Stochastic Equations for Driven Lattice Models

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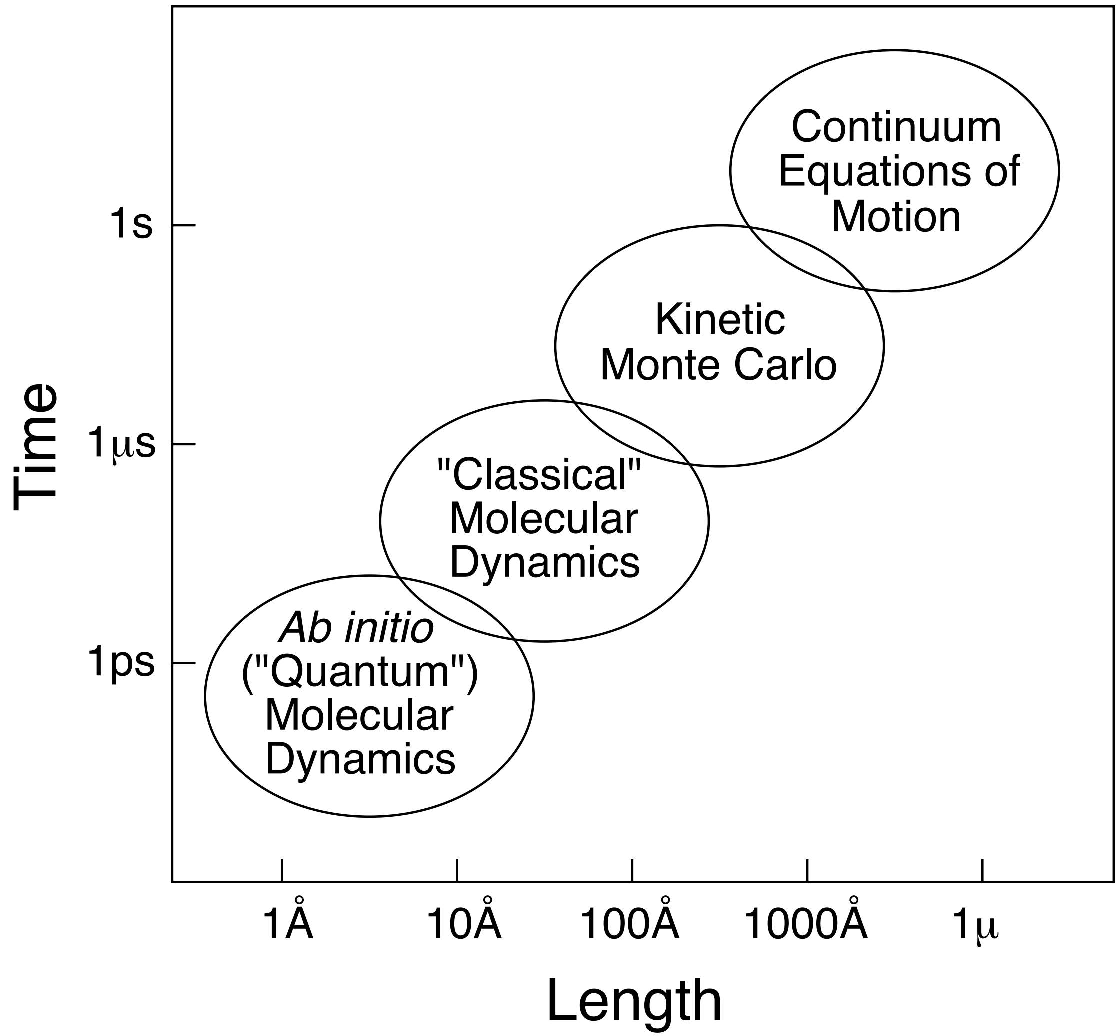
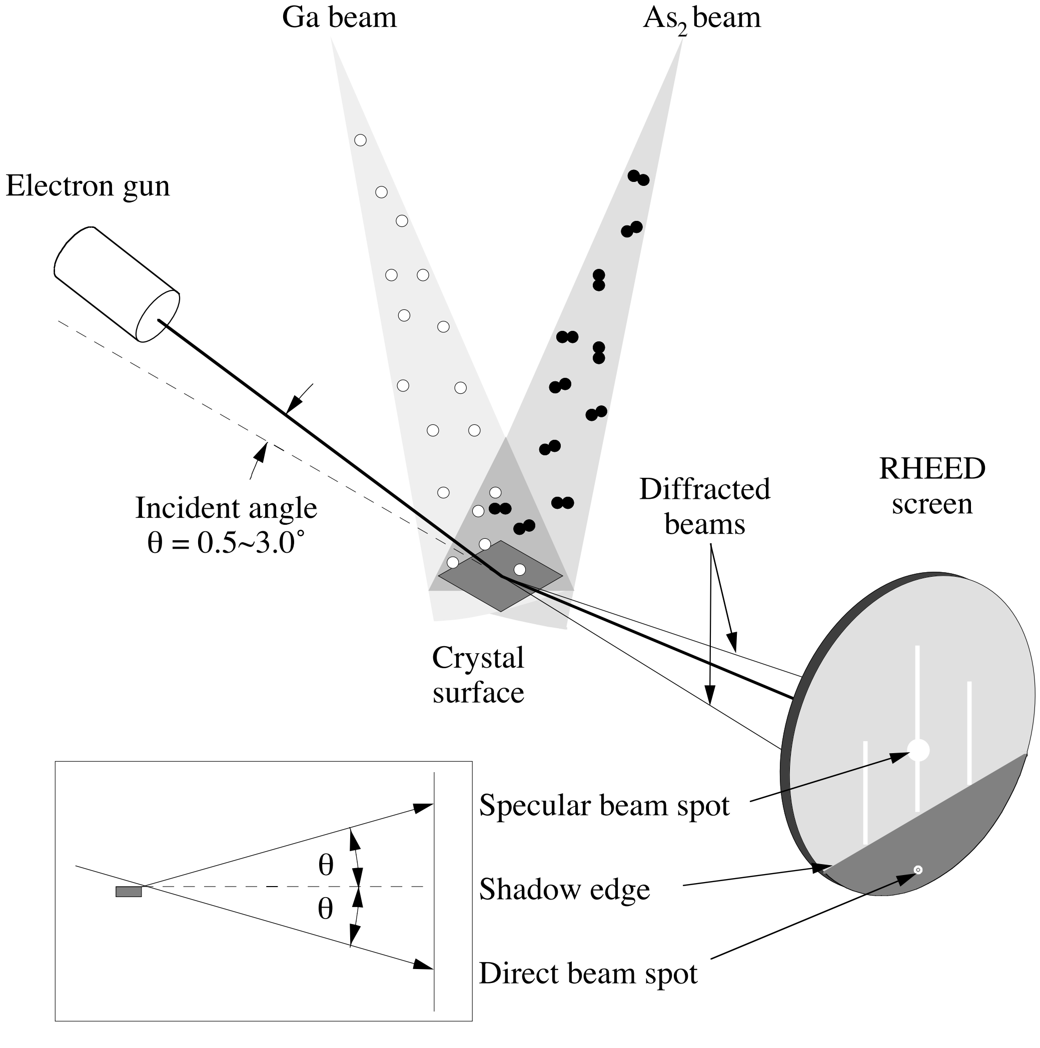
Outline

