Step meandering

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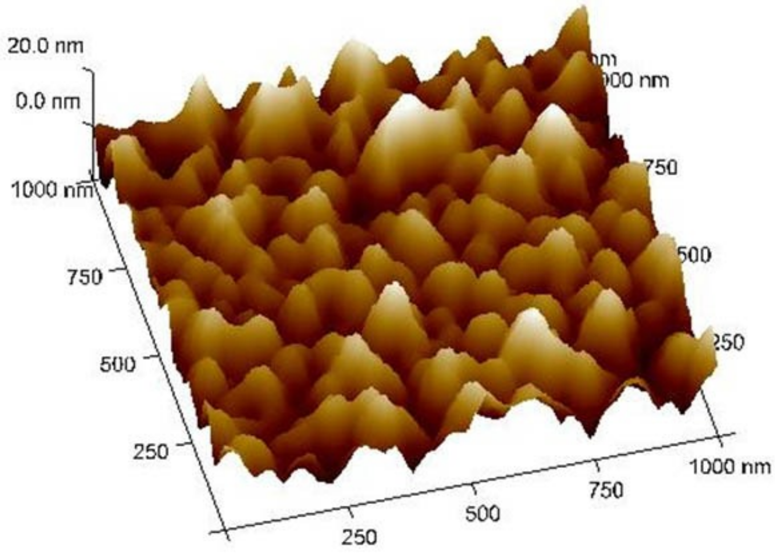
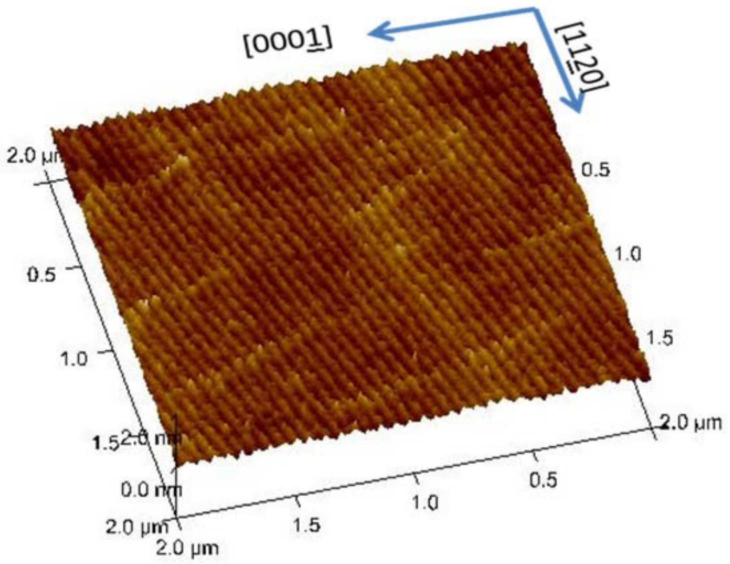
Crystal growth

We want to reach best control over

- growth mode of the crystal
  - smooth, regular formation of monocrystal
- creation of desired surface structures



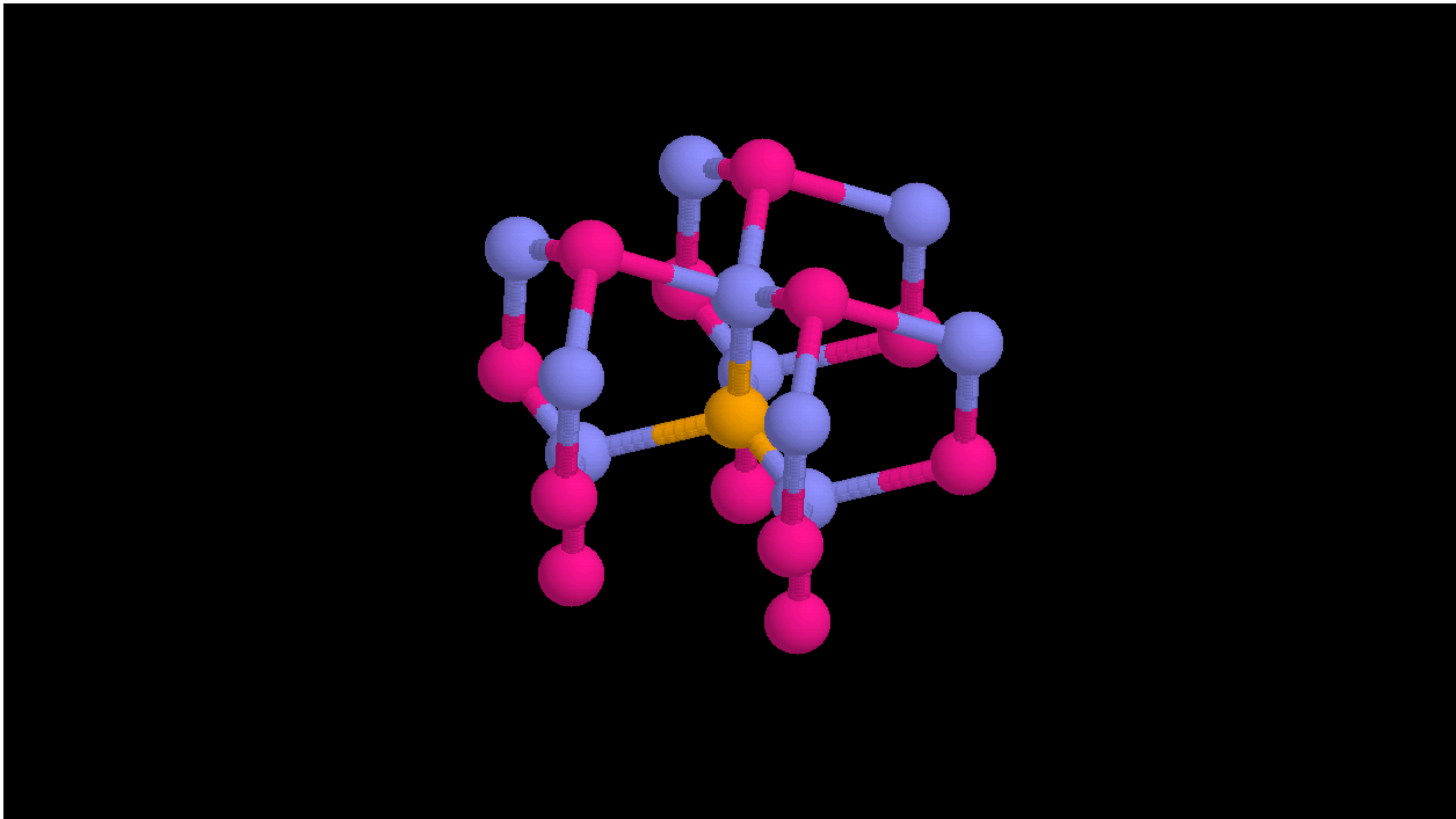


GaN(0001) surface

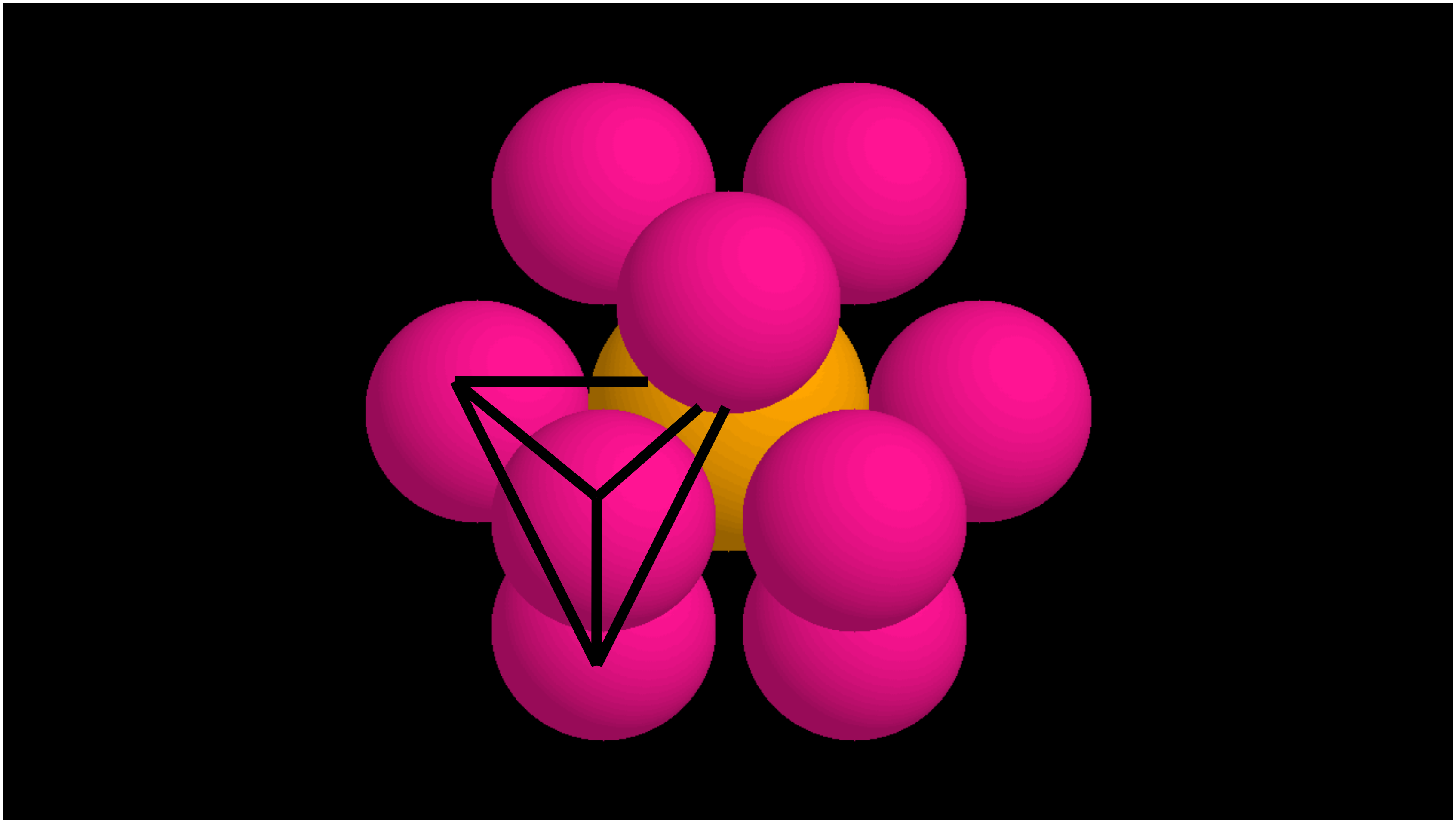
GaN

AFM picture of MOVPE grown GaN layers
Grzegorz Nowak, Institute of High Pressure Physics (UNIPRESS)
PAS

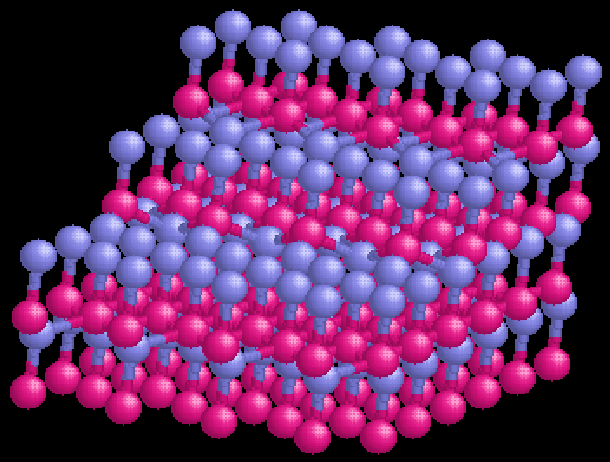
GaN structure – need for many-particle interactions



