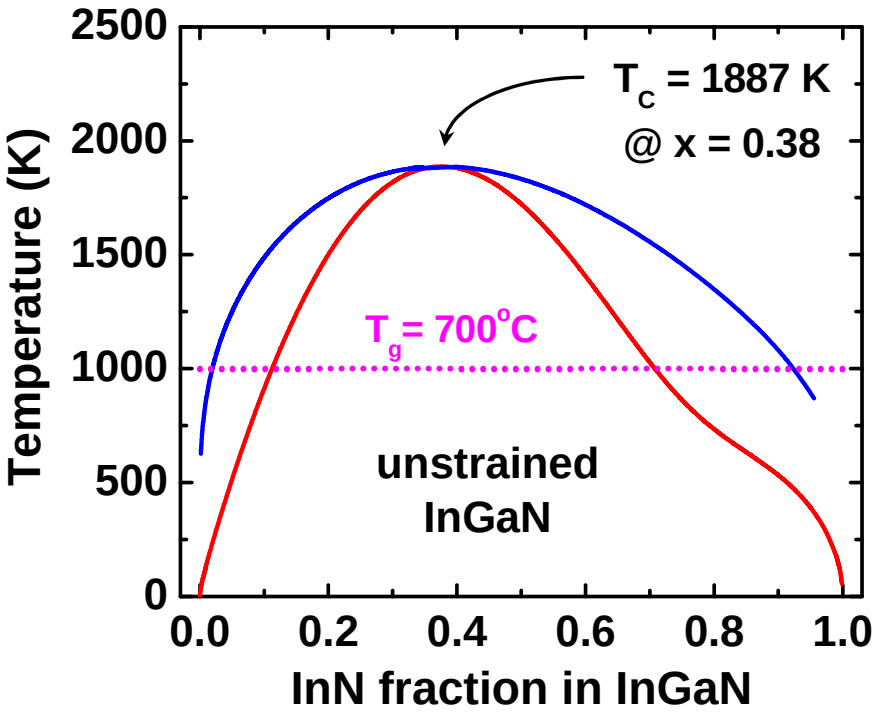


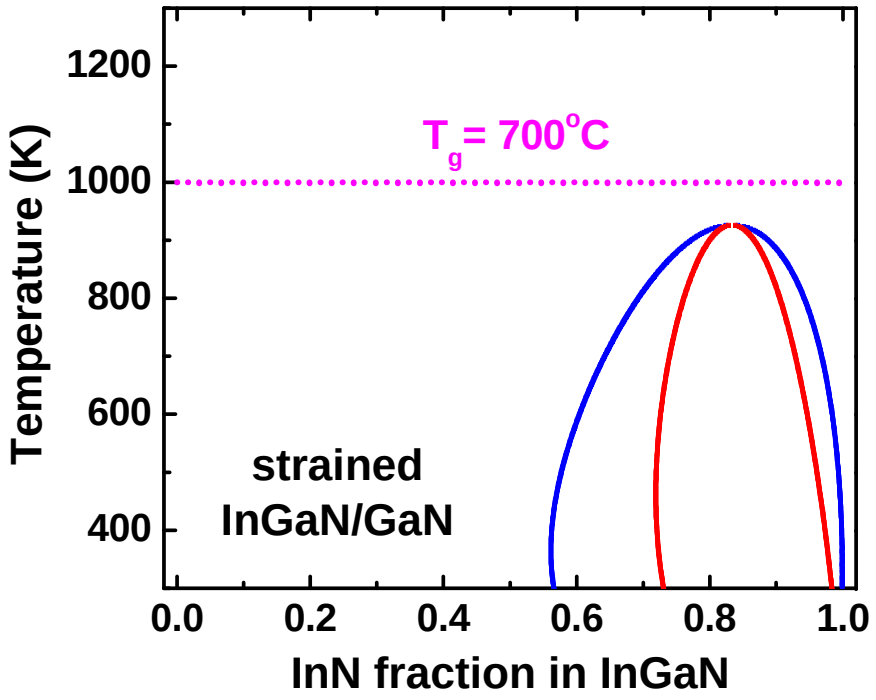
T. Matsuoka, Appl. Phys. Lett. 71 (1997) 105