1. Multiscale Modelling of Materials
2. Epitaxial Phenomena
3. Lattice Models of Growth
4. Lattice Langevin Equation
5. Continuum Equations of Motion
6. Future Directions

Multiscale Modelling

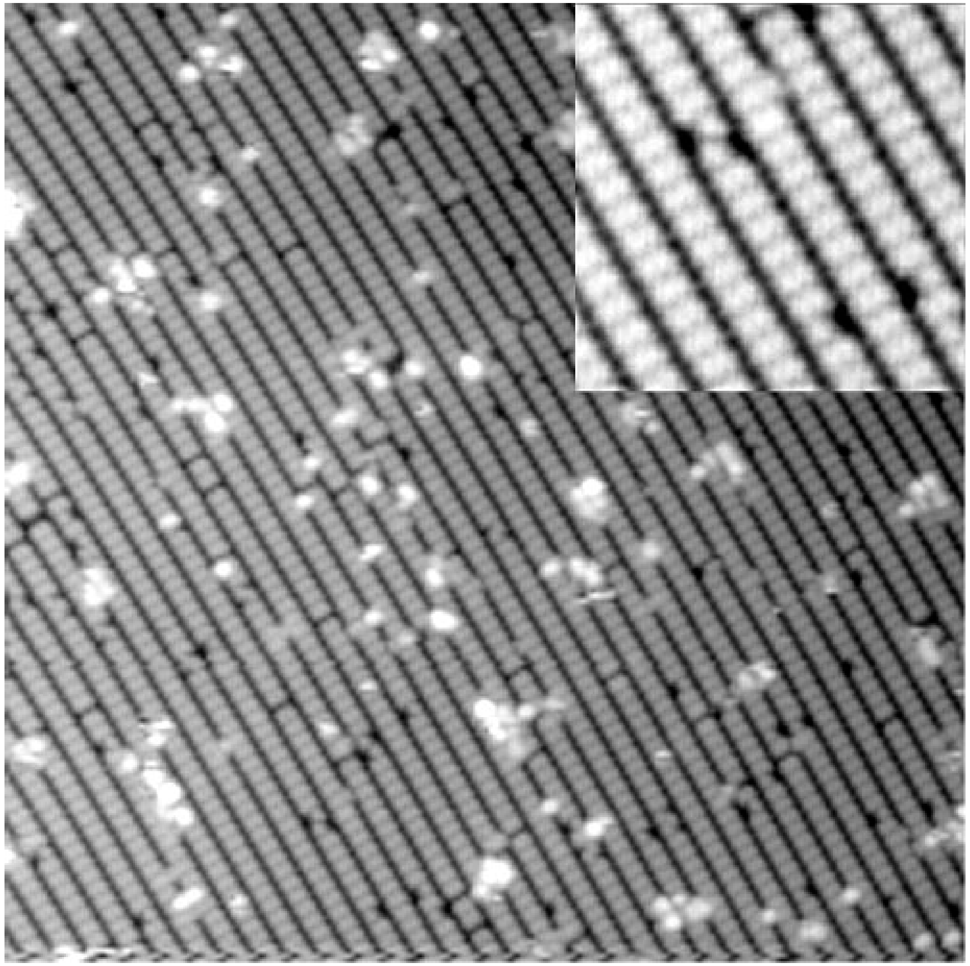


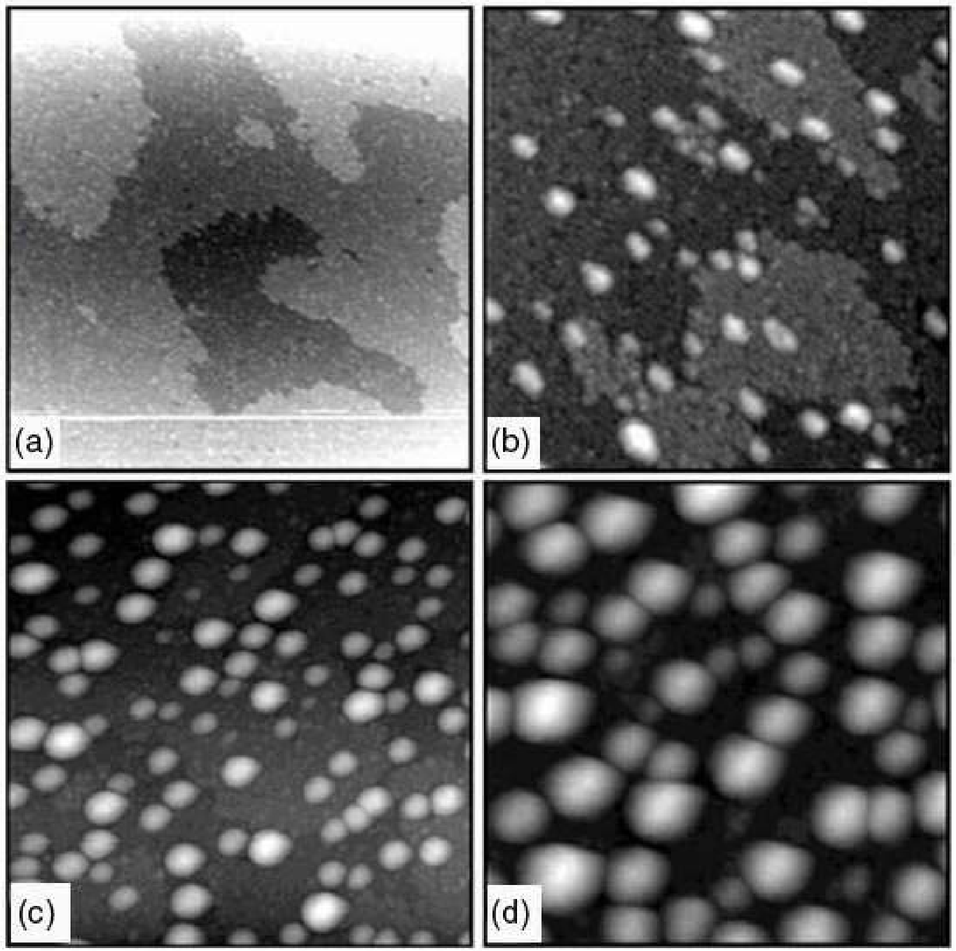
Epitaxial Phenomena



Quantum Dots

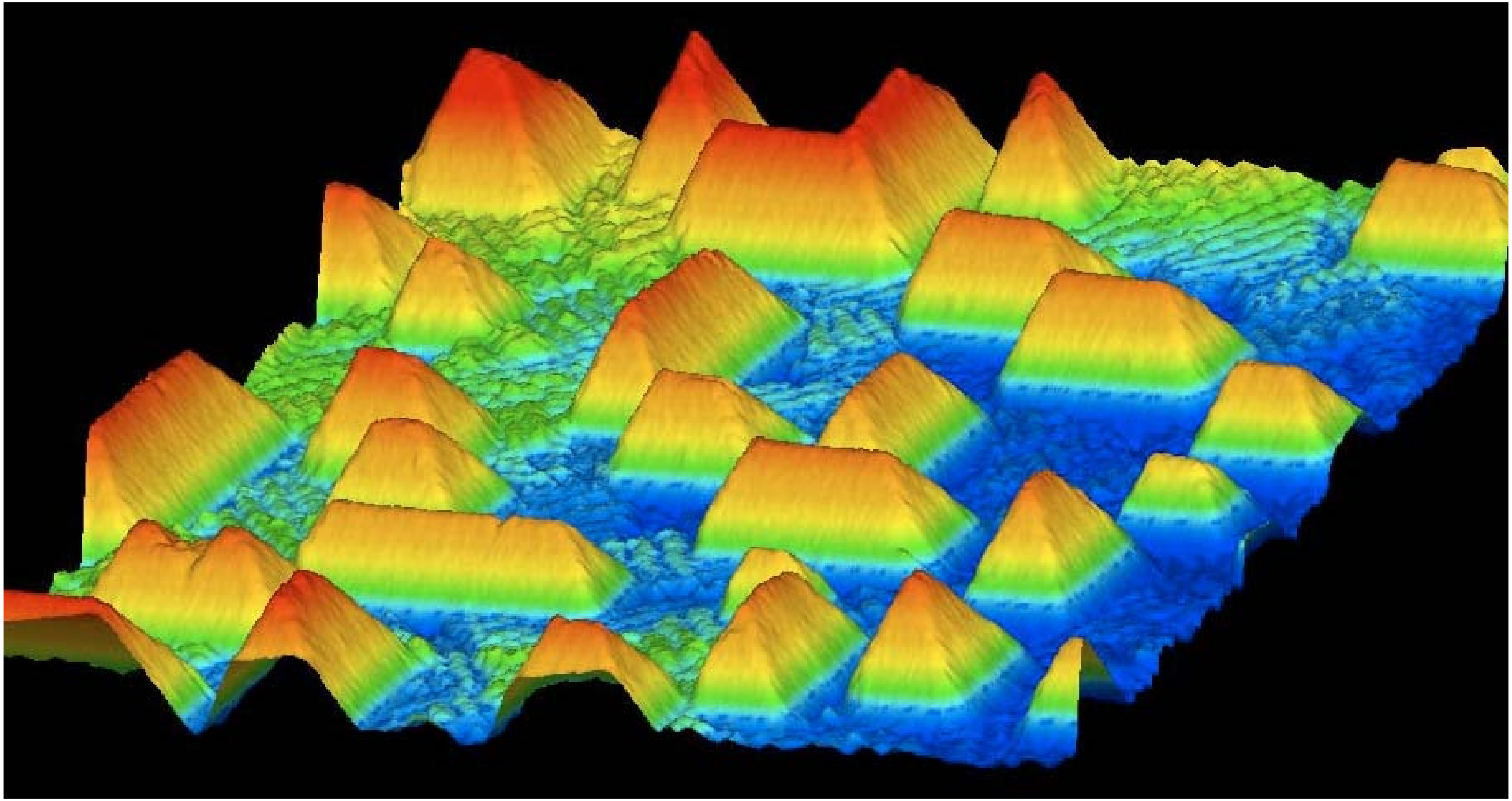
InAs/GaAs(001)



