

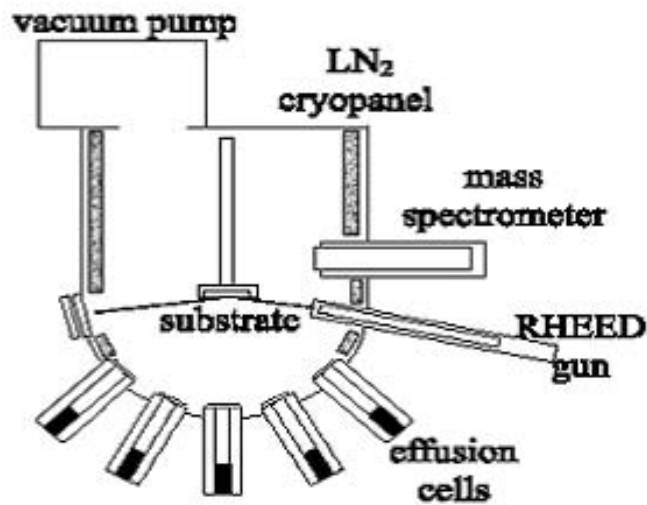
# **An Introduction to MBE Growth**

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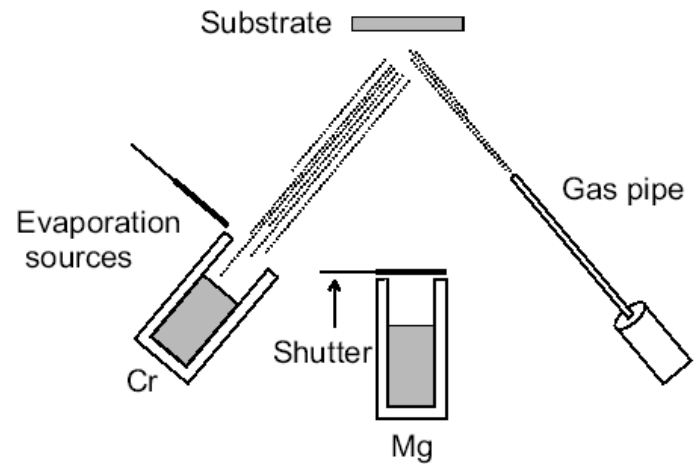
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# Basic description of MBE



A typical MBE system.