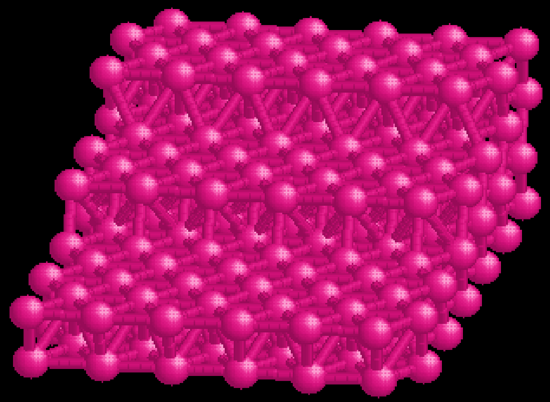
Ga - Ga interaction



Structure of GaN(0001) surface

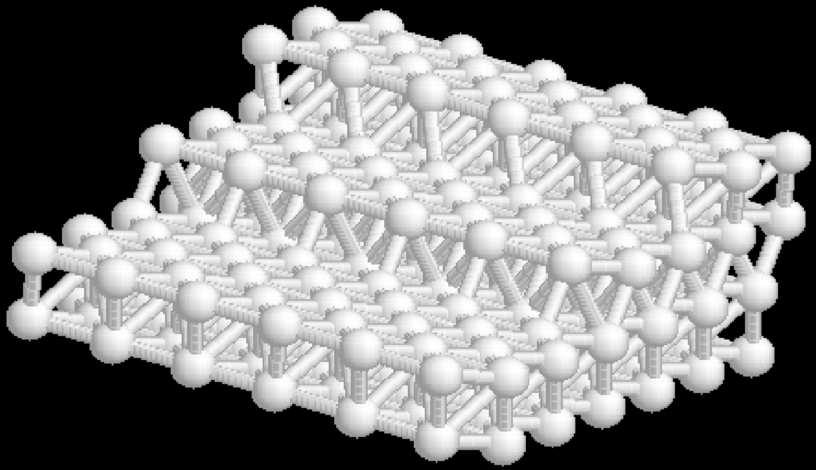


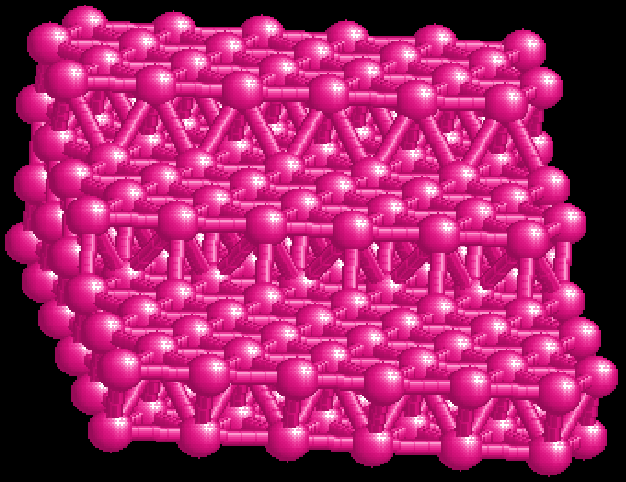
Ga & N



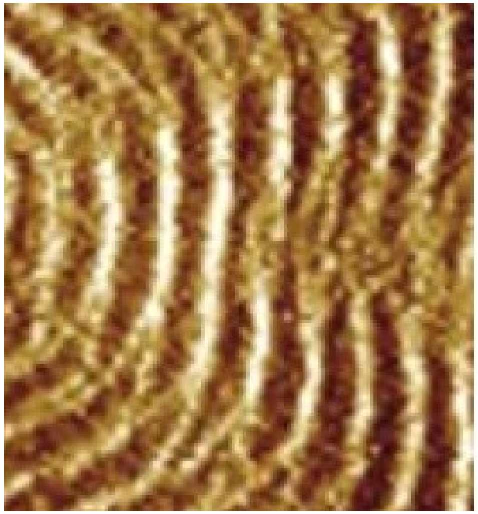
Ga

Ga – double step structure

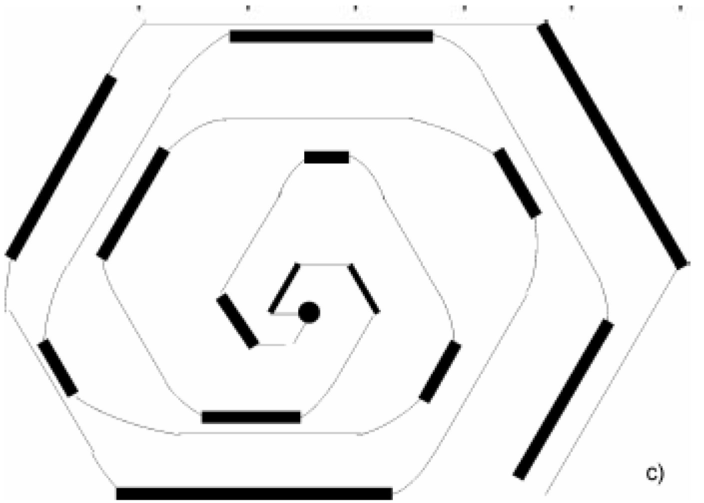


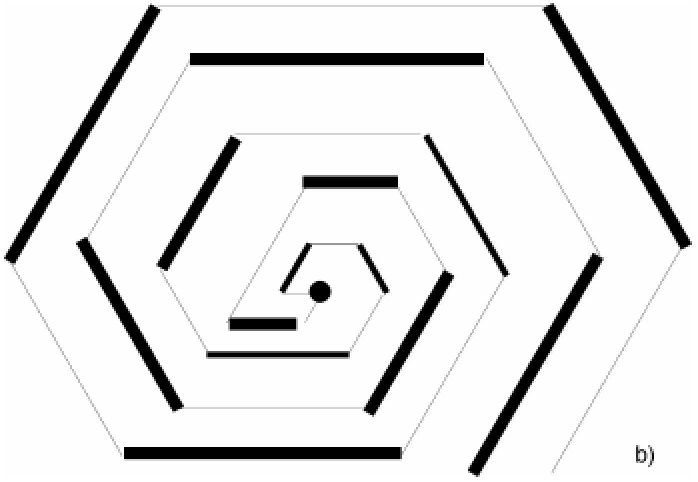


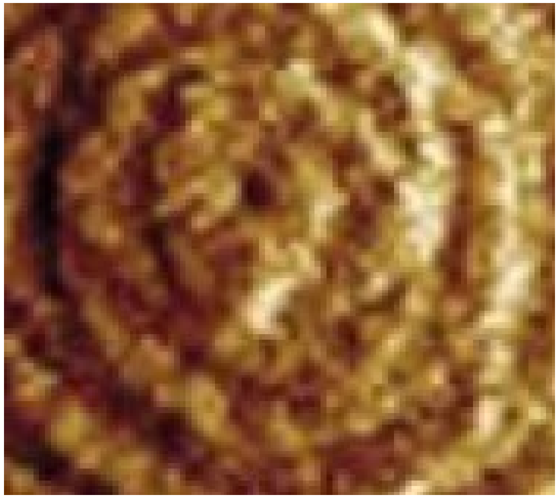
Meandering



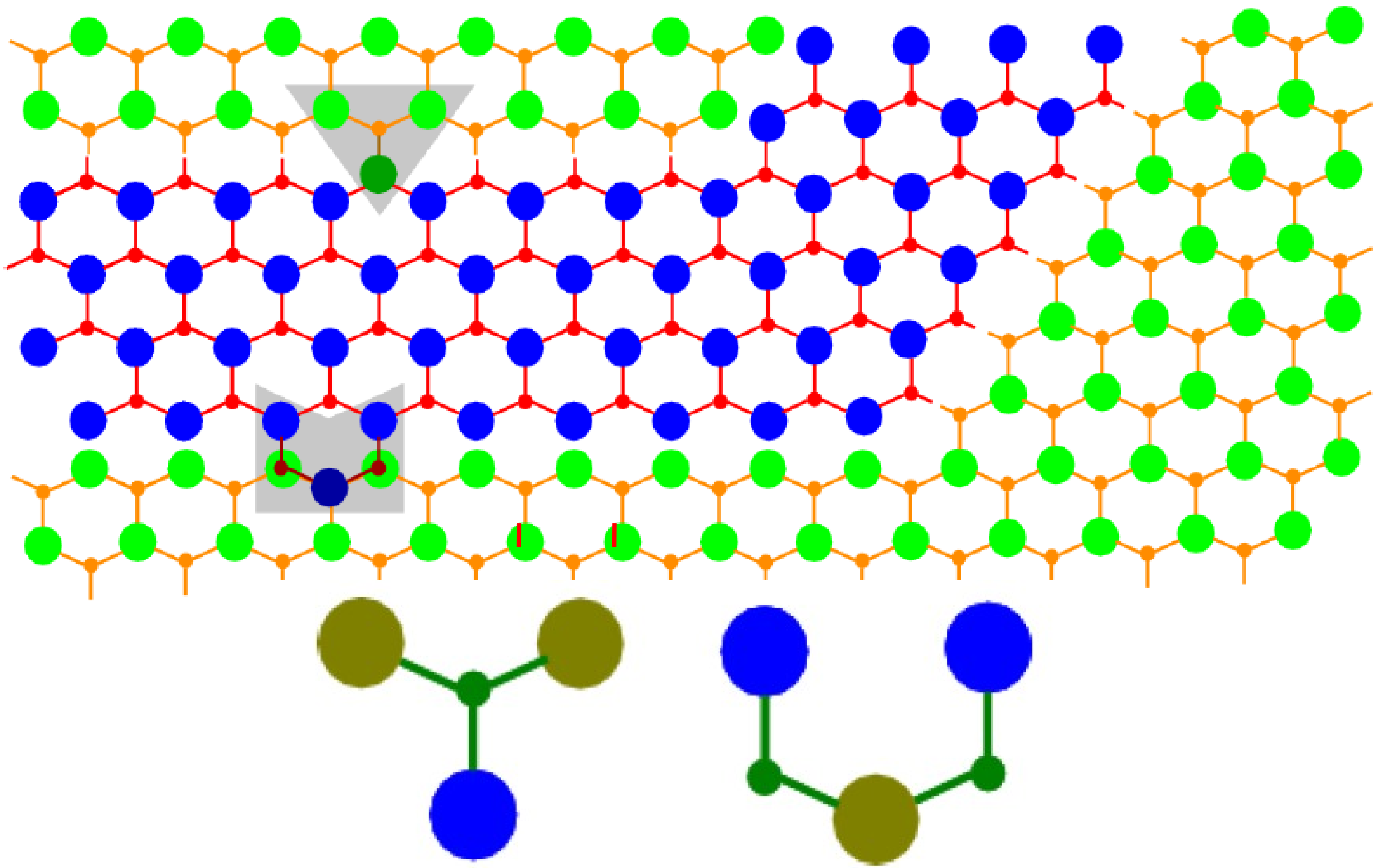
Step evolution



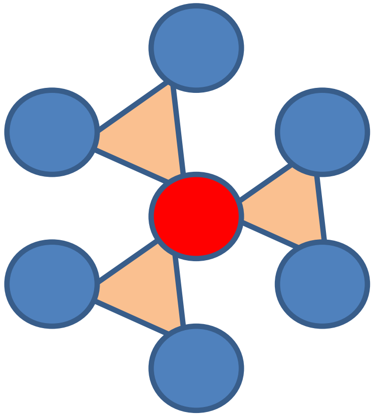




Interaction at steps



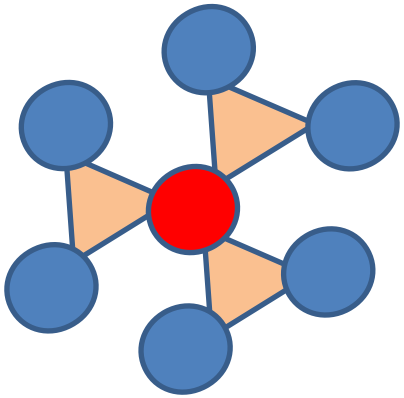
Interaction



$$\eta_i = \begin{cases} 0 & \text{no neighbors} \\ \frac{1}{3}\text{r} & \text{two- body interactions} \\ 1 & \text{four-body interactions} \end{cases}$$