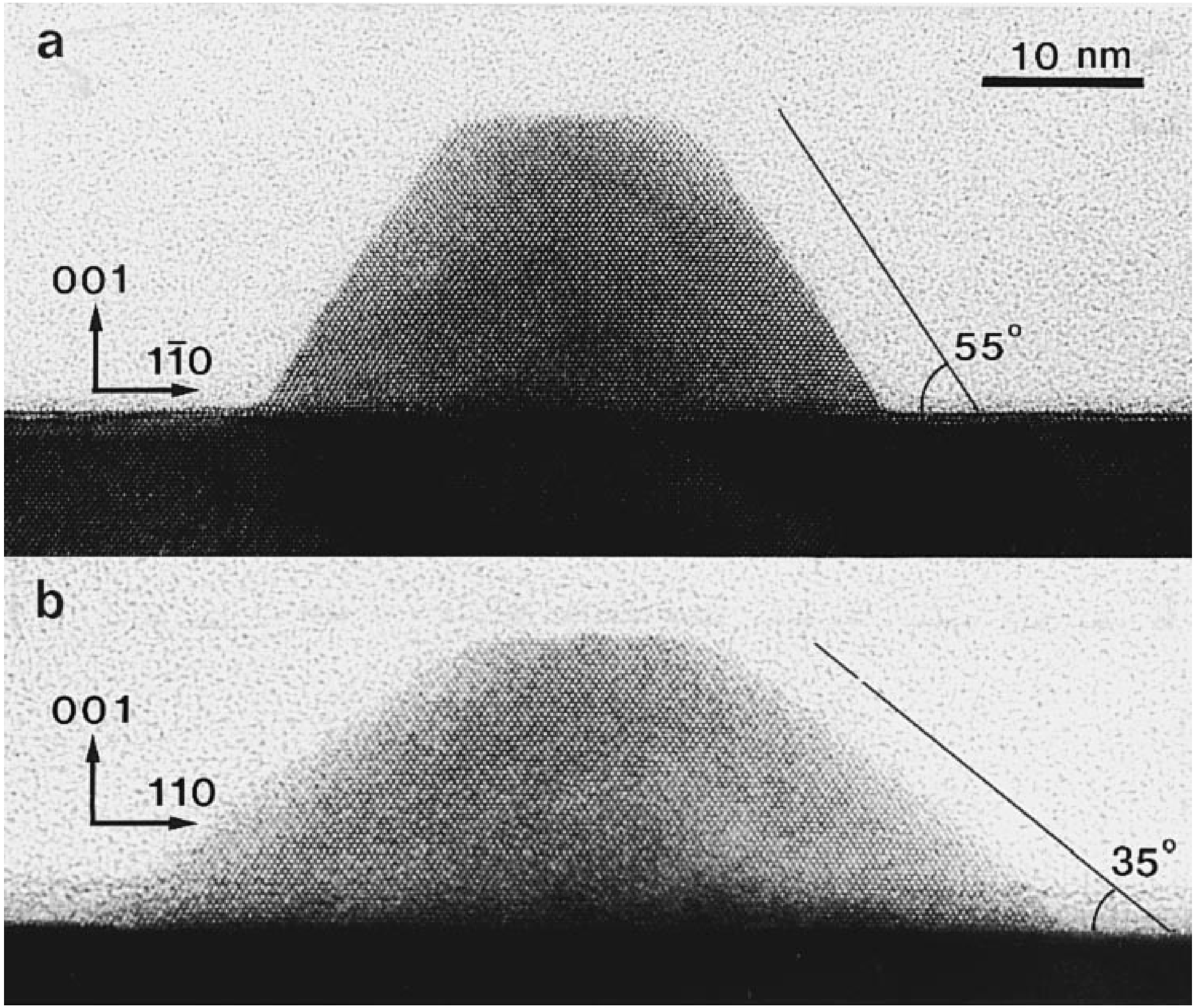


Quantum Dots

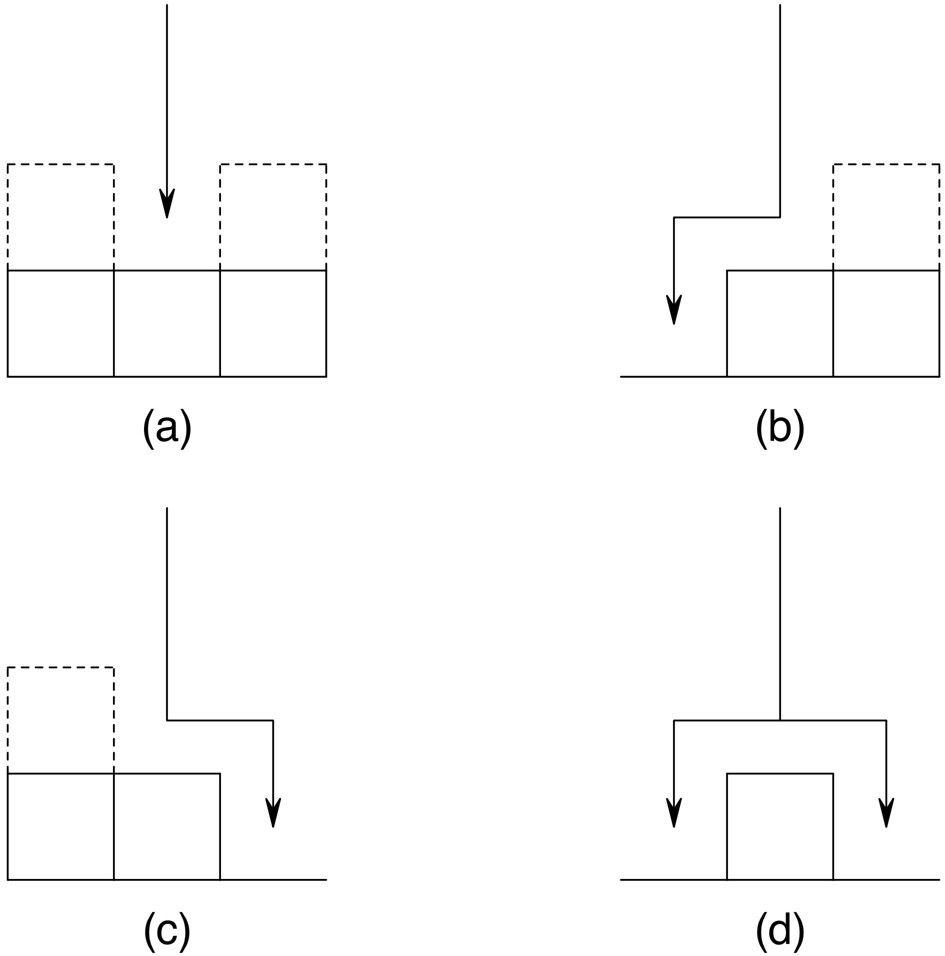
Ge/Si(001) (Courtesy Bert Voigtländer)