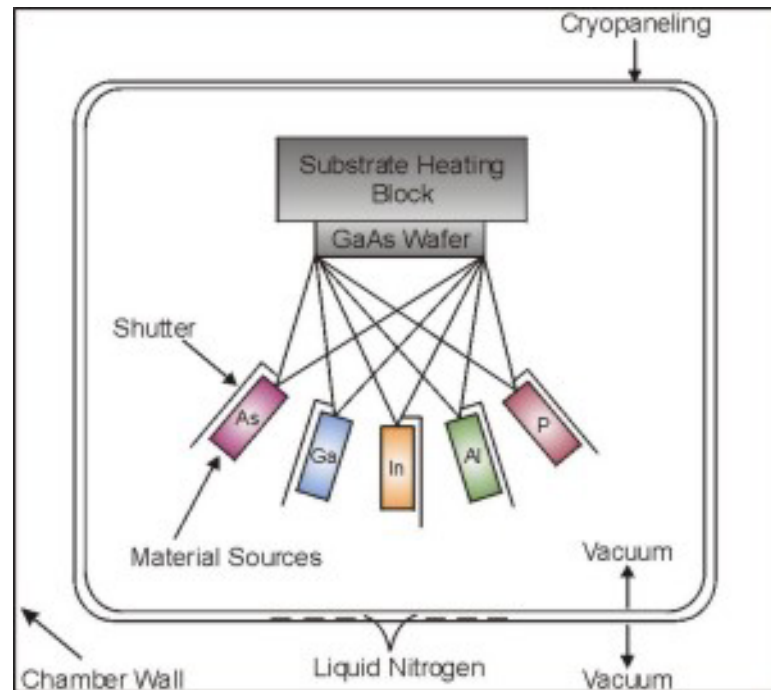


# Layout of an MBE System

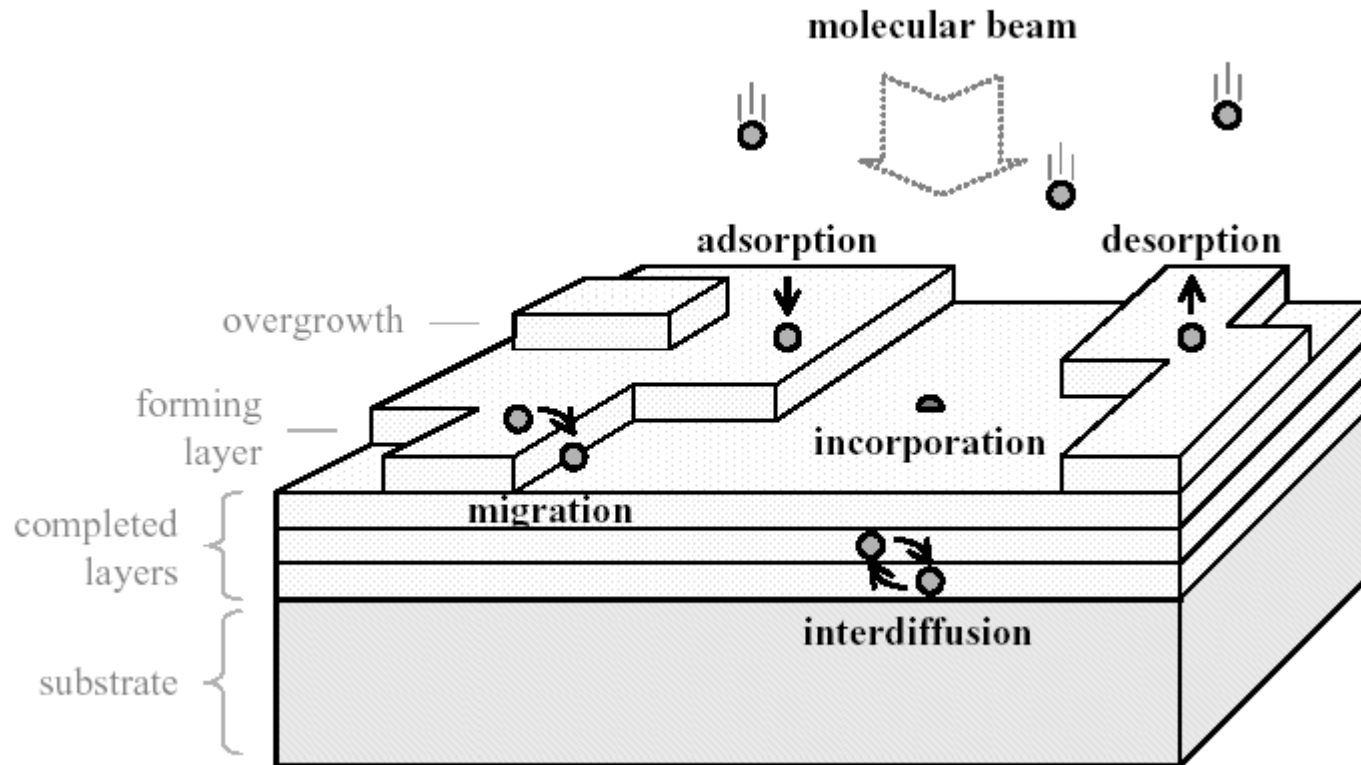
Growth chamber

Load lock

Other modules



# Surface processes during growth



# Features of MBE

- Ultra-High Vacuum (UHV)  
typical pressure in growth chamber  $10^{-11}$  torr
- Growth Rate of 1  $\mu\text{m}/\text{Hr}$  or 1 Atomic Layer/Sec  
only 1/75 the thickness of a hair
- MBE Uses High-Purity Elemental Charge Materials  
available in 7N's purity (99.99999% pure)
- Real-time Monitoring Tools  
Reflective High Energy Electron Diffraction  
(RHEED) system

# Growth models

- Kinetic Monte Carlo simulation (kMC)
- Kardar-Parisi-Zhang equation model(KPZ)
- Coupled growth equation model (CGE)

# Kinetic Monte Carlo simulation

The KMC method is based on a solid-on-solid model (SOS) of epitaxial growth, which assumes a simple cubic lattice structure with neither vacancies nor overhangs. The basic processes included in the model are *deposition of adatoms* and subsequent *surface diffusion*.