Even terrace

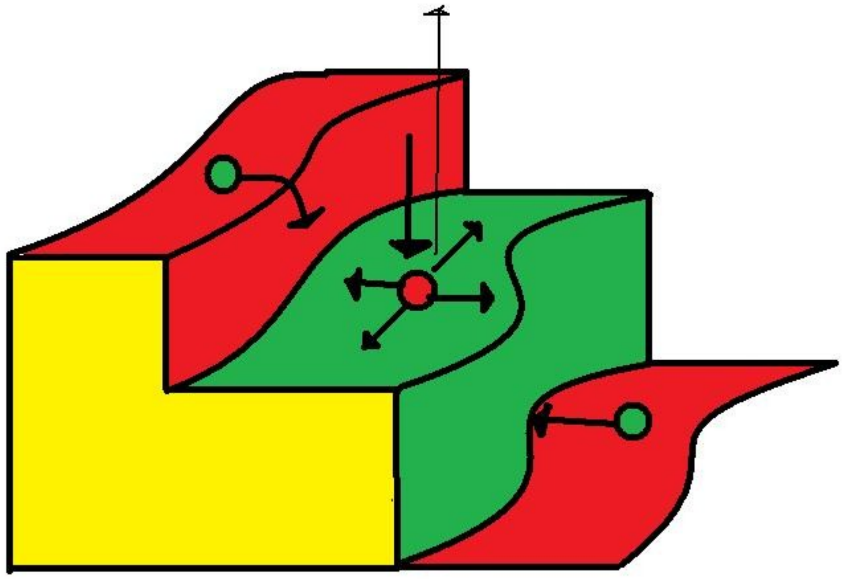
$$E(J) = J\sum_{i=1}^{4}\eta_i$$



For $r_o = 1$ steps are identical

Odd terrace

Model of crystal growth



Terrace adsorption

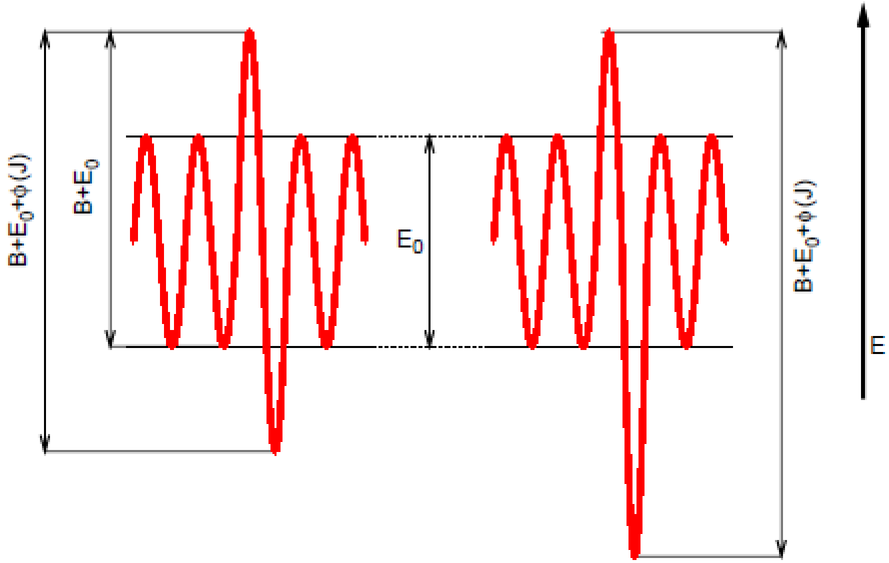
Surface diffusion

Step adsorption

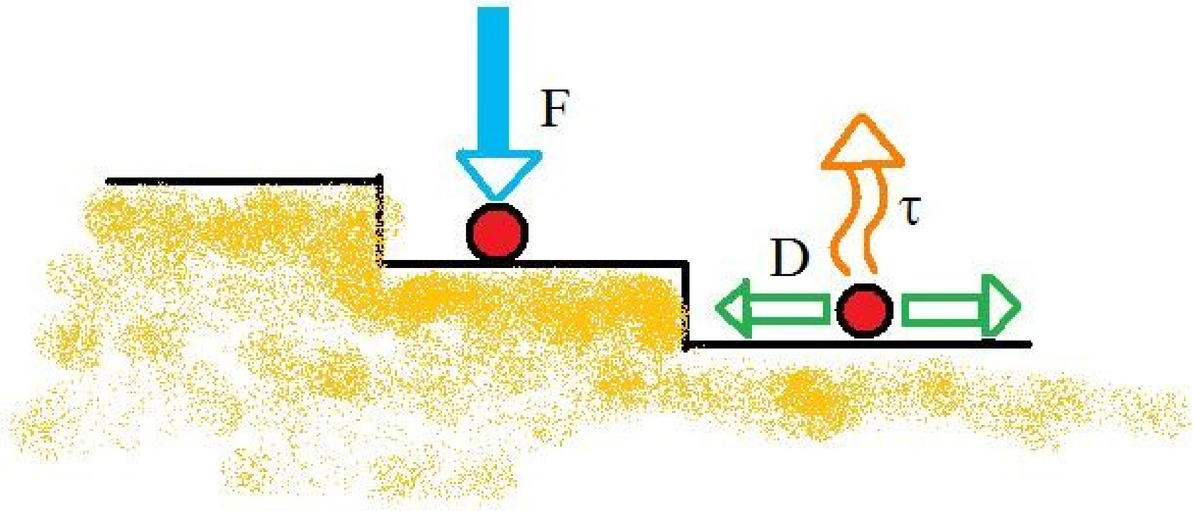
Jump step up and step down
– Schwoebel barrier

External particle flux

Potential at steps



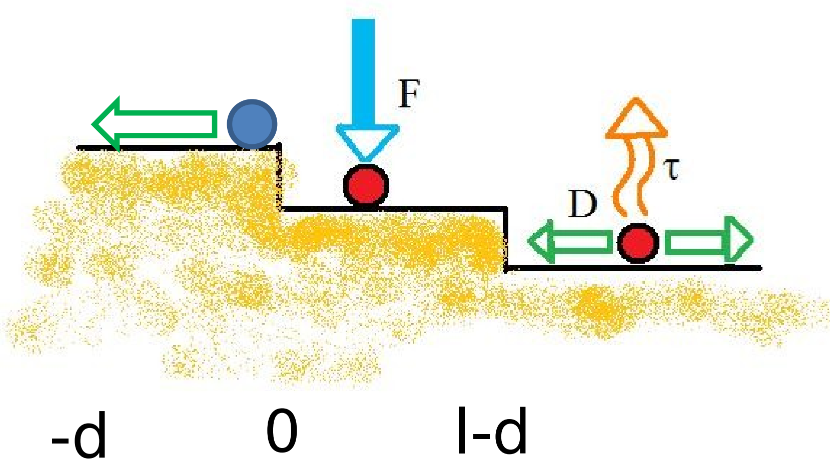
Surface growth Burton-Carbera-Franck analysis



$$D\Delta\rho + F - \frac{1}{\tau}\rho = \frac{d}{dt}\rho$$

Analytical model 1D parallel straight steps

$$D\frac{d^2}{(dz)^2}\rho + F - \frac{\rho}{\tau} + V\frac{d}{dz}\rho = 0$$



$$D\frac{d\rho}{dz}\,|_{(-d)+} \;=\; k_1(\rho - \rho^+{}_1)\,|_{(-d)+}$$

$$-D\frac{d\rho}{dz}\,|_{0-} \;=\; \kappa_2(\rho - \rho^-{}_2)\,|_{0-}$$

$$D\frac{d\rho}{dz}\,|_{0+} \;=\; k_2(\rho - \rho^+{}_2)\,|_{0+}$$

$$-D\frac{d\rho}{dz}\,|_{(l-d)-} \;=\; \kappa_1(\rho - \rho^-{}_1)\,|_{(l-d)-}$$

$$V = D\frac{d\rho}{dz}\,|_{0+} + D\frac{d\rho}{dz}\,|_{0-} = D\frac{d\rho}{dz}\,|_{(-d)+} + D\frac{d\rho}{dz}\,|_{(l-d)-}$$

Solution

$$\rho(z) \;=\; F\tau - A\cosh(\lambda z) - B\sinh(\lambda z)$$

$$\lambda = \sqrt{\frac{1}{D\tau}}$$

Pair of steps d and l-d. Width d is given by:

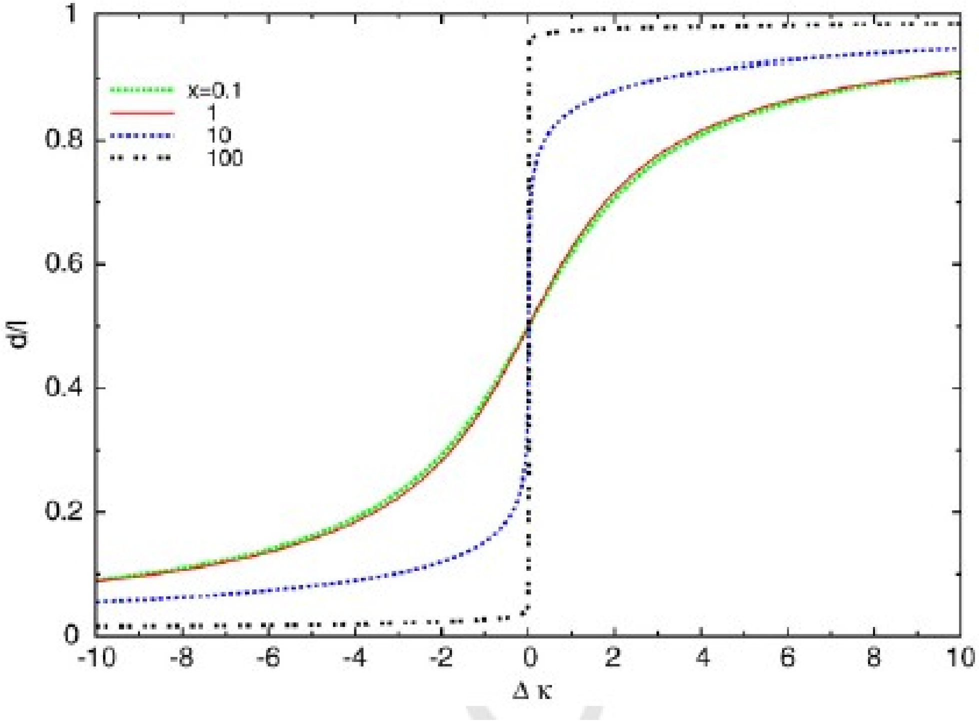
$$\frac{k_1+\kappa_2}{k_1-\kappa_2}\coth(\lambda d) - \frac{k_2+\kappa_1}{k_2-\kappa_1}\coth[\lambda(l-d)] = \frac{\kappa_1 k_2+\lambda^2 D^2}{\lambda D(k_2-\kappa_1)} - \frac{\kappa_2 k_1+\lambda^2 D^2}{\lambda D(k_1-\kappa_2)}$$

for: $(k_1-\kappa_2)(k_2-\kappa_1) > 0$

else: d=0 double step structure

Relative terrace width

x=λl

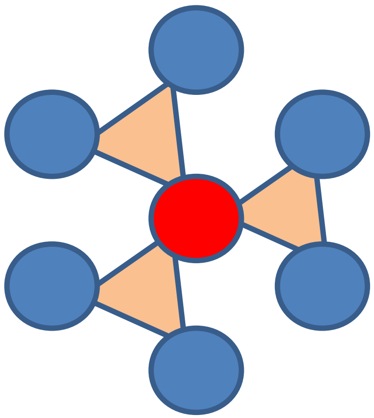


For high Schwoebel barrier

$$\coth(\lambda a) - \coth(\lambda(l-a)) = \frac{1}{\tau\lambda}\left(\frac{1}{\kappa_2} - \frac{1}{\kappa_1}\right)$$

$$\Delta\kappa = \frac{1}{\kappa_2} - \frac{1}{\kappa_1}$$

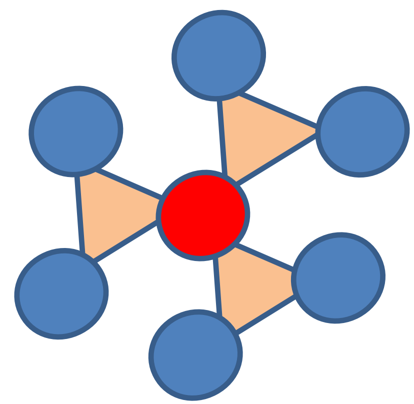
Monte Carlo simulation 2D+1



Even terrace

$$\eta_i = \begin{cases} 0 & \text{no neighbors} \\ \frac{1}{3}r & \text{two- body interactions} \\ 1 & \text{four-body interactions} \end{cases}$$