Quantum Dots

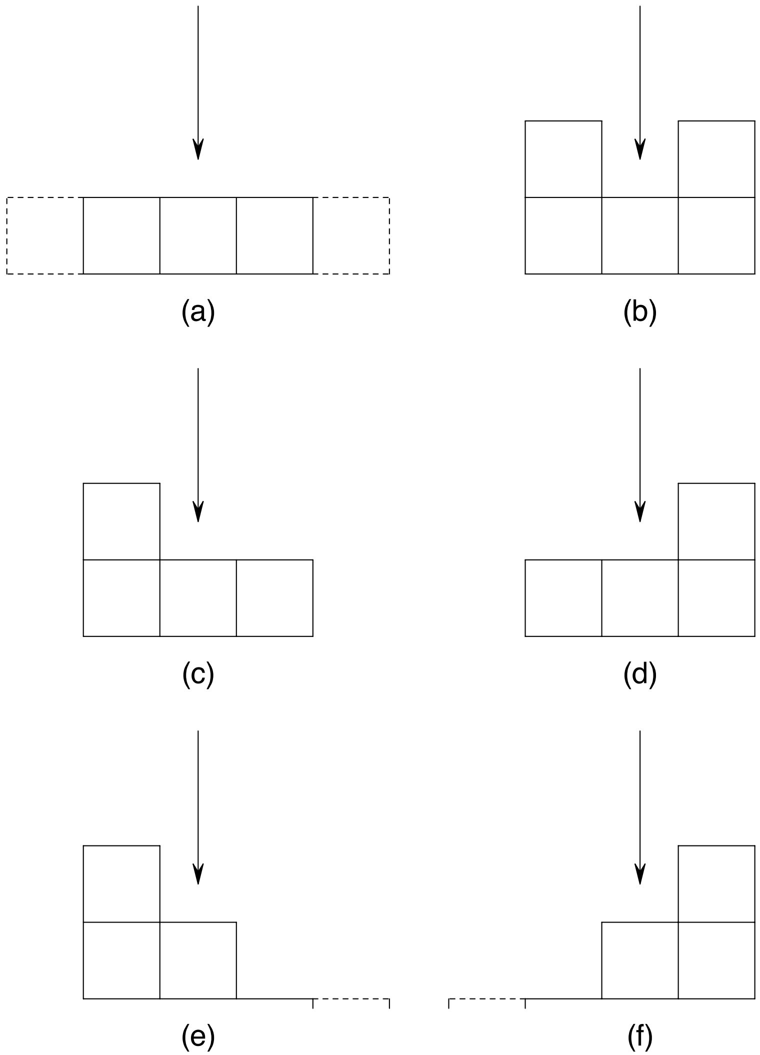


Edwards–Wilkinson Model



Originally introduced to model sedimentation; model for “hot-atom” effects near step edges.

Wolf-Villain Model



Introduced as “toy” model; used earlier for low-temperature growth on Si(001) and Ge(001).

Coarse Graining "Road Map"

$$\frac{\partial P}{\partial t} = \sum_{\mathbf{r}} [W(\mathbf{H}-\mathbf{r};\mathbf{r})P(\mathbf{H}-\mathbf{r},t) - W(\mathbf{H};\mathbf{r})P(\mathbf{H},t)]$$

$$\downarrow$$

$$\frac{dh_i}{dt} = K_i^{(1)}(\mathbf{H}) + \eta_i\,, \qquad \langle \eta_i(t)\eta_j(t')\rangle = K_{ij}^{(2)}(\mathbf{H})\delta(t-t')\,.$$

$$K_i^{(1)}(\mathbf{H}) = \sum_{\mathbf{r}} r_i W(\mathbf{H};\mathbf{r})\,, \qquad K_{ij}^{(2)}(\mathbf{H}) = \sum_{\mathbf{r}} r_i r_j W(\mathbf{H};\mathbf{r})$$

$$\downarrow$$

$$\frac{\partial h}{\partial t} = \nu\frac{\partial^2 u}{\partial x^2} + \lambda_1\frac{\partial^2}{\partial x^2}\left(\frac{\partial u}{\partial x}\right)^2 + \lambda_2\frac{\partial}{\partial x}\left(\frac{\partial h}{\partial x}\right)^3 + K\frac{\partial^4 u}{\partial x^4} + \eta$$

Edwards–Wilkinson Model

$$\frac{dh_i}{d\tau} = K_i^{(1)} + \eta_i\,, \qquad K_i^{(1)} = \frac{1}{\tau_0}\left[w_i^{(1)} + w_{i+1}^{(2)} + w_{i-1}^{(3)}\right]$$

$$\eta_i(\tau)\eta_j(\tau'))\rangle = K_i^{(1)}\delta_{ij}\delta(\tau-\tau')\,.$$

$$w_i^{(1)} = \theta(h_{i+1}-h_i)\theta(h_{i-1}-h_i)\,,$$
$$w_i^{(2)} = \theta(h_{i+1}-h_i)[1-\theta(h_{i-1}-h_i)] + \tfrac{1}{2}[1-\theta(h_{i+1}-h_i)][1-\theta(h_{i-1}-h_i)]\,,$$
$$w_i^{(3)} = \theta(h_{i-1}-h_i)[1-\theta(h_{i+1}-h_i)] + \tfrac{1}{2}[1-\theta(h_{i+1}-h_i)][1-\theta(h_{i-1}-h_i)]\,.$$

$$\theta(x) = \begin{cases} 1, & \text{if } x \geq 0; \\ 0, & \text{if } x < 0. \end{cases}$$

Kinetic Roughening

$$W(L,t) = \left[\langle h^2(t)\rangle - \langle h(t)\rangle^2\right]^{1/2}$$

$$\langle h(t)\rangle = L^{-1}\sum_i h_i(t)\,, \qquad \langle h^2(t)\rangle = L^{-1}\sum_i h_i^2(t)$$

$$W(L,t) \sim L^\alpha f(t/L^z)$$

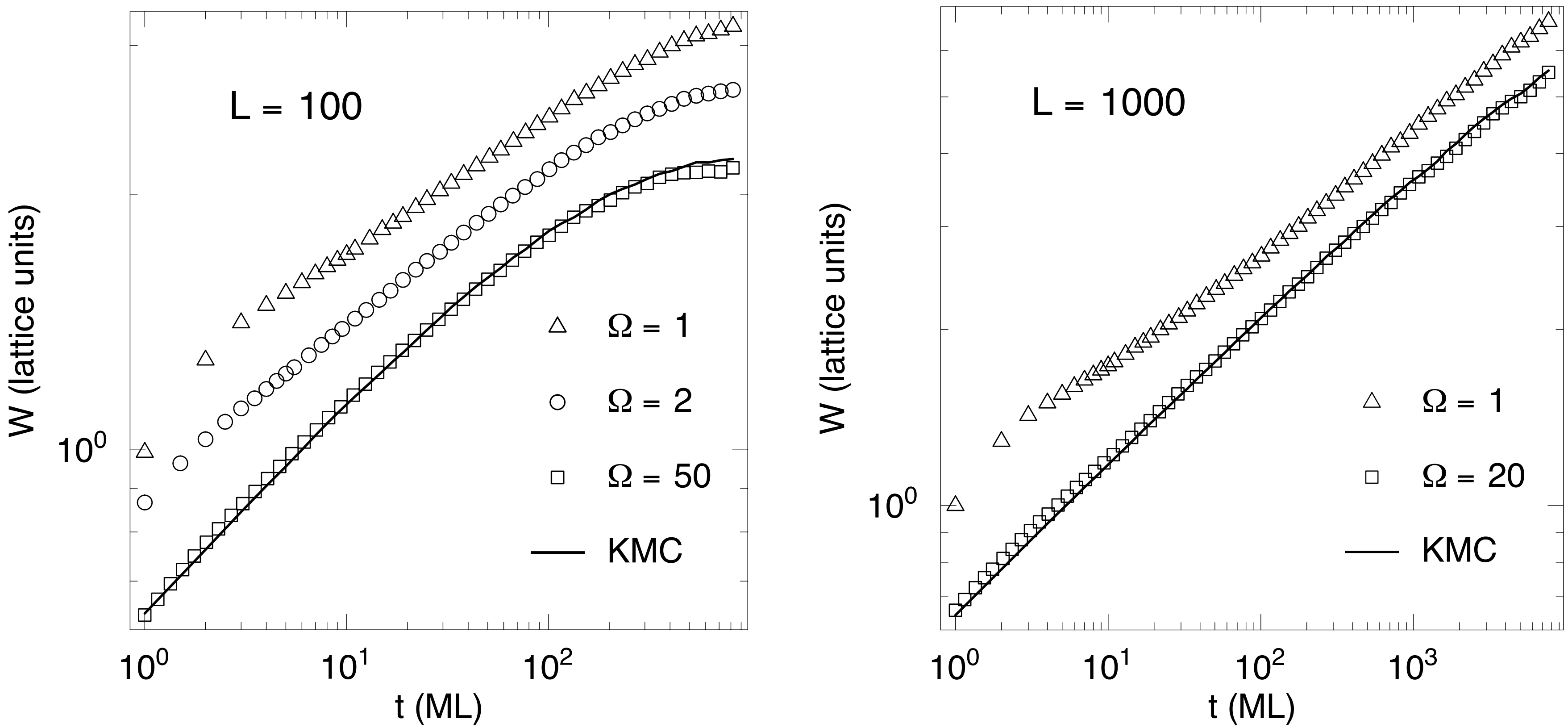
$$f(x) \sim \begin{cases} x^\beta, & \text{for } x \ll 1 \\ \text{constant}, & \text{for } x \gg 1 \end{cases}$$