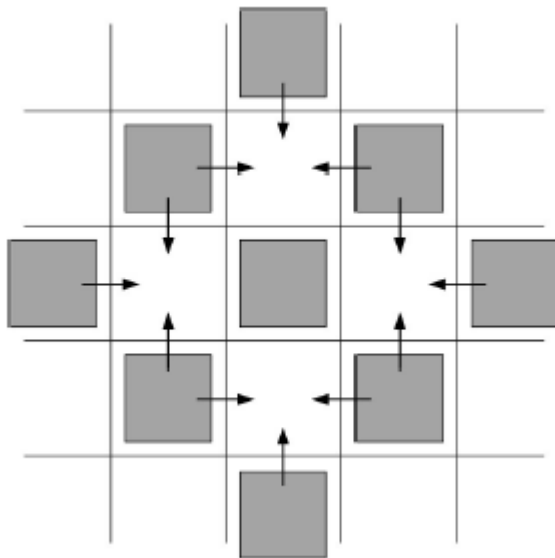
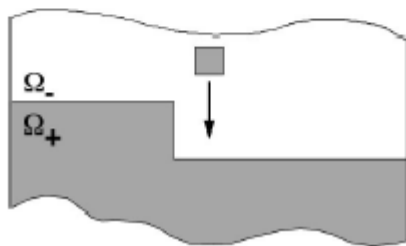
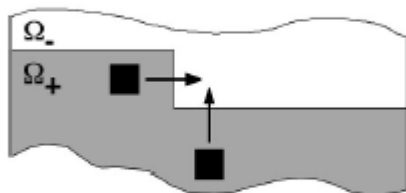
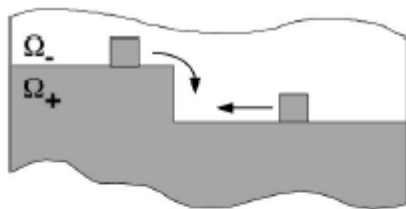
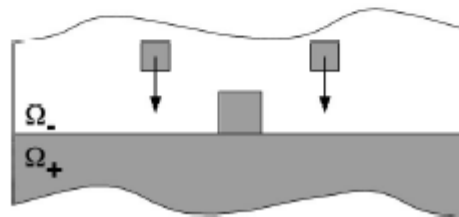
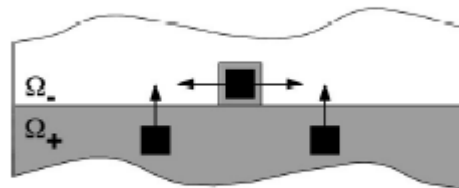
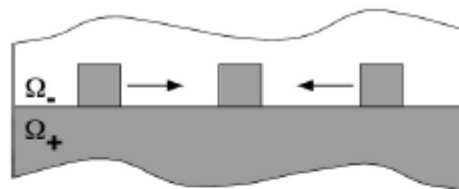


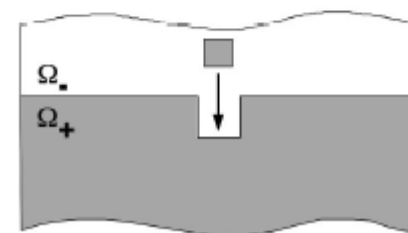
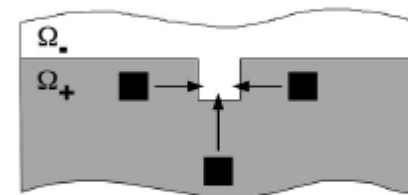
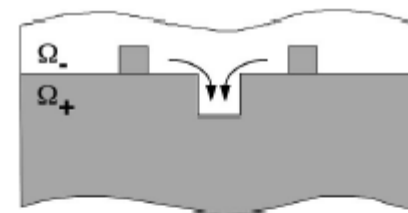
Illustration of the nucleation process. For a fixed adatom (center), this shows the  $C_m=12$  ways that a second adatom can attach to nucleate a new island.



This shows the number of ways that an adatom can hop to a fixed kink site:  
 $cw=2$  for edge adatom (top);  
 $cw=2$  for an adatom from the upper terrace (middle);  
 $cw=1$  for an adatom from the lower terrace (bottom).



This shows the number of ways that an atom can hop to a fixed edge adatom:  
 $cg=2$  for an edge adatom (top);  
 $cg=4$  for an adatom from the upper terrace (middle);  
 $cg=2$  for an adatom from the lower terrace (bottom).