$$E(J) = J\sum_{i=1}^{4}\eta_i$$



Odd terrace

For $r_o = 1$ steps are identical

Particle kinetics

Diffusion

$$D = \nu_d e^{-\beta(E(J) - E'(J))} \quad \text{for } E(J) - E'(J) > 0$$

$$D = 0 \quad \text{otherwise}$$

$$\beta = 1/(k_B T)$$

Adsorption + desorption

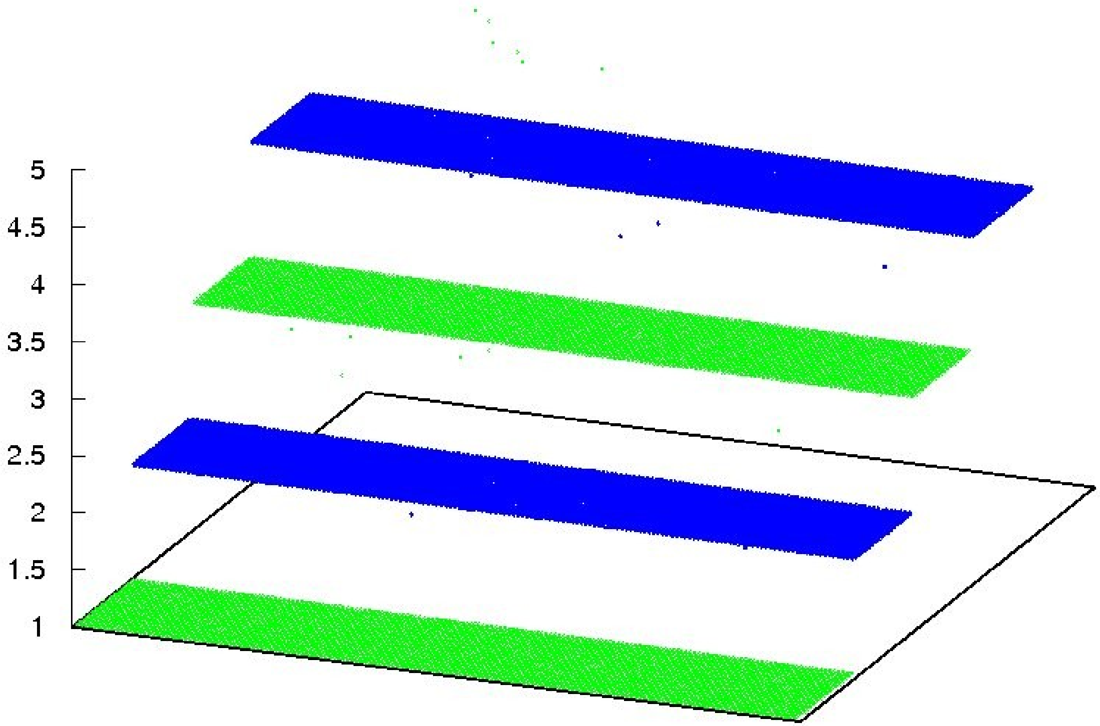
$$F = \nu_a e^{-\beta\mu} = \tau^{-1}$$

Jumps step down and step up

$$P_g = D e^{-\beta b_g}$$

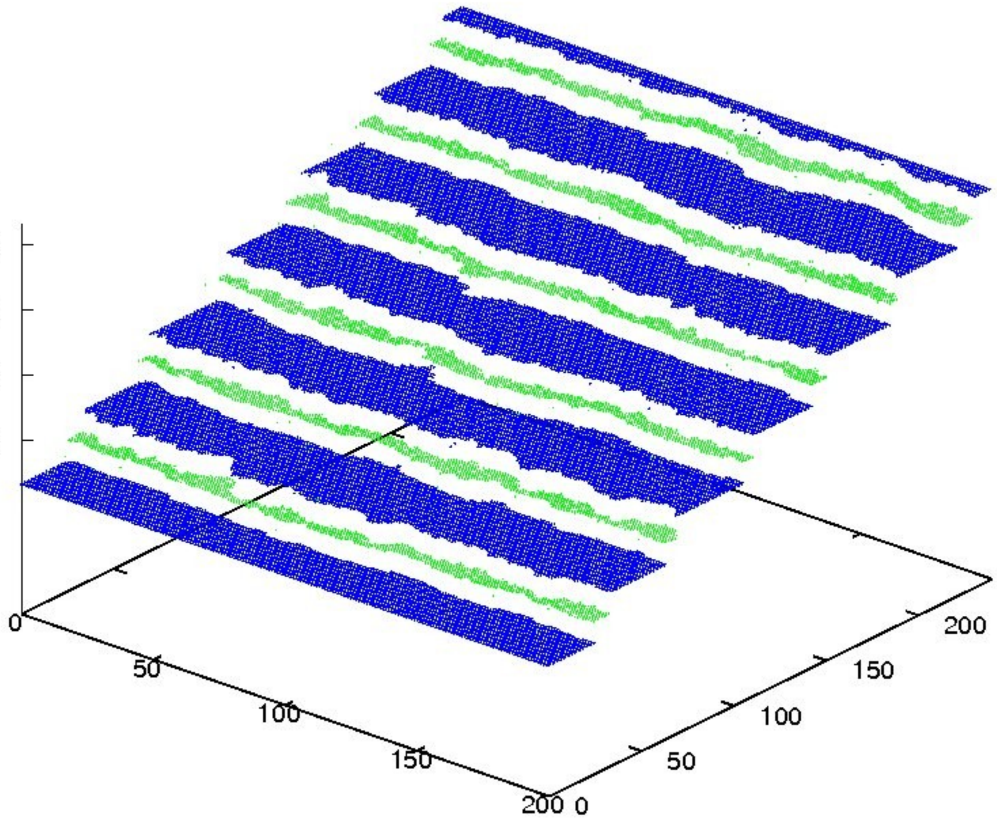
$$P_d = D e^{-\beta b_d}$$

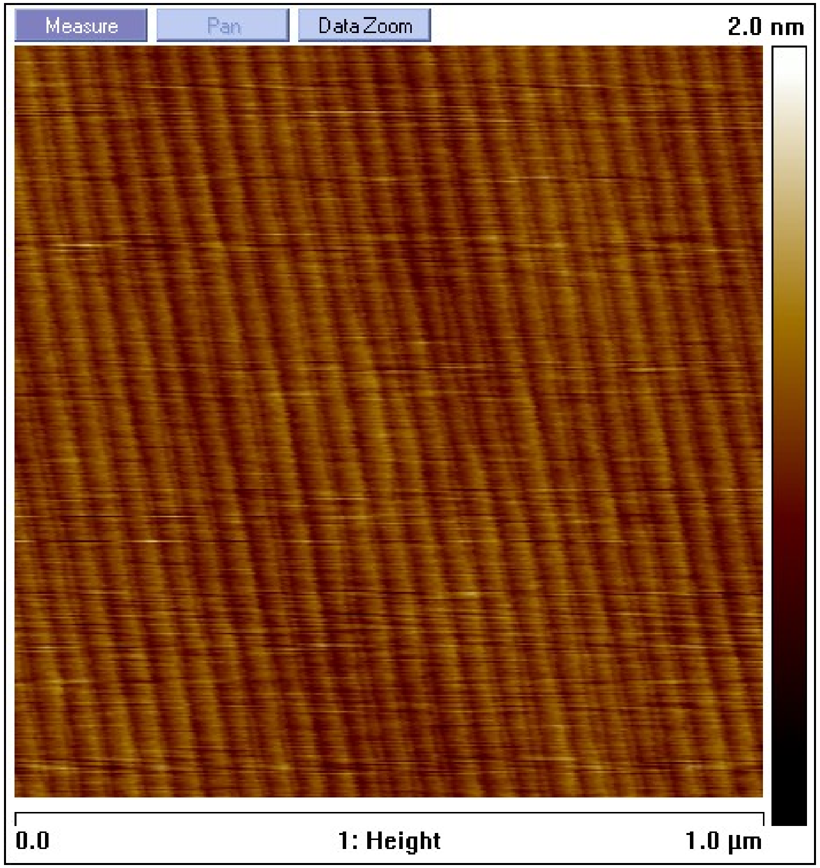
Initial configuration



Narrow terraces,high temperatures

$r = 0.4$, β J=5 , $\beta\mu$=15, β b=0,
[01$\underline{1}$0]





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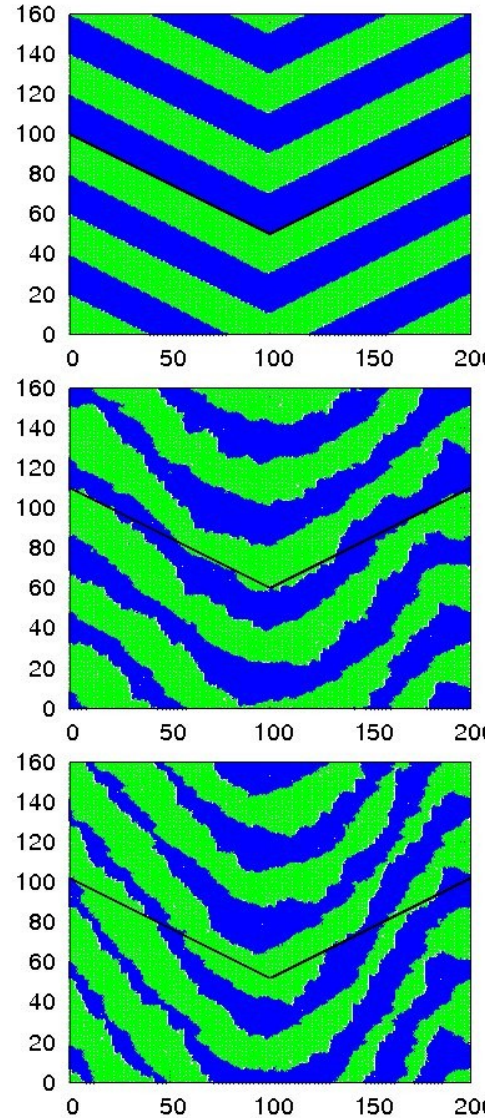
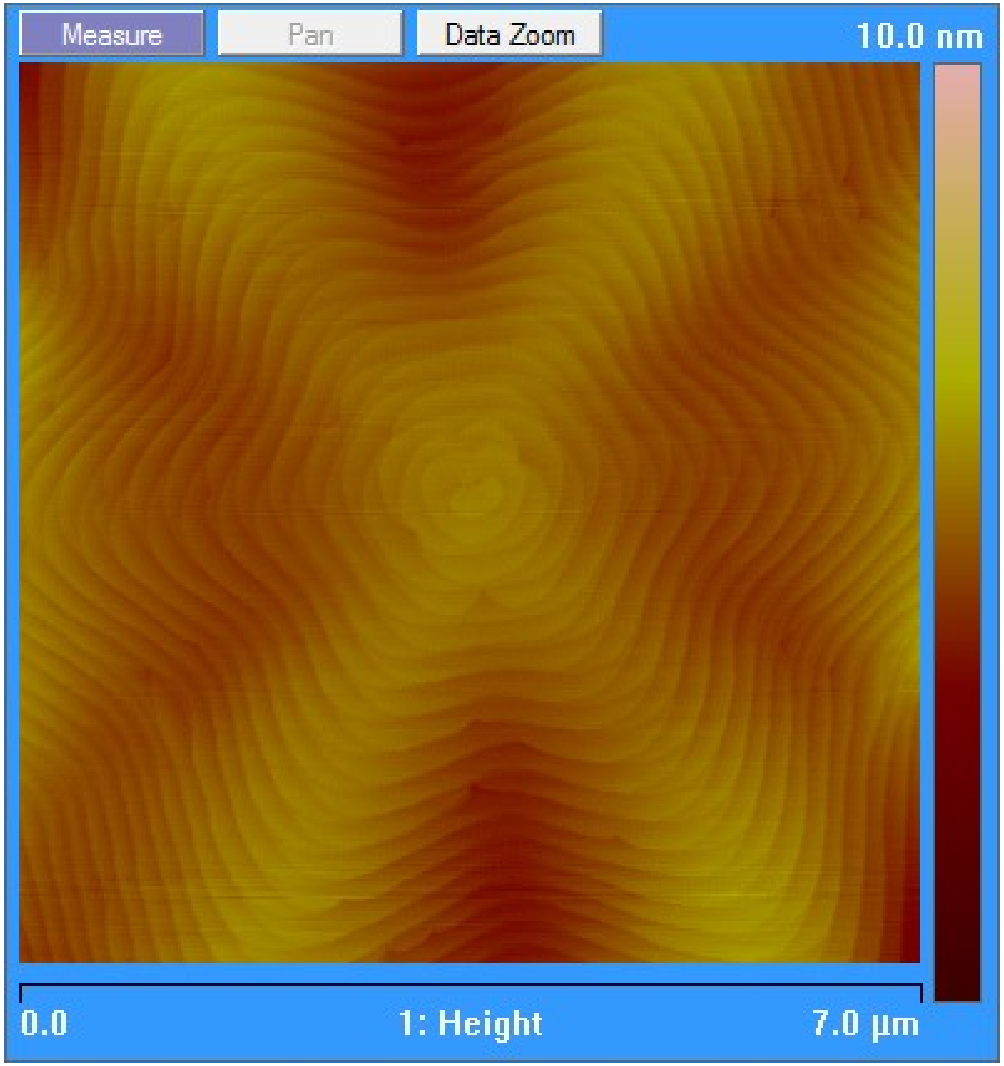


r= 0.4, β J=5 , βμ=15, β b=0, [01$\underline{1}$0], [010$\underline{1}$]