$$\alpha: \text{roughness exponent}$$

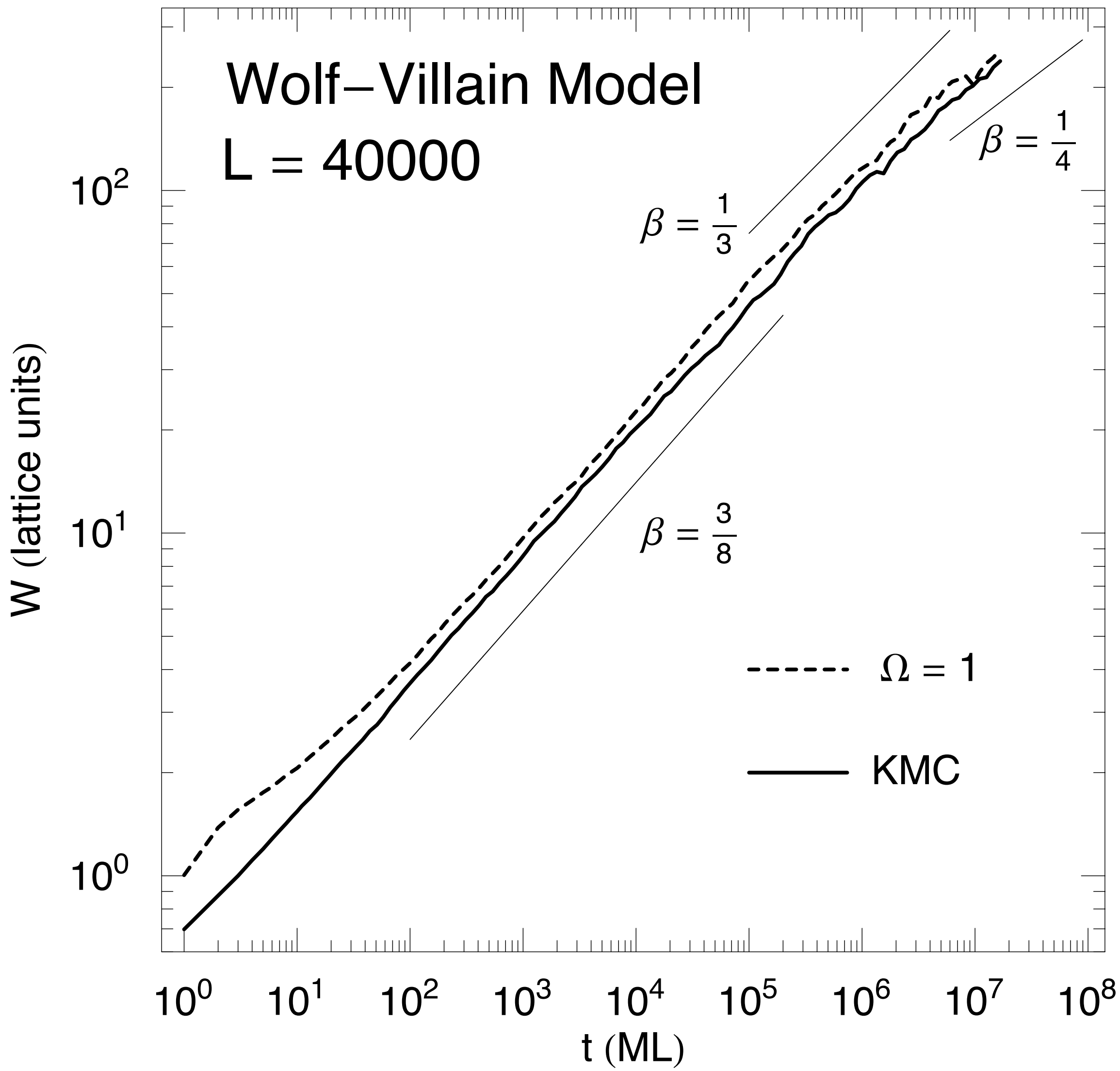
$$z = \alpha/\beta: \text{dynamic exponent}$$

$$\beta: \text{growth exponent}$$

Edwards–Wilkinson Model



Wolf-Villain Model



Summary of Lattice Models

1. Transition rules for processes such as deposition, diffusion, desorption
2. Rates obtained from (i) ab initio calculations, (ii) experiment, (iii) estimates
3. Morphologies obtained from KMC simulations
4. Used for materials-specific and generic studies; simulations reveal intriguing dimensionally-dependent behavior
5. Relation to continuum equations?