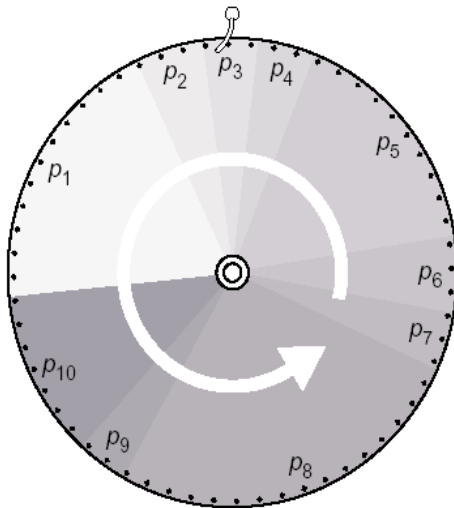
This shows the number of ways that an adatom can fill in an empty site between two kinks:  
 $ch=2$  for an edge adatom (top);  
 $ch=3$  for an adatom from the upper terrace (middle);  
 $ch=1$  for an adatom from the lower terrace (bottom).



The diffusion rate of a single adatom is defined as the probability of a diffusion jump per unit time, and it is given by the Arrhenius-type expression:

$$k(E, t) = k_0 \exp(-E / k_B T)$$

$$E = E_S + nE_N + E_B$$



**Schematic representation of various competing thermally activated diffusional processes. The large sectors represent jump paths with large jump rates and vice versa.**

$$\text{Circumference} = \sum p_i$$

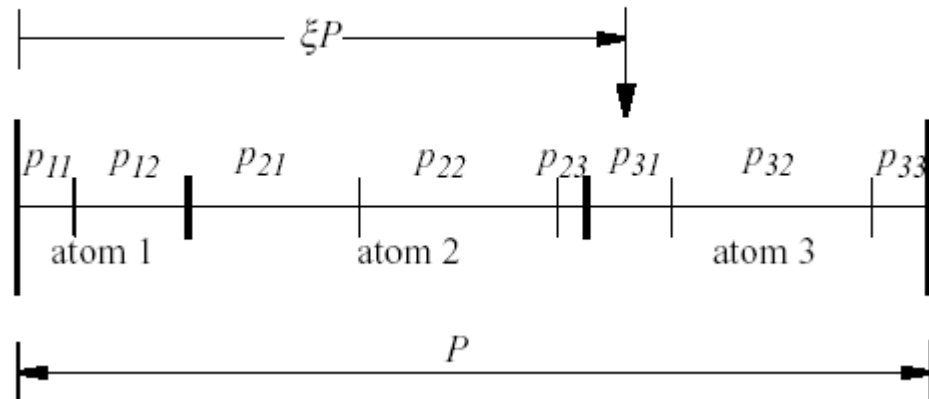
where

$$p_i = v_0 \exp\left(-\frac{E_i}{kT}\right)$$

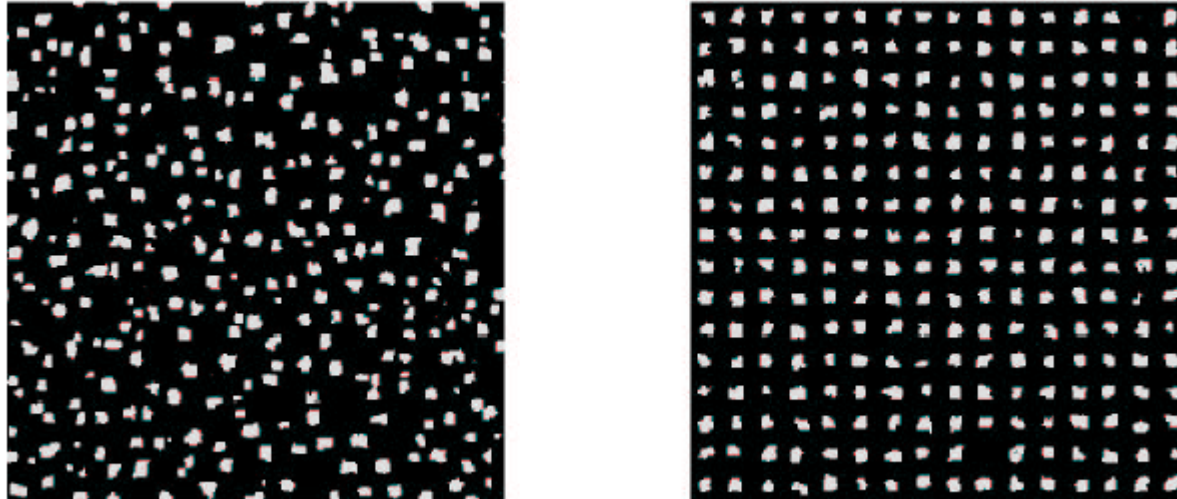
The key steps lie in the execution of the thermal diffusion loop and can be described as follows:

- (1) Select a jump path at random weighting by individual rate;**
- (2) Make the jump;**
- (3) Update and sum up jump rates;**
- (4) Turn ahead simulation clock;**
- (5) Iterate step 1 through 4 until designated number of atoms is deposited.**

## Linear search



**A schematic illustration of the linear procedure used to select the jump path. Path  $p_{31}$  is a randomly chosen event on a line segment of length  $P$ .**



Examples of configurations generated by KMC simulations at the temperature of 390 K and at the adatoms coverage of 15 %. On the left is illustrated the results from simulations where the substrate was homogeneous. On the right is the lattice from simulations using model A for a patterned substrate. Dark areas designate the substrate and light areas the first layer of adatoms.

## Conventional modeling of weak surface texture

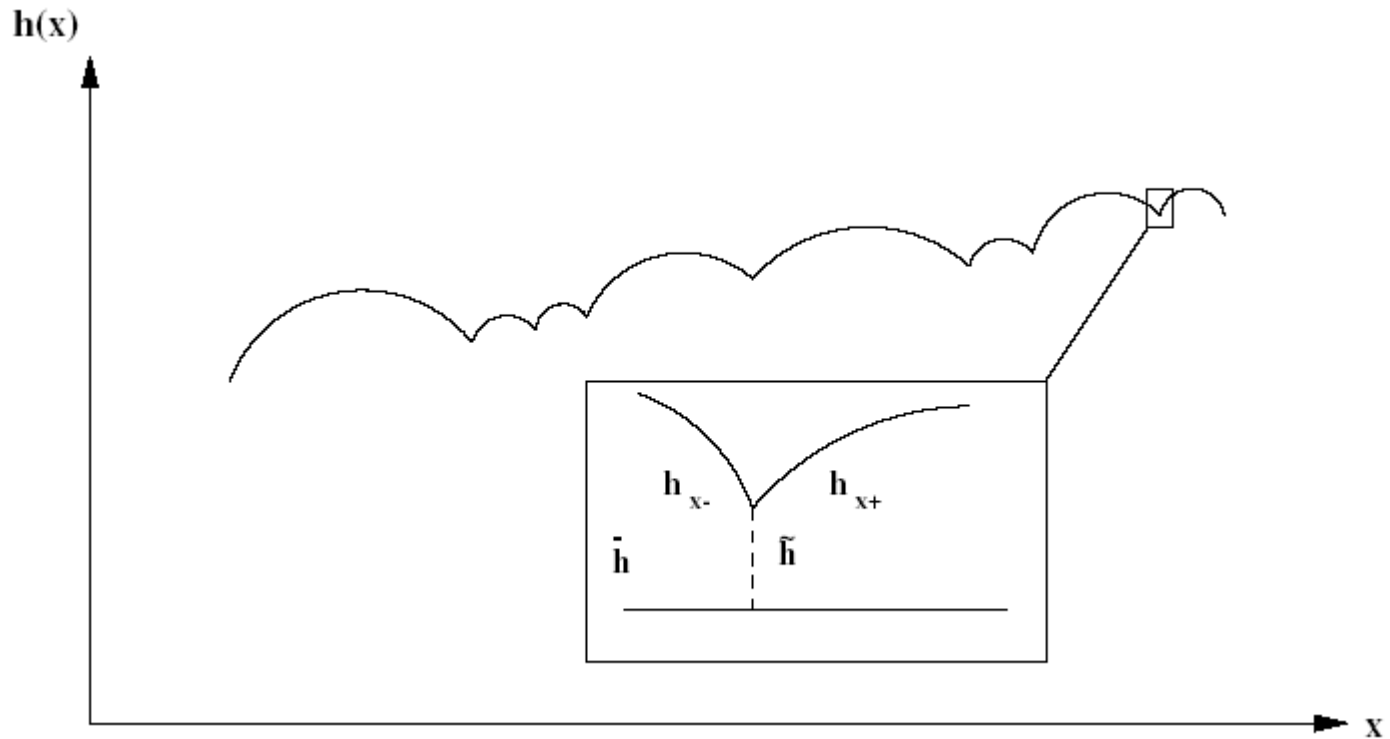
Kardar-Parsi-Zhang equation (KPZ) :

$$\partial_t h = \nu \nabla^2 h + \frac{\lambda}{2} (\nabla h)^2 + F + \eta(x, t)$$