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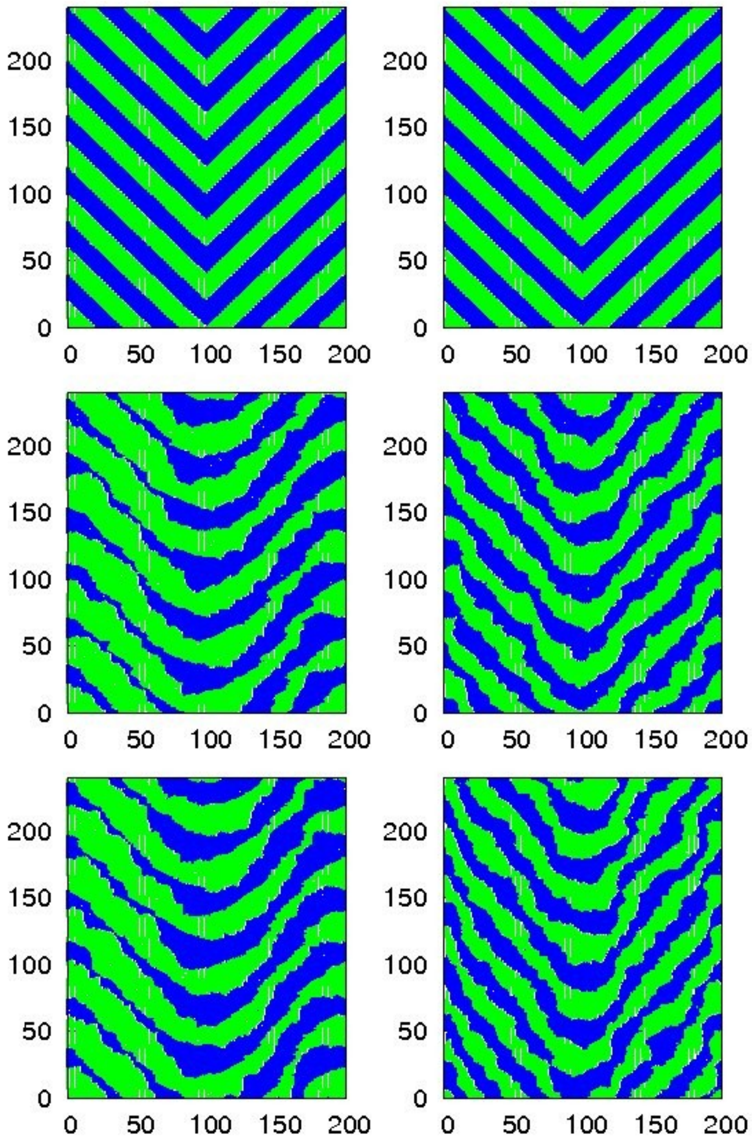
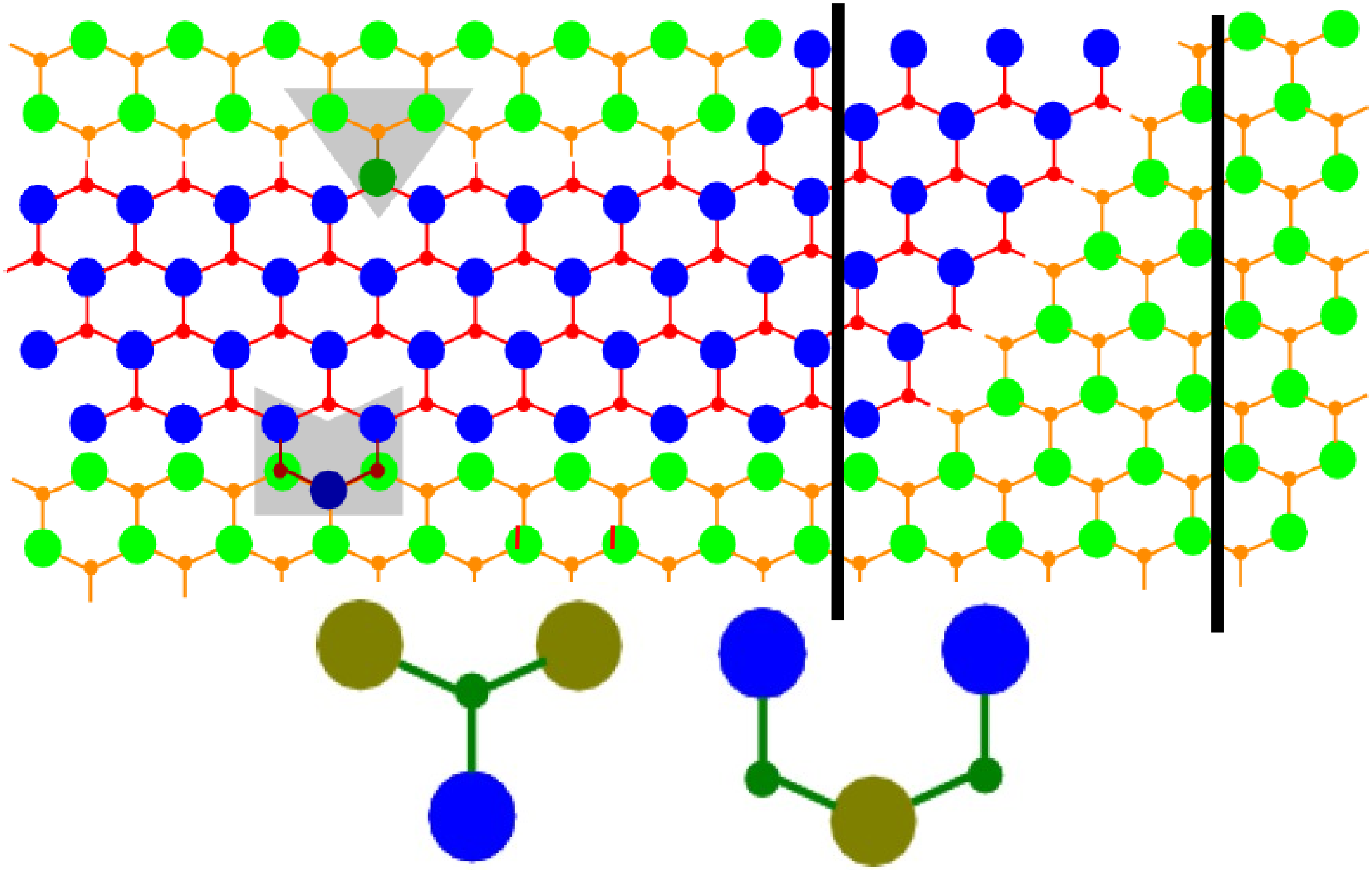


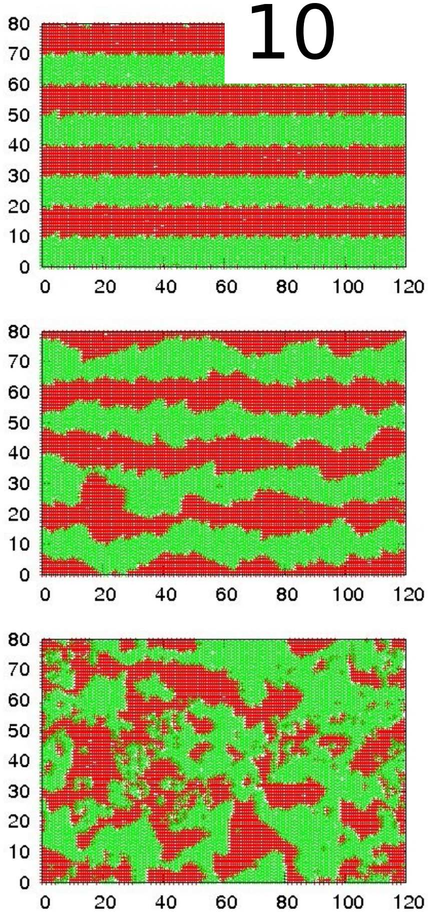
$r=0.4$ $\beta J=5$, $\beta\mu=15$, $\beta b=0$, 20° $r=1$ [01$\underline{1}$0] , [010$\underline{1}$]

Step [11$\underline{2}$0]

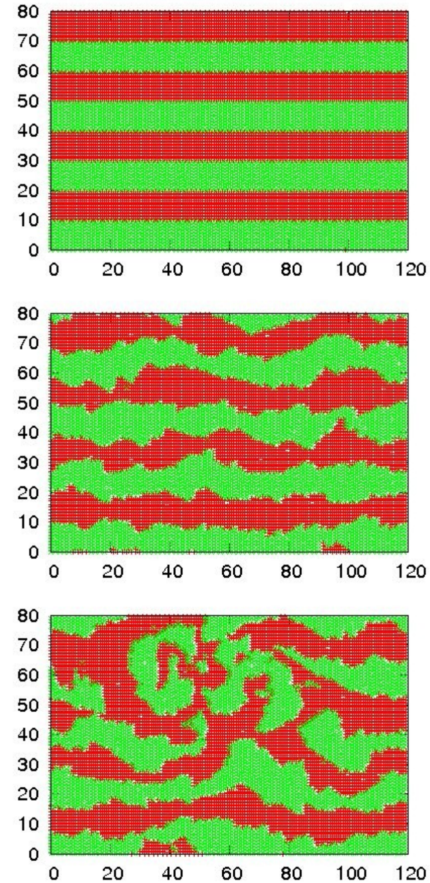


Vertical cut

r=0.4 βJ=5, d= 10

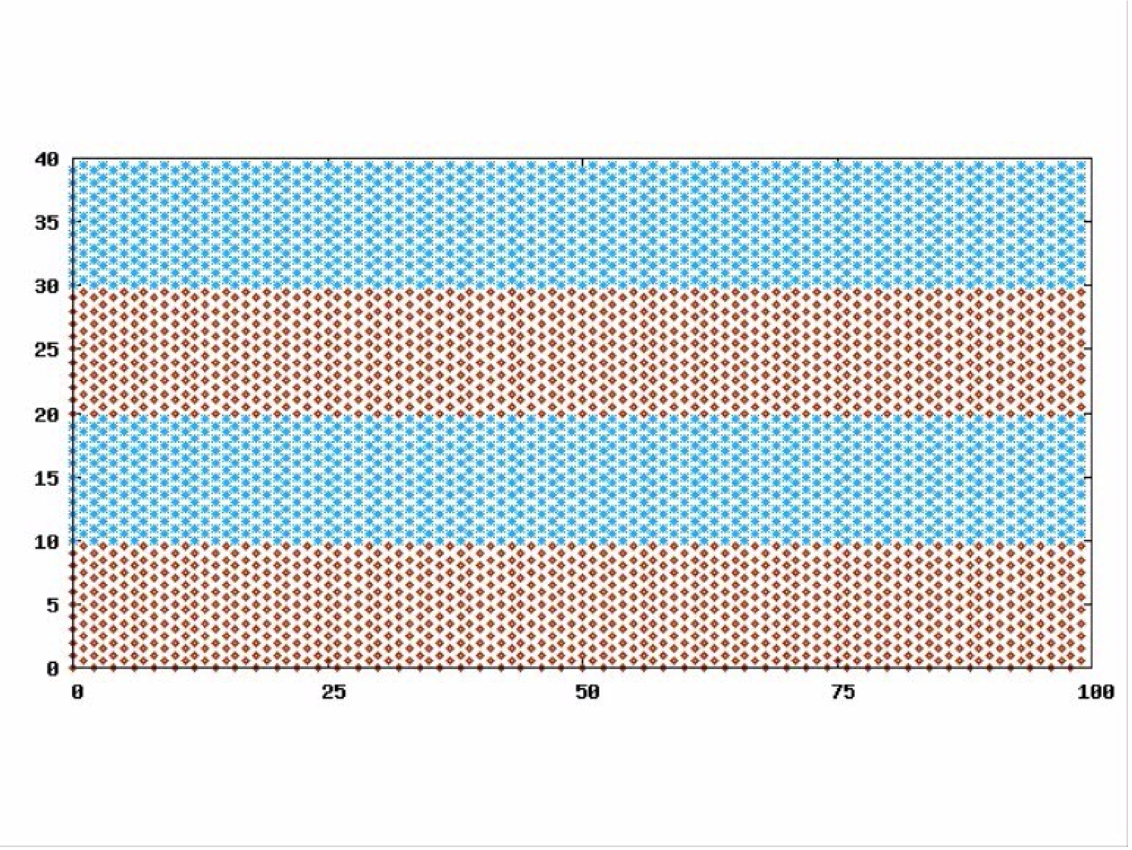


b=1.5



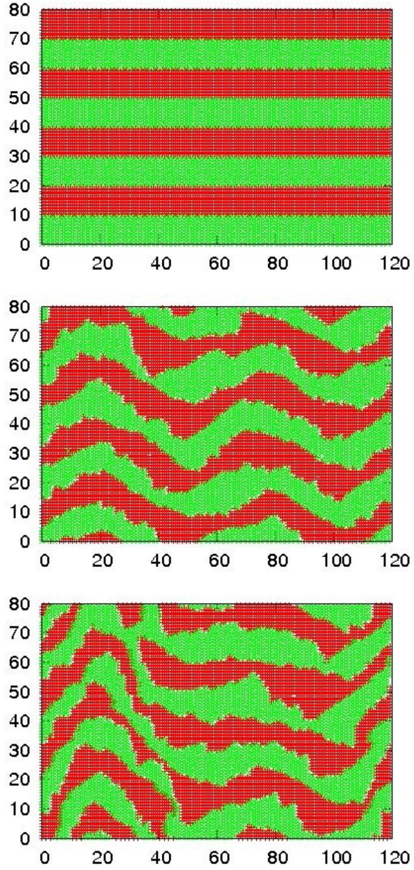
b=1.05

Lower temperature

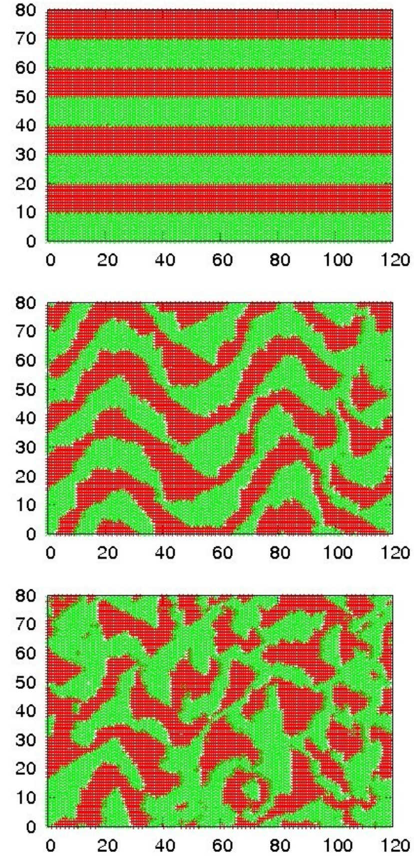


r= 0.4, β J=5.8 , βμ=15, β b=0,
[11$\underline{2}$0]