Continuum Limit: The Issues

1. Methods of “derivation”: phenomenological and symmetry arguments, universality, real-space renormalization
2. Analytic coarse graining inhibited by step functions (used to characterize local environment)
3. Any regularization of step functions must yield finite coefficients in the continuum limit
4. Coefficients must contain rates of particular atomistic processes

Continuum Equations of Surface Growth

$$\frac{\partial h}{\partial t} = -\nabla^4 h + \eta \quad (\mathrm{Mullins-Herring})$$

$$\frac{\partial h}{\partial t} = \nabla^2 h + \eta \quad (\mathrm{Edwards-Wilkinson})$$

$$\frac{\partial h}{\partial t} = \nabla^2 h + (\nabla h)^2 + \eta \quad (\mathrm{Kardar-Parisi-Zhang})$$

$$\frac{\partial h}{\partial t} = -\nabla^4 h - \nabla^2 (\nabla h)^2 + \eta \quad (\mathrm{Villain-Lai-Das\ Sarma})$$

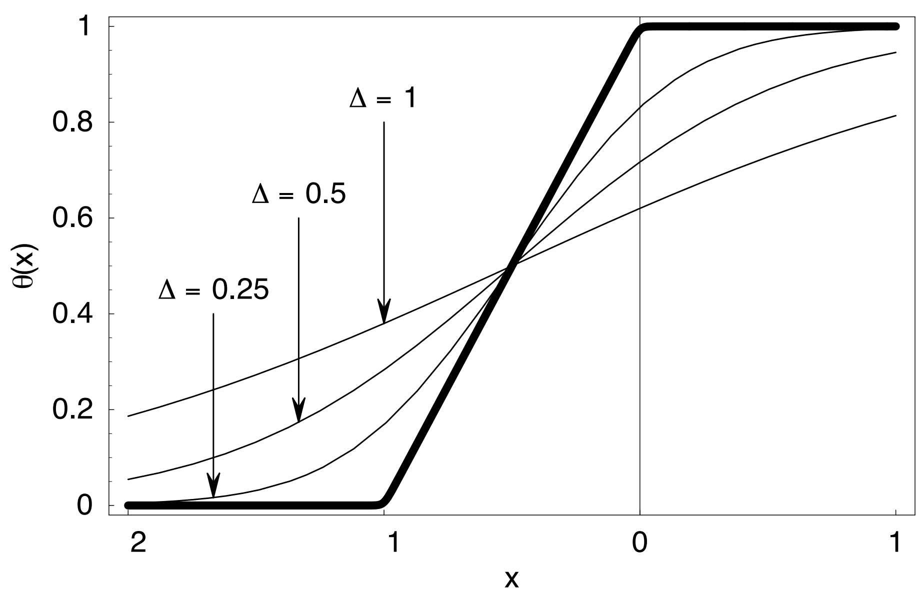
Regularization of Step Function

$$\max(x, y) = \lim_{\epsilon \to 0^+} \left[\epsilon \ln(e^{x/\epsilon} + e^{y/\epsilon}) \right]$$

$$\theta(x) = \max(x + a, 0) - \max(x, 0)$$

$$= \lim_{\Delta \to 0^+} \left\{ \frac{\Delta}{a} \ln \left[\frac{e^{(x+a)/\Delta} + 1}{e^{x/\Delta} + 1} \right] \right\}$$

$$= A + \frac{Bx}{2} - \frac{B^2 x^2}{8\Delta} + \cdots$$



Coarse-Graining the Edwards–Wilkinson Model

$$\frac{dh_i}{dt} = \frac{1}{\tau_0}\left[w_i^{(1)} + w_{i+1}^{(2)} + w_{i-1}^{(3)}\right] + \eta_i$$

$$x = i\epsilon\,, \quad t = \epsilon^z \tau/\tau_0\,, \quad u(x,t) = \epsilon^\alpha \left(h_i - \frac{\tau}{\tau_0}\right)$$

$$\epsilon^{z-\alpha}\frac{\partial u}{\partial t} = \nu\epsilon^{2-\alpha}\frac{\partial^2 u}{\partial x^2} + K\epsilon^{4-\alpha}\frac{\partial^4 u}{\partial x^4} + \lambda_1\epsilon^{4-2\alpha}\frac{\partial^2}{\partial x^2}\left(\frac{\partial u}{\partial x}\right)^2 + \epsilon^{(1+z)/2}\xi$$

$$\nu = B\,, \qquad K = \frac{1}{12}(4-3A)\,, \qquad \lambda_1 = \frac{B^2}{8} - \frac{B^2}{8\Delta}(1-A)$$

$$\epsilon \to 0 \longrightarrow \frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + \xi\,, \quad \langle \xi(x,t)\xi(x',t')\rangle = \delta(x-x')\delta(t-t')$$

Coarse-Graining the Wolf–Villain Model

$$\epsilon^{z-\alpha}\frac{\partial u}{\partial t} = \nu\epsilon^{2-\alpha}\frac{\partial^2 u}{\partial x^2} + \lambda_1\epsilon^{4-2\alpha}\frac{\partial^2}{\partial x^2}\left(\frac{\partial u}{\partial x}\right)^2$$

$$+ \lambda_2\epsilon^{4-3\alpha}\frac{\partial}{\partial x}\left(\frac{\partial h}{\partial x}\right)^3 + K\epsilon^{4-\alpha}\frac{\partial^4 u}{\partial x^4} + \epsilon^{(1+z)/2}\xi$$