S. Yu. Karpov at al., Phys. Rev. B 70 (2004) 235203

Effect of biaxial strain on phase separation of InGaN alloys

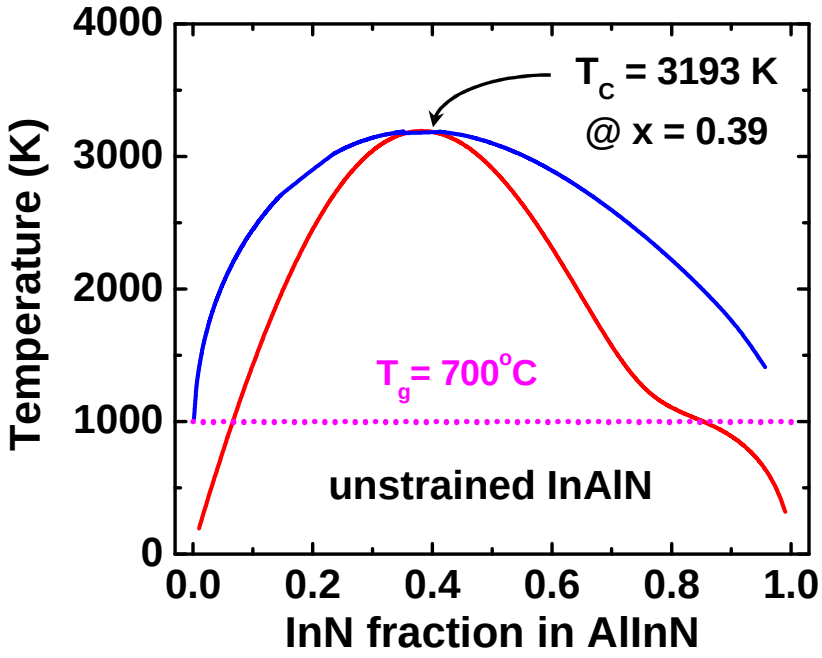
S. Yu. Karpov, MRS J. Nitride Semicond. Res. 3 (1999) 16

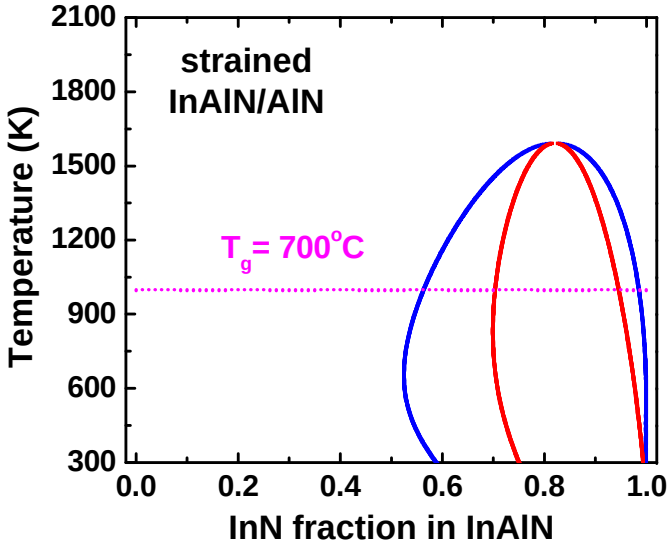


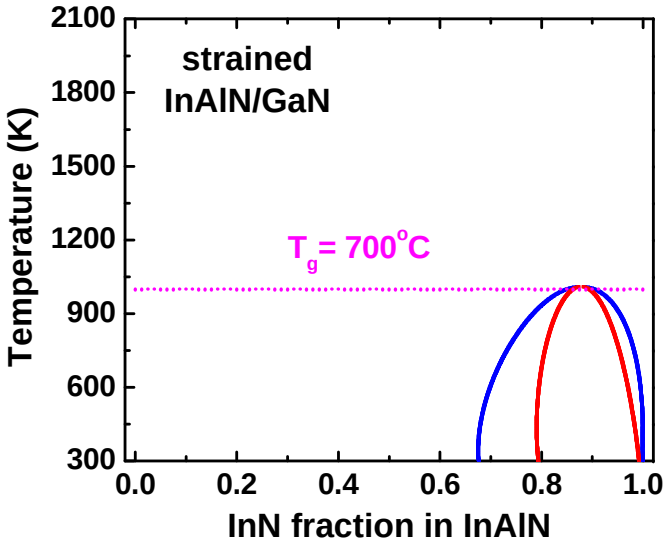


uniform biaxial strain results in considerable suppression of phase separation in III-nitride alloys; in particular, phase separation in strained InGaN/GaN is predicted to be completely suppressed at typical growth temperature of 700°C