Where  $h(x,t)$  is the height of the interface above a substrate, the coefficients in this equation are constants characterizing the microscopic atomic processes.

$F$  is the deposition rate from vapor

$\eta(x, t)$  simulate the random arrival of atoms at an average rate  $F$ .



The sharp valley solutions in KPZ equation are demonstrated while the variables characterising the vallies, namely  $hx_-$ ,  $hx_+$  and  $h^-$  are shown.

In the limit of the  $\nu \rightarrow 0$  unforced KPZ equation develops singularities for the given dimension. In one spatial dimension it develops sharp valleys in the finite time. The geometrical picture in Fig. 1 consists of a collection of sharp valleys intervening a series of hills in the stationary state. Obviously the height itself is a continuous quantity while in the sharp valleys the first derivative is discontinuous. Higher derivatives are singular *on the sharp valleys* and only can be described as distributions.

To summarize, the KPZ equation provides an accurate description of the surface morphology under certain restricted conditions (constant growth rate, low surface slope and long wavelength surface structure). In addition, the origin of the Nonlinearity in KPZ is still unclear in the case of MBE growth.

# Coupled growth equation model(CGE)

*(Developed by A. Ballestad, T. Tiejie, etc)*

Two 1D coupled growth equations:

$$\partial_t n + \nabla \cdot j = F - a_{//}^{-1} \partial_t (a_+^{-1} h) \quad (1)$$

$$\partial_t (a_+^{-1} h) = \beta D n^2 + \beta D n S - a_{//} \kappa S \quad (2)$$

**F** is the deposition rate from the vapor

**D** the adatom diffusion coefficient

**S** the density of steps

$\kappa$  the rate of thermal detachment of atoms from step edges into the adatom phase



In Eq. (2), any adatom that attaches to a step edge is assumed to have incorporated into the film.

We also define:

$$j = -D(a_+ \zeta n \nabla h + \nabla n),$$

$$S = \sqrt{S_0^2 + (a_+ \nabla h)^2}$$

$j$  is the surface current of adatoms

$\zeta$  is a proportionality constant which describes the net direction drift of adatoms.

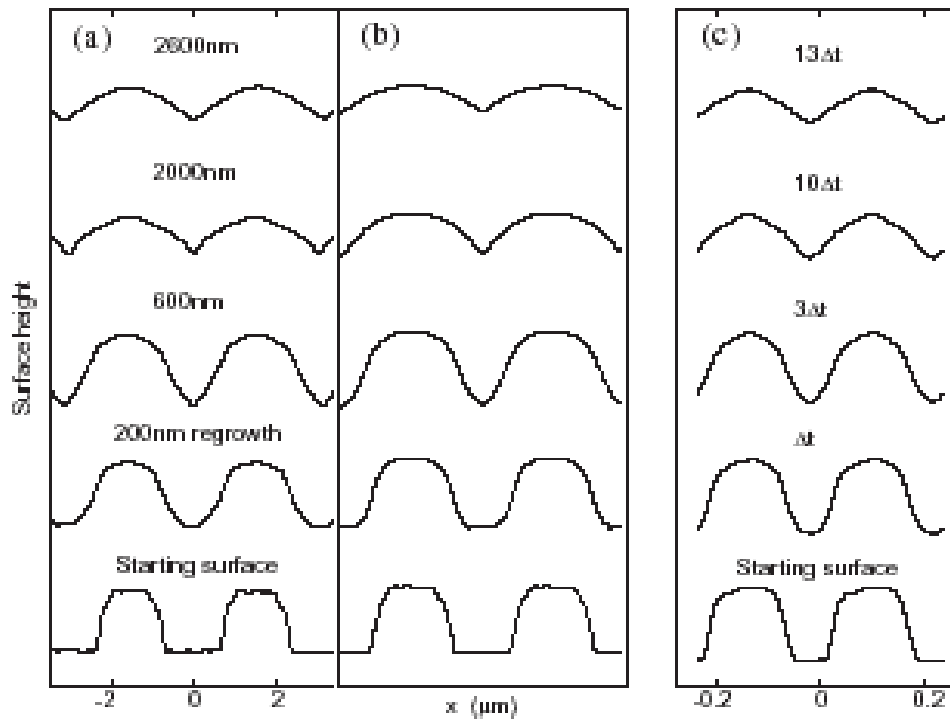
For low amplitudes and long wavelength ( $\nabla h < S_0$ ) the adatom density will be nearly constant as a function of position and time, and approximately equal to