Lower temperatures

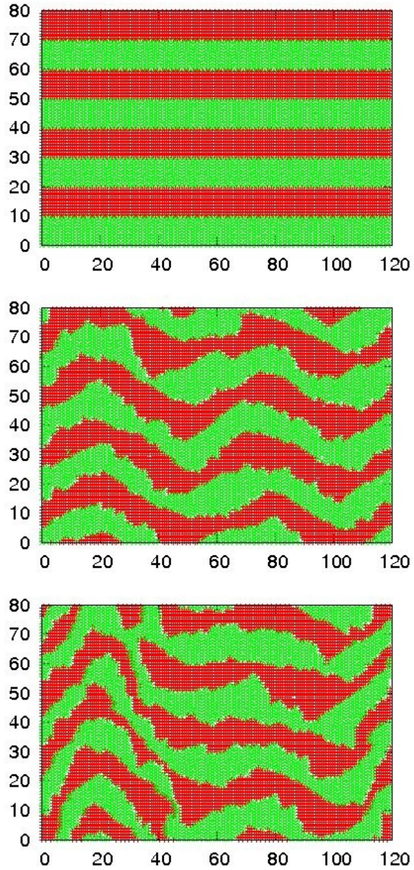


$r = 0.4$, $\beta J=6$, $\beta\mu=15$, $\beta b=0.7$, $[11\underline{2}0]$

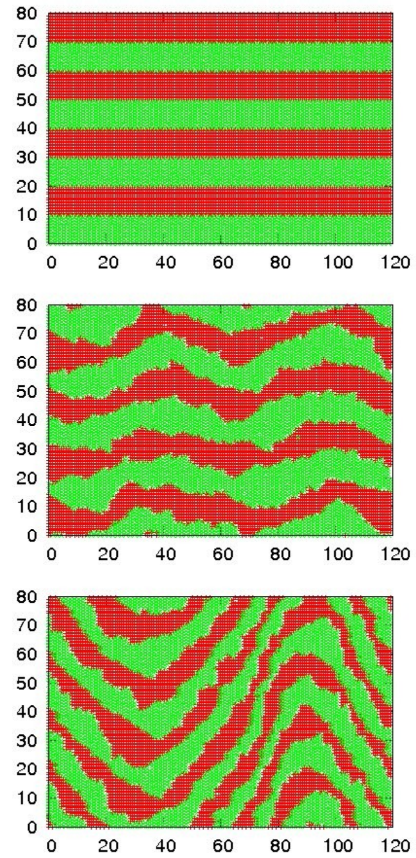


$r = 0.4$, $\beta J=6.5$, $\beta\mu=15$, $\beta b=0.7$, $[11\underline{2}0]$

Low Schwoebel barrier

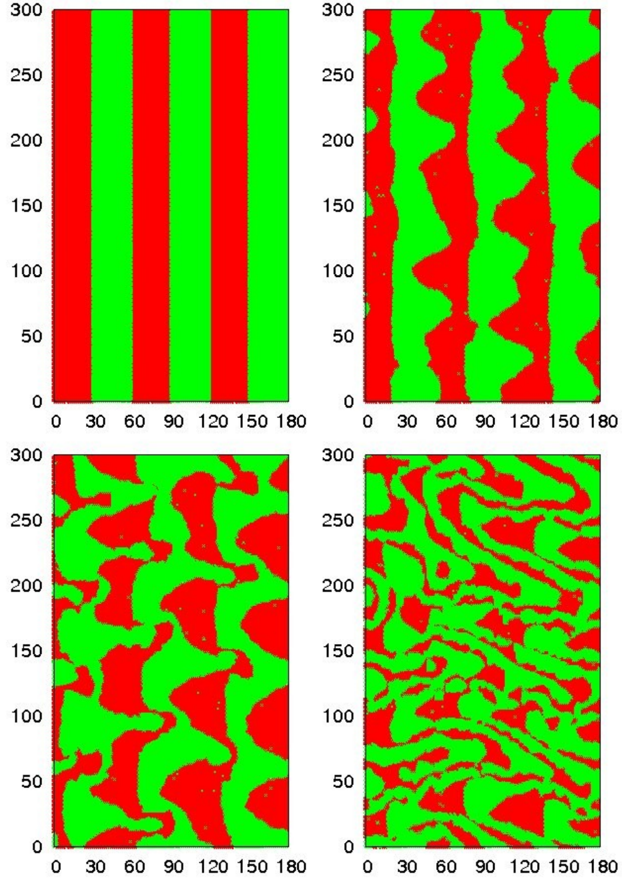


r$=0.4$, β J=6, $\beta\mu$=15, β b=0.7, $[11\underline{2}0]$

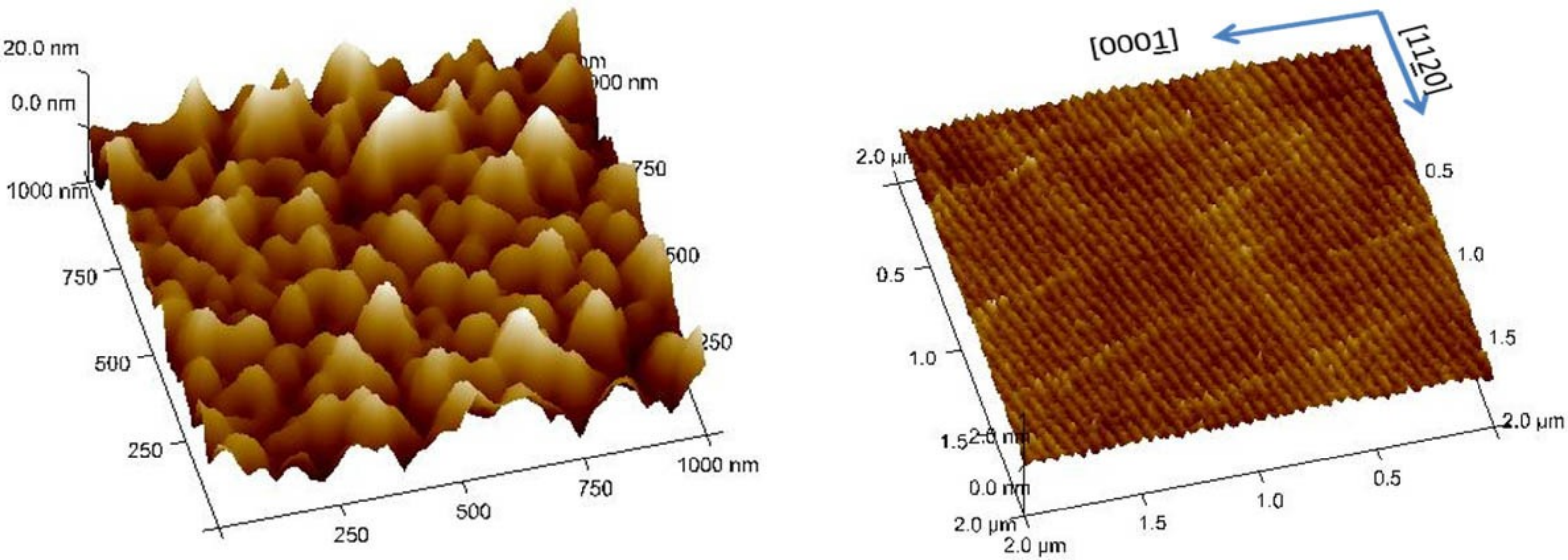


r$=0.4$, β J=6 , $\beta\mu$=15, β b=0., $[11\underline{2}0]$

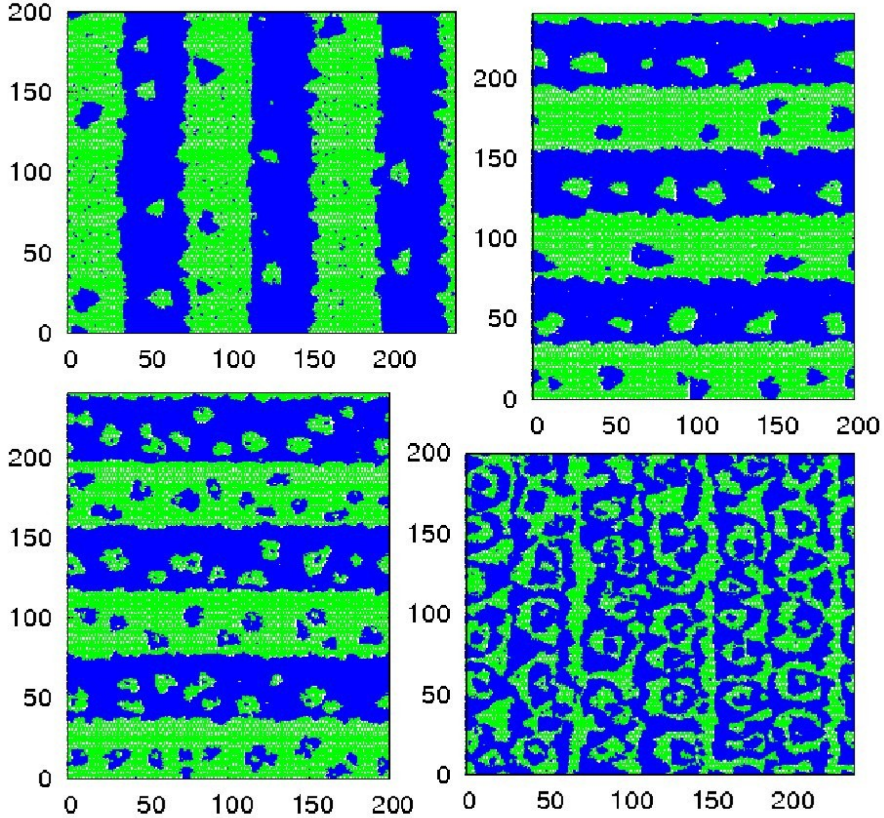
Wider steps, lower temperatures, Schwoebel barrier



r= 0.4, β J=6 , βμ=16, β b=0.5, [01$\underline{1}$0]

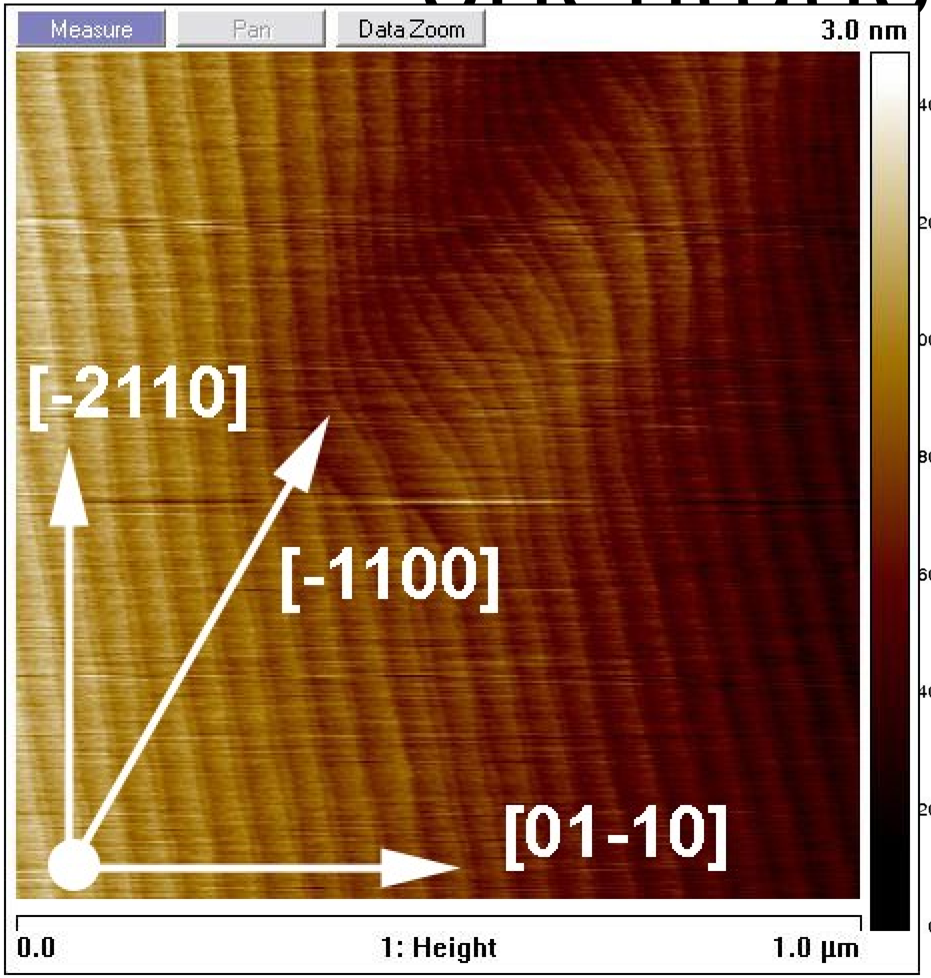

20.0 nm
0.0 nm
1000 nm
750
500
250
250
500
750
1000 nm
[0001]
[1120]
2.0 µm
0.5
1.0
1.5
2.0 µm
0.0 nm
2.0 µm
2.0 µm
1.5
1.0
0.5
0.5
1.0
1.5
2.0 µm