Effect of biaxial strain on phase separation of InAlN alloys

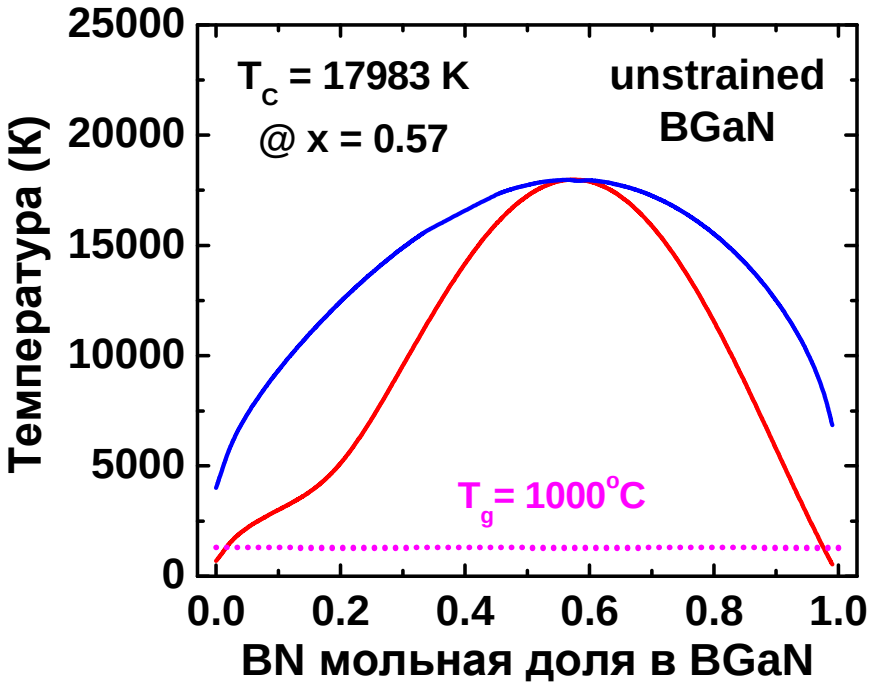


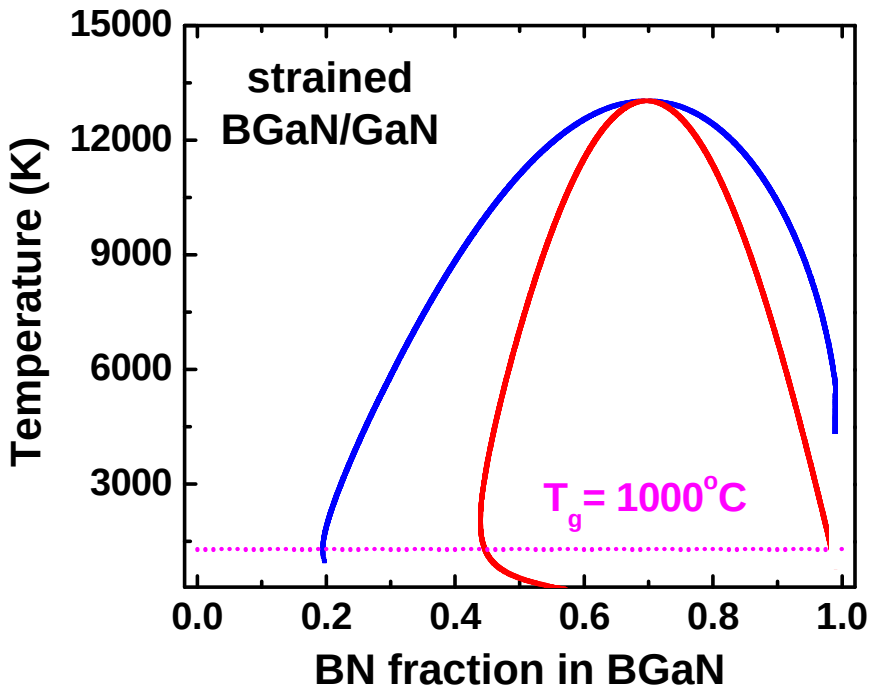




suppression of phase separation in InAlN alloys depends substantially on the substrate/template layer on which the alloys is grown