$$n_0 = (F + \kappa S_0) / \beta D S_0$$

In this case, Eqs (1) and (2) reduce to,

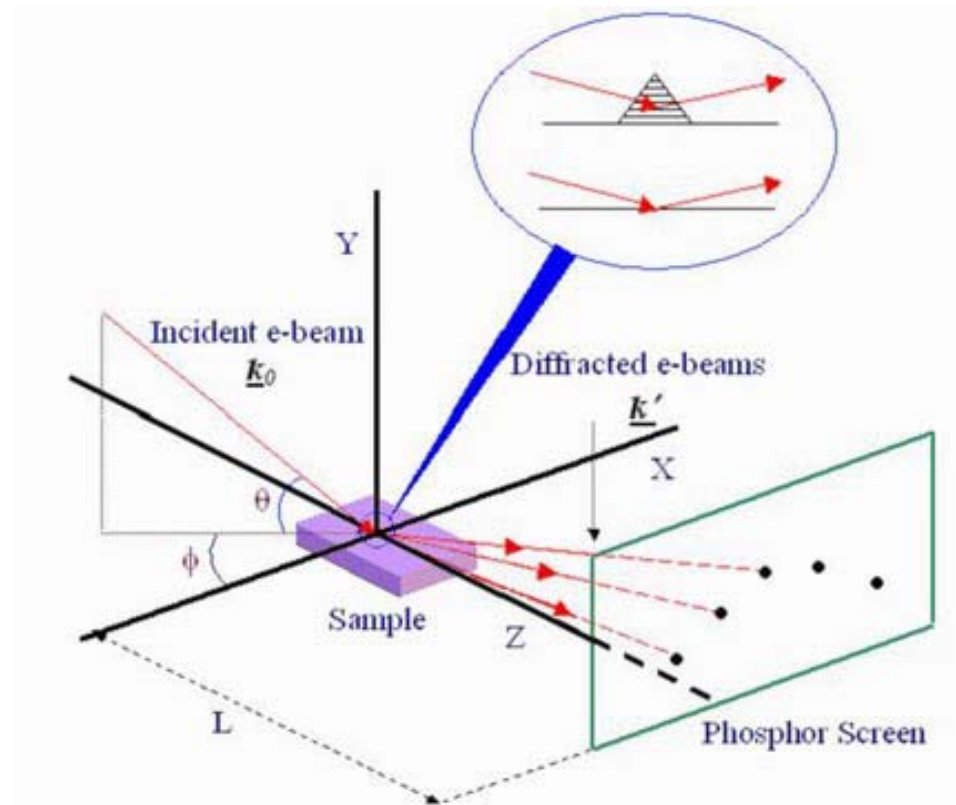
$$\frac{\partial h}{\partial t} = \frac{\zeta}{\beta} \left( \frac{F}{S_0} + \kappa \right) \nabla^2 h + F \quad (3)$$