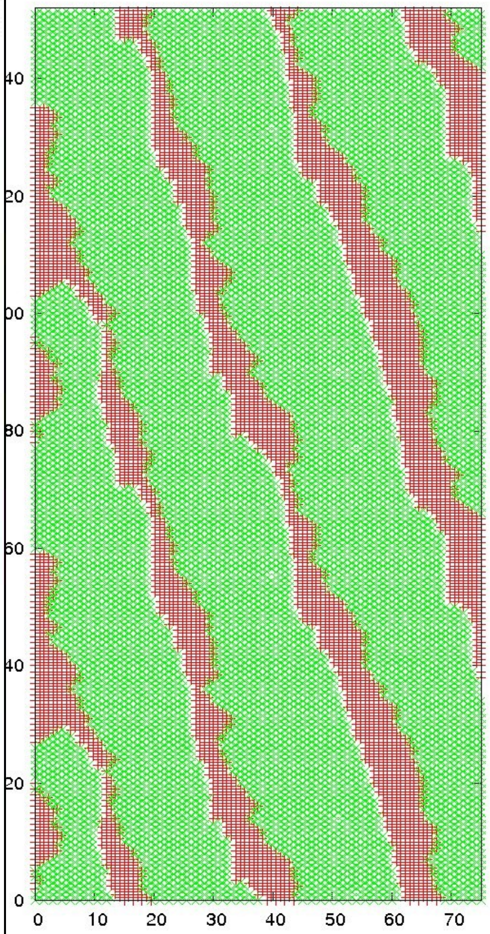
Too large particle flux



$r = 0.2$, $\beta J = 5$, $\beta\mu = 13$, $\beta b = 0$,
$[01\underline{1}0]$

Dependence on the step orientation





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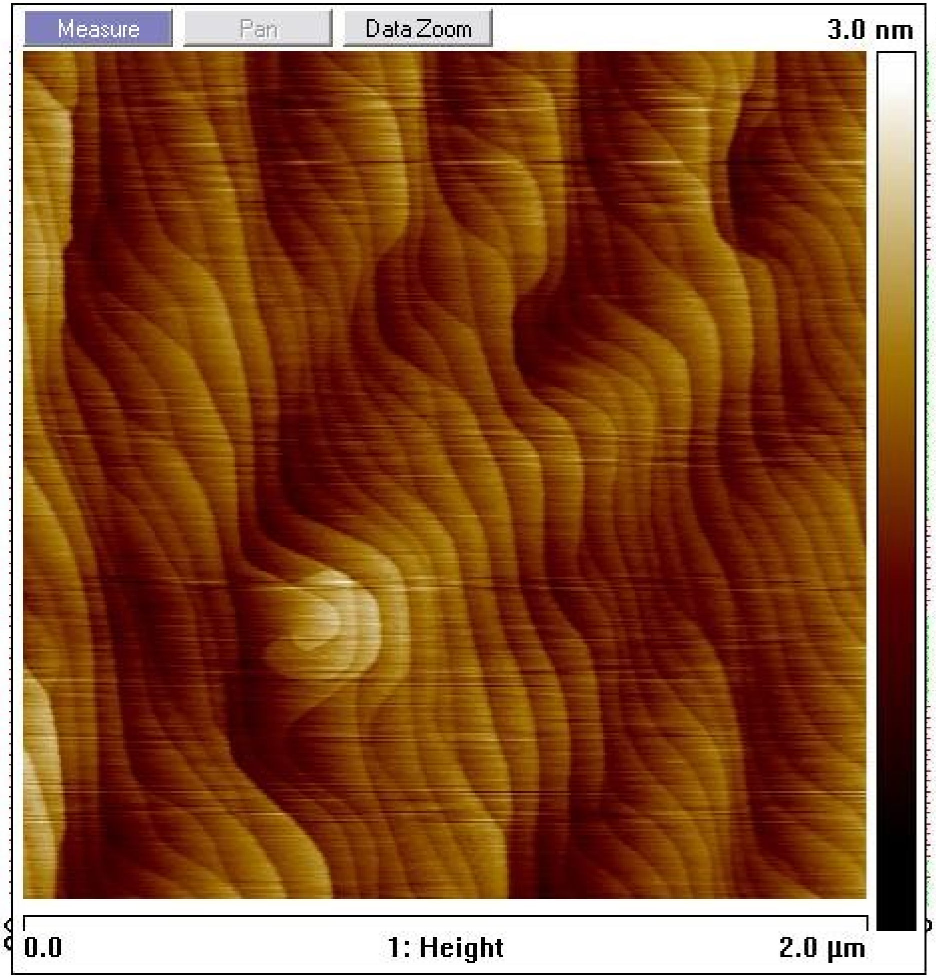
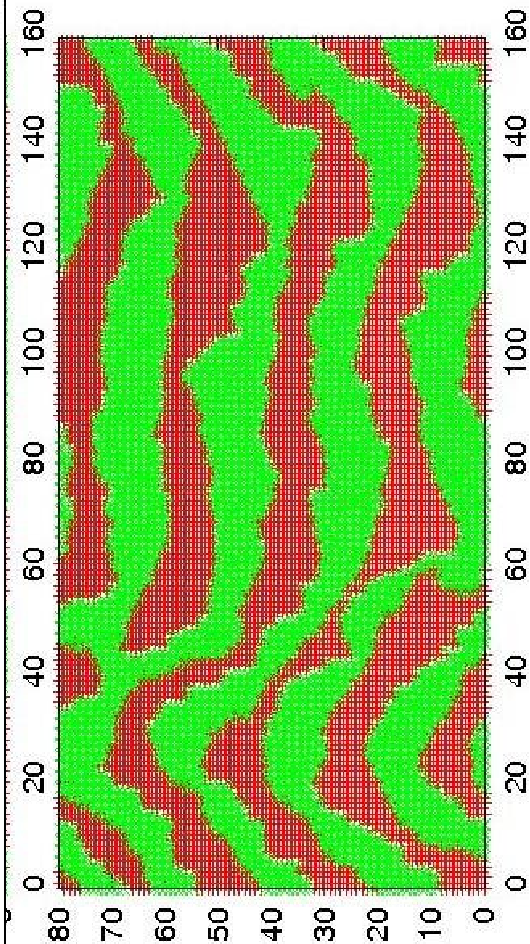
[1210] orientation