Effect of biaxial strain on phase separation of BGaN alloys



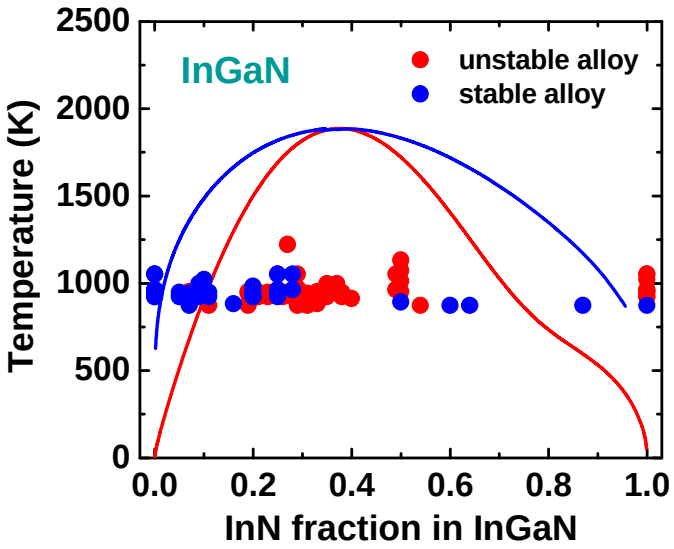


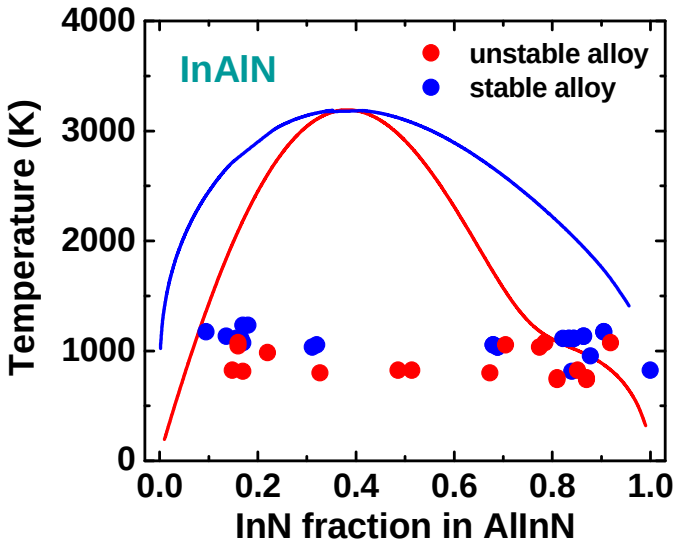
biaxial strain leads to considerable narrowing of the immiscibility gap in BGaN/GaN alloys and increase of boron solubility in GaN; the effect occurs in the practically important range of alloy compositions

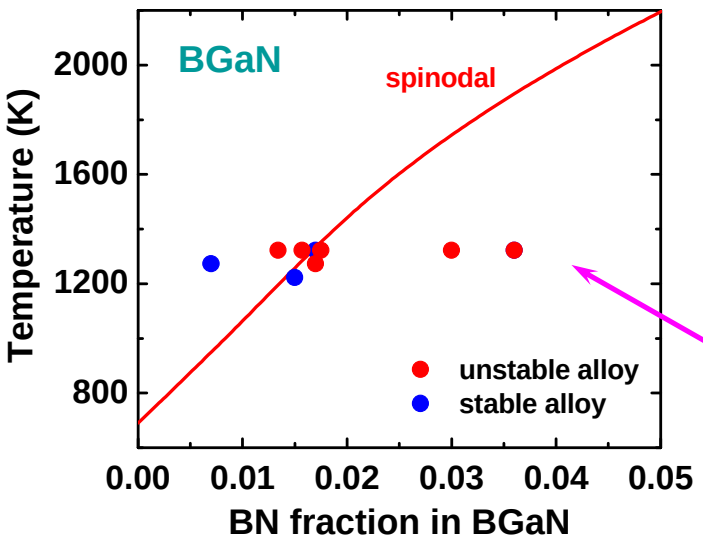
Observations of phase separation in III-nitride alloys