## Film thickness evolution

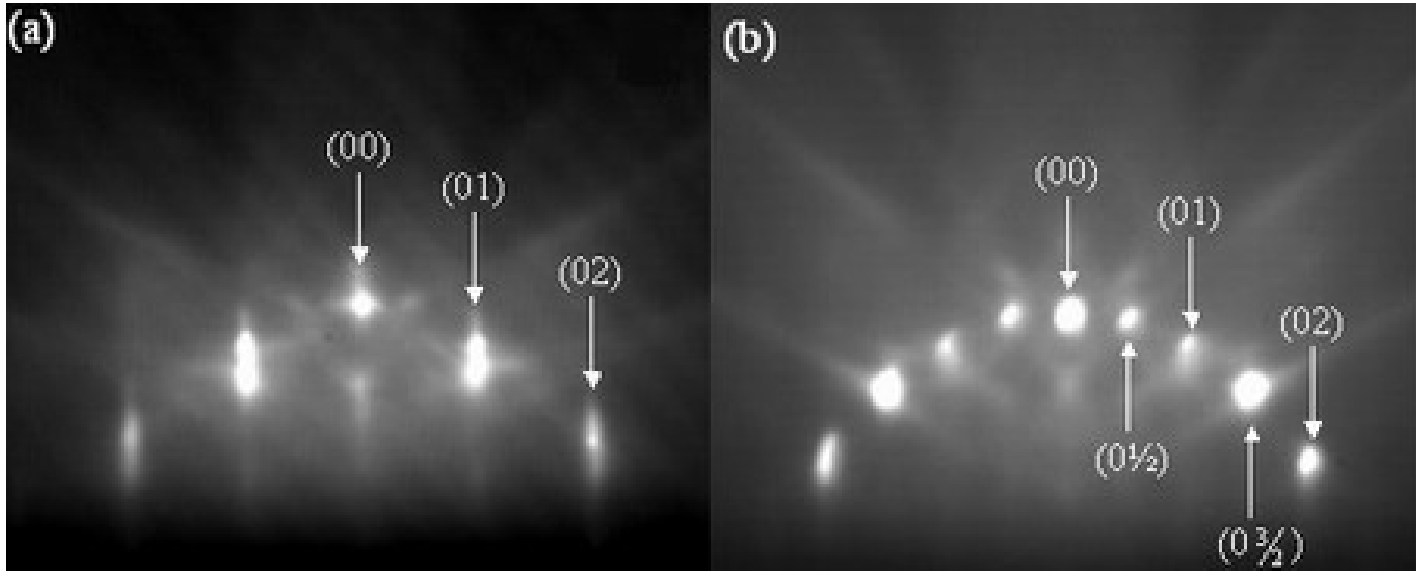


Film thickness dependence: (a) AFM scan lines for regrowth On 100nm deep gratings orientated perpendicular to the [110] Direction; (b) Scan lines from CGE calculation; (c) Scan lines From 2D kMC simulation of 10 nm high grating structure.

# Real-time monitoring tool: RHEED

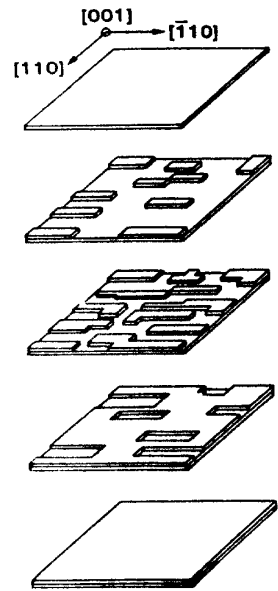


An illustration of the fundamentals of RHEED. The inset shows two kinds of reflection: transmission-reflection diffraction scattering by three-dimensional crystalline island (top) and surface scattering from flat surface (bottom).

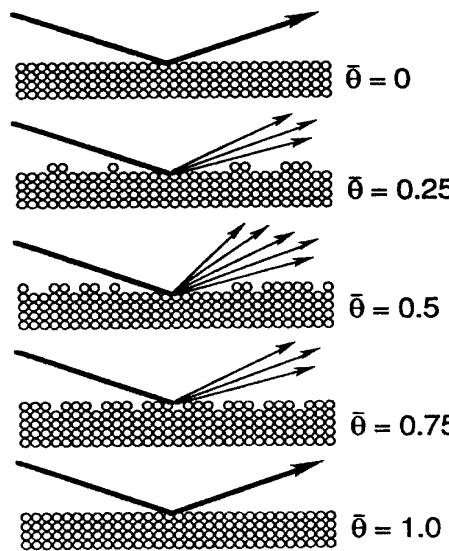


RHEED is sensitive for surface structures and reconstructions. (a) Si(100)-1x1 obtained by chemically cleaning the sample and loading it to the vacuum within few minutes [electron beam is incident in the  $\langle 110 \rangle$  with 8.6 keV], (b) Si(100)-2x1 reconstructed surface, obtained by chemically-cleaning the sample then baking the system for two days and flashing it up to 1200 °C [electron beam is incident in the  $\langle 110 \rangle$  with 8.6 keV]

MONOLAYER GROWTH



ELECTRON BEAM



RHEED SIGNAL