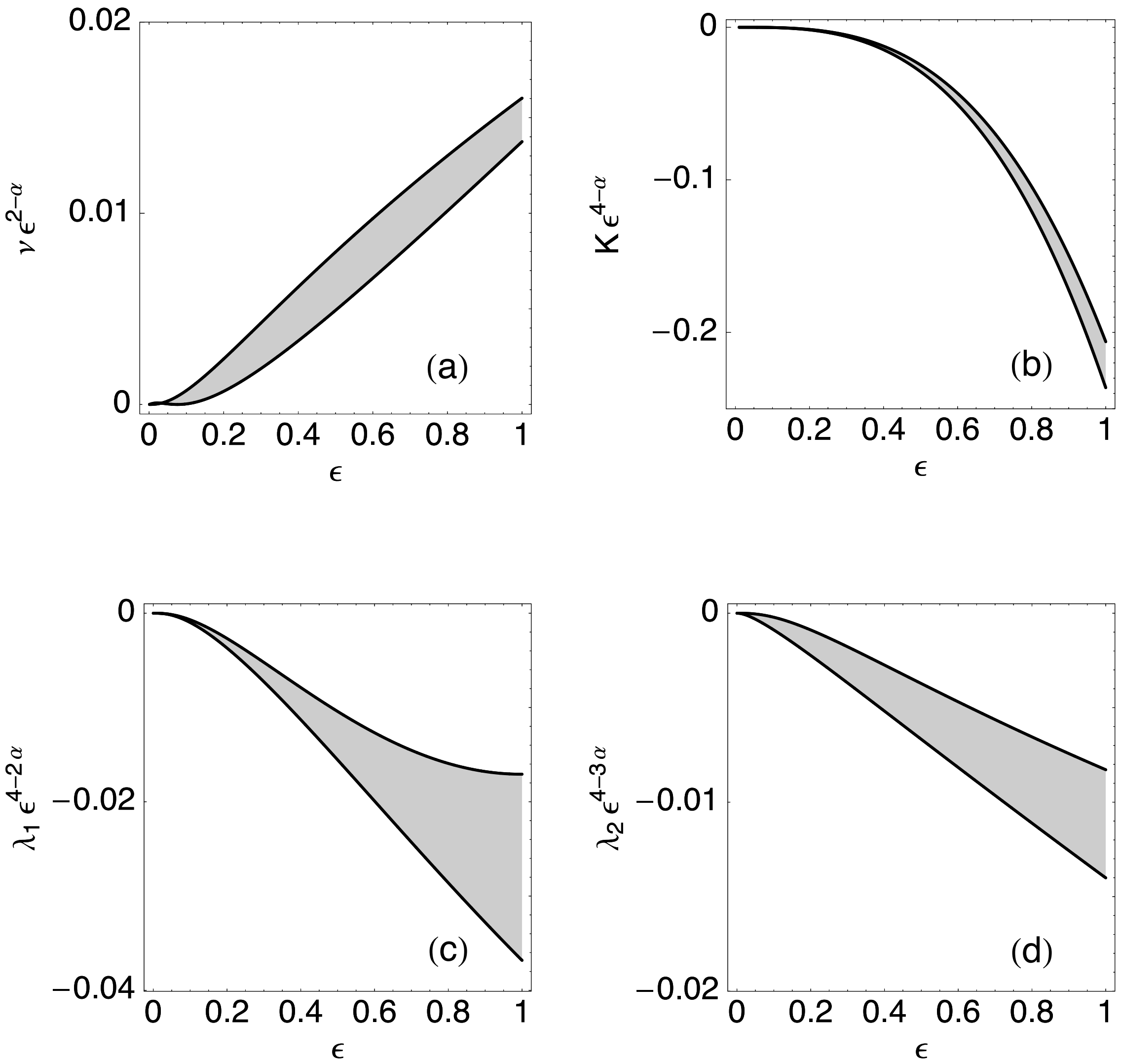
$$\nu = \frac{B}{a^4}(2A-a)(A-a)^2$$

$$\lambda_1 = \frac{B^2}{4a^4}(a^2+2aA-4A^2) + \frac{B^2}{4a^4\Delta}(4A^3-8aA^2+5a^2A-2a^3)$$

$$\lambda_2 = -\frac{B^3}{4a^4}(2A-a) - \frac{B^3}{4a^4\Delta}(3A-2a)(A-a) - \frac{C}{3a^4\Delta^2}(2A-a)(A-a)^2$$

$$K = \frac{B}{12a^4}(44A^3-95aA^2+64a^2A-19a^3)$$

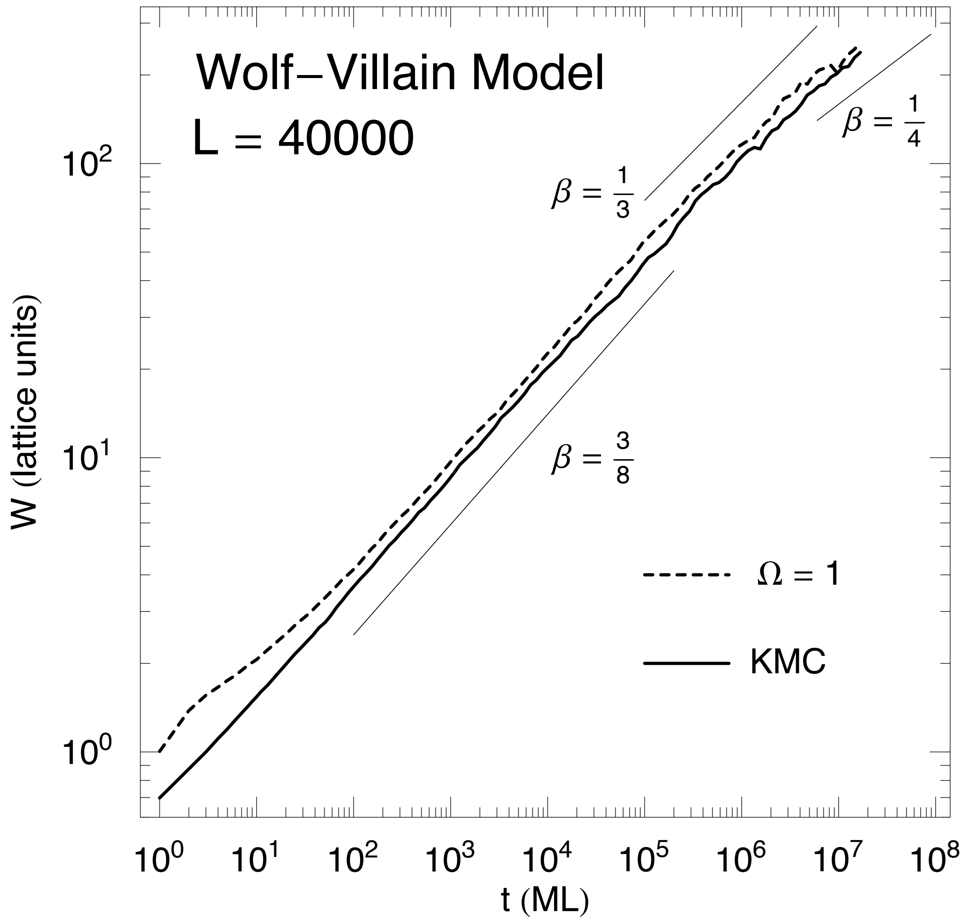
Coarse-Graining the Wolf–Villain Model



Coarse-Graining the Wolf–Villain Model

$$\frac{\partial h}{\partial t} = -K\frac{\partial^4 h}{\partial x^4} + \eta \quad \text{(smoothed lattice model)}$$

$$\frac{\partial h}{\partial t} = \nu\frac{\partial^2 h}{\partial x^2} + \eta \quad \text{(continuum model)}$$



Summary, Conclusions, Future Work

1. Analytic theory of Edwards-Wilkinson and Wolf–Villain models for one-dimensional substrates
2. Extension to two-dimensional substrates in progress
3. Applications to growth in the presence of strain