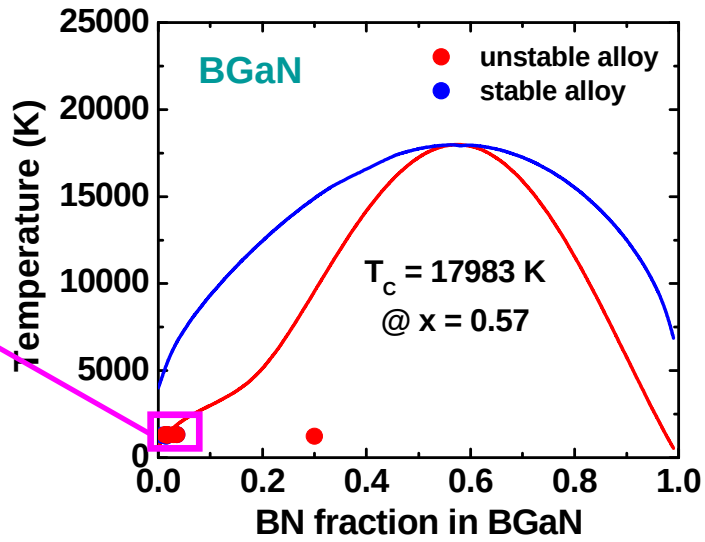
N. I. Podolskaya, PhD Thesis (2011) 205 p.

there is a correlation between observed phase separation and predicted spinodal curves; however, it depends strongly on the degree of strain relaxation in particular epitaxial material !!



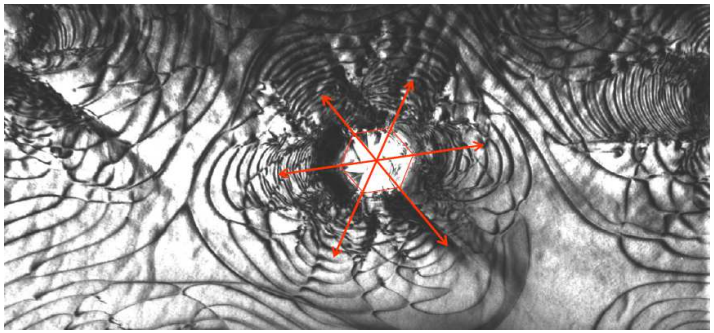






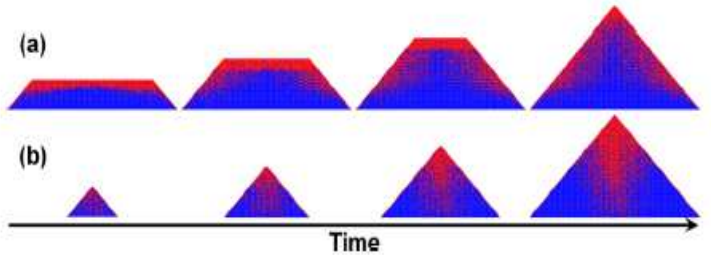
Still open questions for further studies

- how to control strain relaxation in bulk epilayer, quantum wells, and superlattices made of III-nitride alloys?



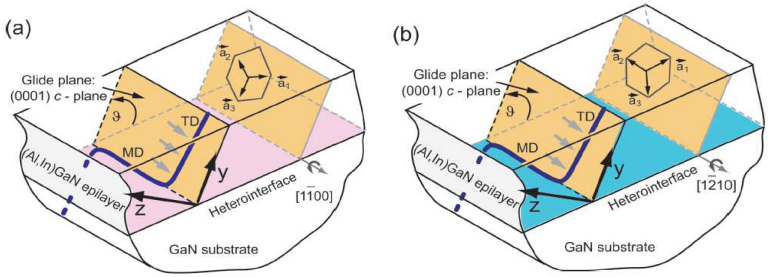
R. Liuet al., Appl. Phys. Lett. 89 (2006) 201911

- how phase separation occurs in strain-inhomogeneous objects: in quantum dots, around threading and misfit dislocations, etc.?



X. Niu et al., Appl. Phys. Lett. 99 (2011) 213102

- how the strain in semipolar epilayers affects the phase separation of III-nitride alloys?
- how anisotropic strain relaxation observed in semipolar epilayers may influence the phase separation?



A E. Romanov et al., Appl. Phys. Lett. 109 (2011) 103522