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Model parameters

Step asymmetry and temperature

r $\beta J = J/(k_B T)$

External particle flux

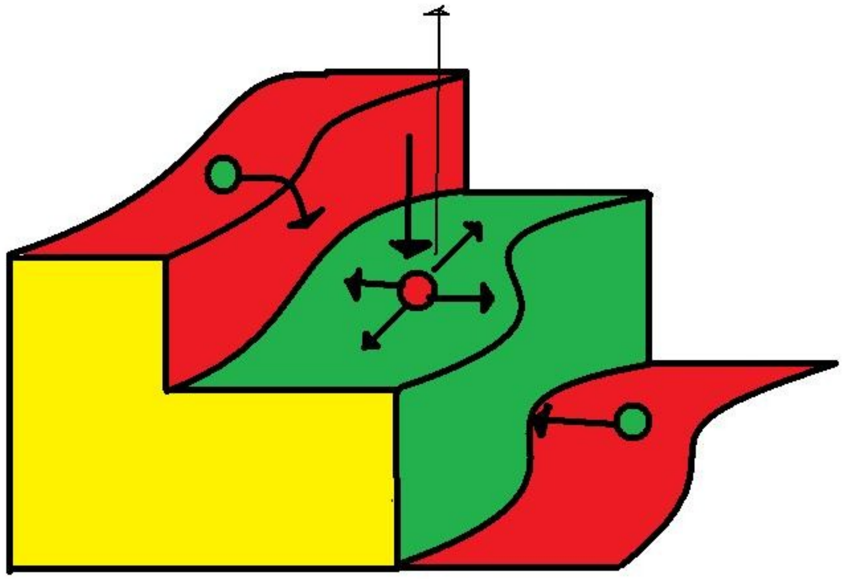
$$F = \nu_a e^{-\beta\mu} = \tau^{-1}$$

Schwoebel barrier

$$P_g = De^{-\beta b_g}$$

$$P_d = De^{-\beta b_d}$$

Control parameters



Terrace width

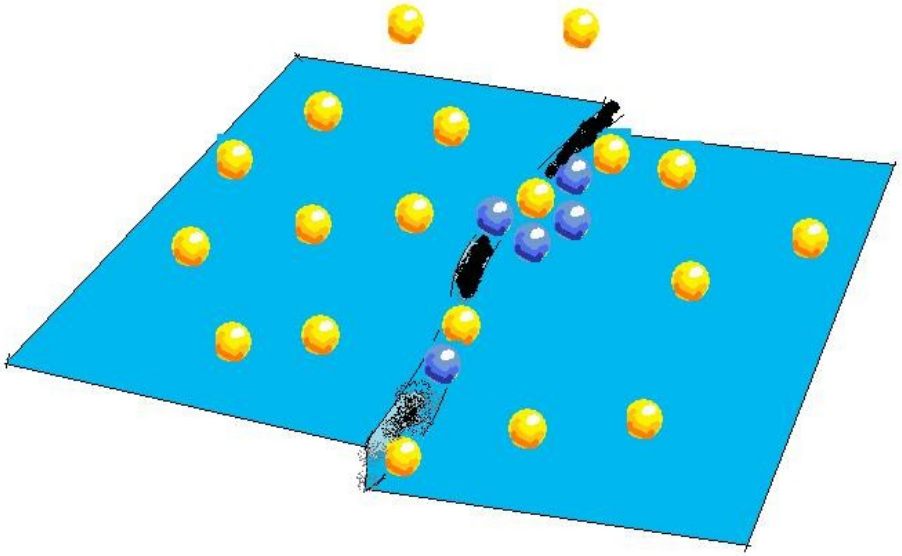
Orientation of steps

Temperature

External particle flux

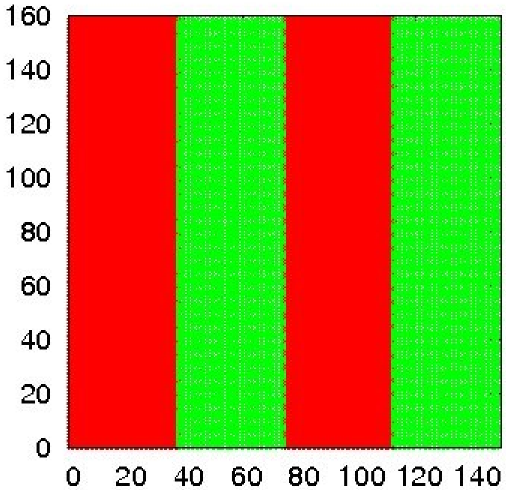
Other particles i.e.: Indium

GaN+Indium



One more component in the model

ndium


160
140
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100
80
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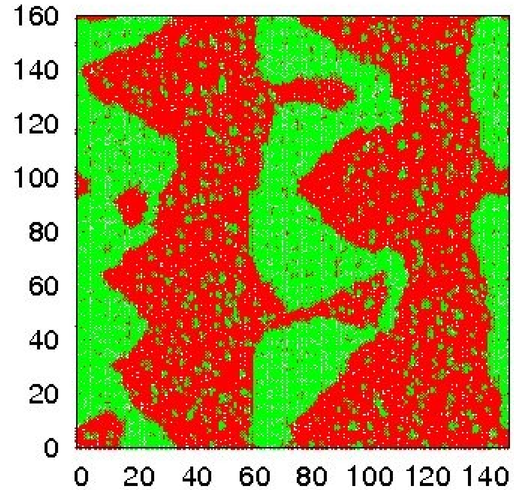
0 20 40 60 80 100 120 140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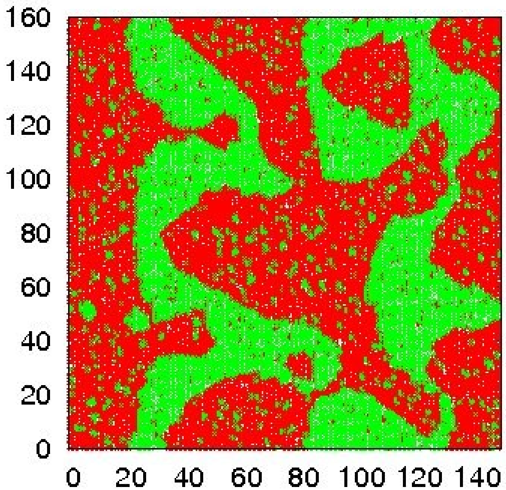
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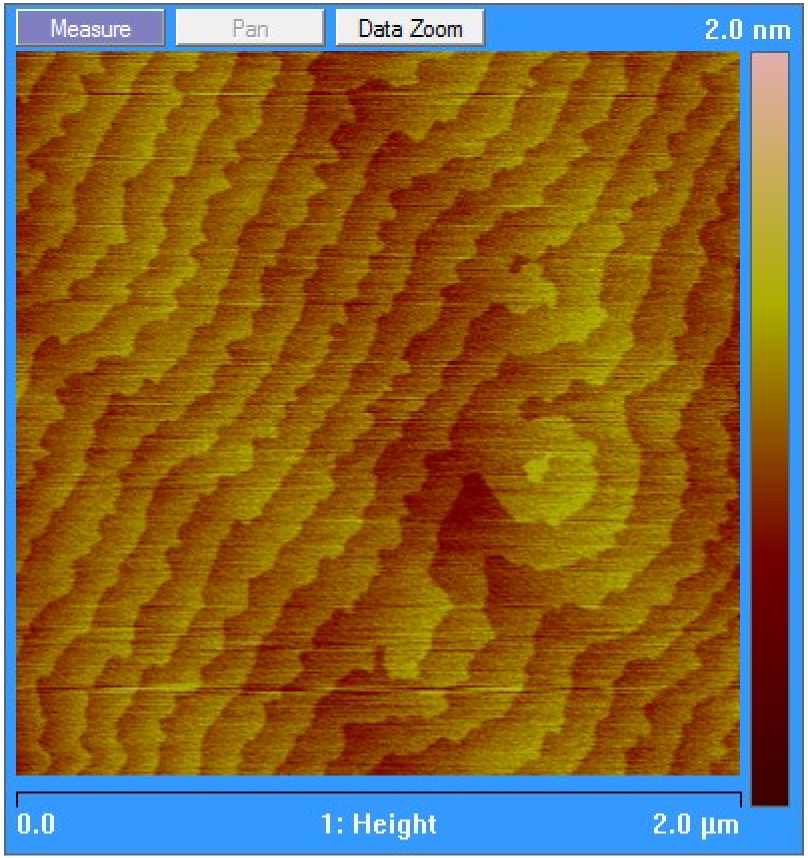
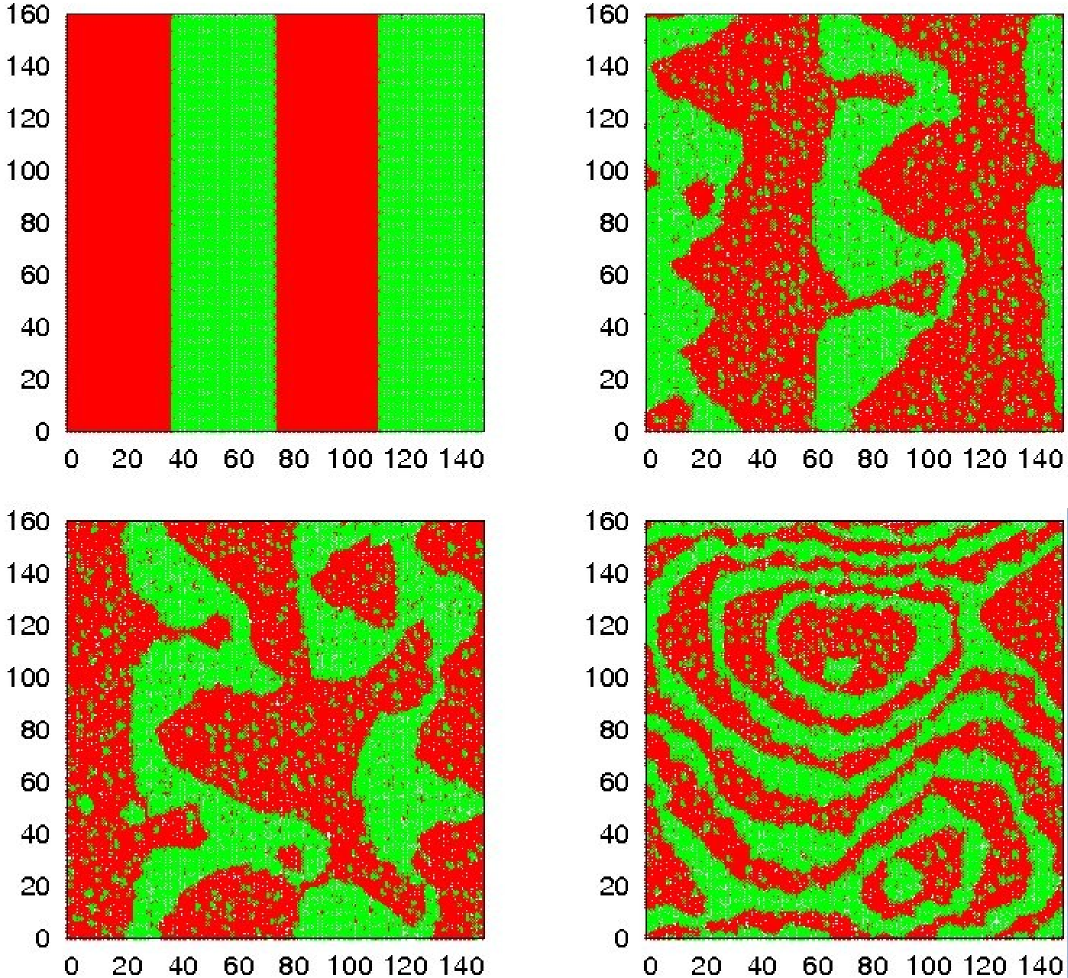

Measure
Pan
Data Zoom
2.0 nm
0.0
1: Height
2.0 µm

Indium



160
140
120
100
80
60
40
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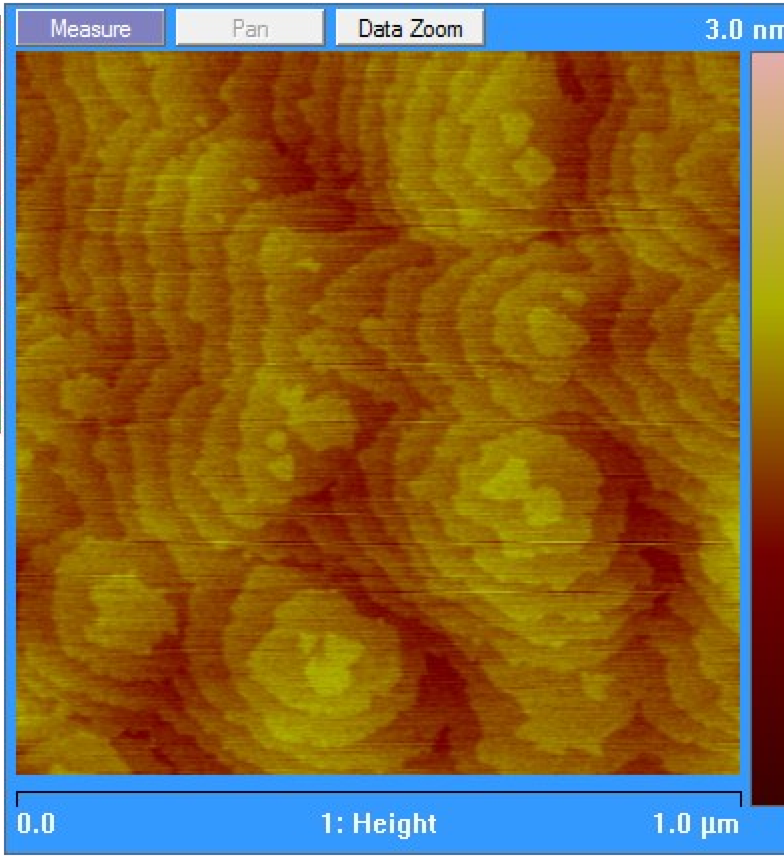
0
0 20 40 60 80 100 120 140



Measure
Pan
Data Zoom
3.0 nm
0.0
1: Height
1.0 µm

Summary

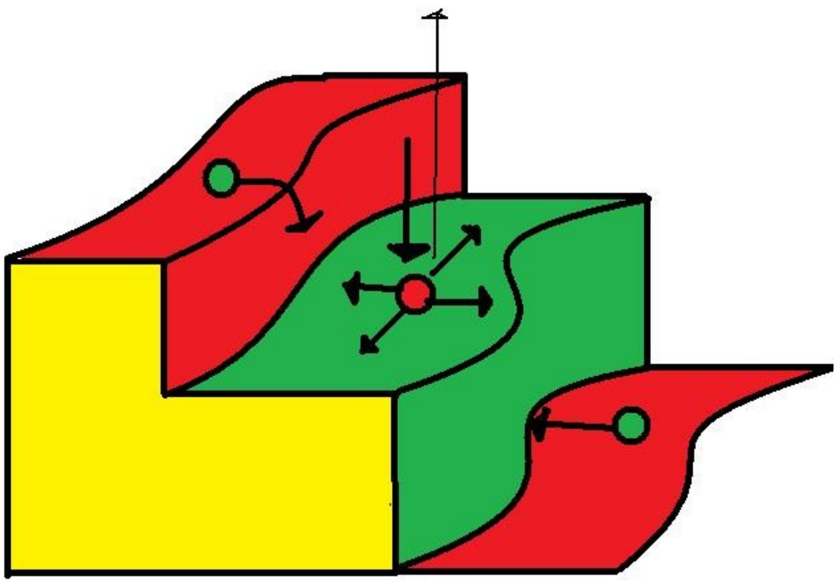
1.Three regimes of step flow during growth on GaN(0001) surface are observed:
  - low misorientation – very large terrace width – single straight step flow
  - medium misorientation – medium terrace width – step meandering
  - large misorientation – small terrace width – double and multiple straight step flow

1.Depending on the orientation of the step – two different crystallographic consecutive step structure can be created on GaN(0001) surface:
2.Rotation by 60 arc deg exchanges these two steps types.
3.Monte Carlo simulations describes:
  - 2-d nucleation controlled growth mode for large supersaturations
  - step flow mode for smaller supersaturations.

1.Monte Carlo simulations recovers step meandering and transition to double step flow modes.
2.Step meandering emerges in the result of diffusive interaction between steps and step anisotropy.

Analytical model 1D – parallel straight steps

$$D\frac{d^2}{(dz)^2}\rho + F - \frac{\rho}{\tau} + V\frac{d}{dz}\rho = 0$$



$$D\frac{d\rho}{dz}\mid_{(-d)+} \;=\; k_1(\rho - \rho^{+}{}_1)\mid_{(-d)+}$$

$$-D\frac{d\rho}{dz}\mid_{0-} \;=\; \kappa_2(\rho - \rho^{-}{}_2)\mid_{0-}$$

$$D\frac{d\rho}{dz}\mid_{0+} \;=\; k_2(\rho - \rho^{+}{}_2)\mid_{0+}$$

$$-D\frac{d\rho}{dz}\mid_{(l-d)-} \;=\; \kappa_1(\rho - \rho^{-}{}_1)\mid_{(l-d)-}$$

$$V = D\frac{d\rho}{dz}\mid_{0+} + D\frac{d\rho}{dz}\mid_{0-} = D\frac{d\rho}{dz}\mid_{(-d)+} + D\frac{d\rho}{dz}\mid_{(l-d)-}$$

Stability analysis of steps

When parallel steps start to meander?

$$z_i(x) = {z_i}^0 + \epsilon_i \sin(kx + \omega t)$$

$$\begin{aligned}\rho(x,z,t) &= A_0 \sinh(\lambda z(x,t)) + B_0 \sinh(\lambda z(x,t)) \\ &+ \epsilon[A_1 \sinh(\Lambda z) + B_1 \sinh(\Lambda z)] \sin(kx + \omega t)\end{aligned}$$

$${\rho^{\pm}}_i = {\rho^{\pm}}_{i0} - \Gamma \frac{z_{xx}}{(\sqrt{1+{z_x}^2})^3}$$

$$V = \frac{V_0 + \dot{z}}{\sqrt{1+{z_x}^2}}$$

$$\omega(k_c) = 0 \quad \frac{\partial \omega}{\partial k}_{k=k_c} = 0$$

Solution

Steps destabilize when

$$\frac{\lambda\Gamma}{F\tau}\left[\coth(\lambda d)\frac{k_1+\kappa_2}{k_1-\kappa_2}+\frac{(D\lambda)^2+k_1\kappa_2}{D\lambda(k_1-\kappa_2)}\right]<\frac{1}{2},$$

Double steps destabilize for

$$\frac{\lambda\Gamma}{F\tau}\left[\coth(\lambda l)\frac{k+\kappa}{k-\kappa}+\frac{(D\lambda)^2+k\kappa}{D\lambda(k-\kappa)}\right]<\frac{1}{2}$$

$$(\lambda\Gamma)/(F\tau)<1/2$$

Step dynamics