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Phase-field-crystal model for pinning a sliding of adsorbed layers

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Phase-field crystal model for pinning and sliding of adsorbed layers

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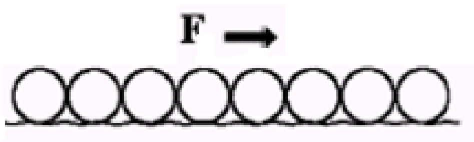
Outline

- Driven adsorbed monolayer: results from particle models
- Phase-field crystal modelling
- Phase-field crystal model of an adsorbed monolayer

Driven monolayer on a periodic potencial

Persson, PRL 71, 112 (1993).



• Lennard-Jones interactions V(r)

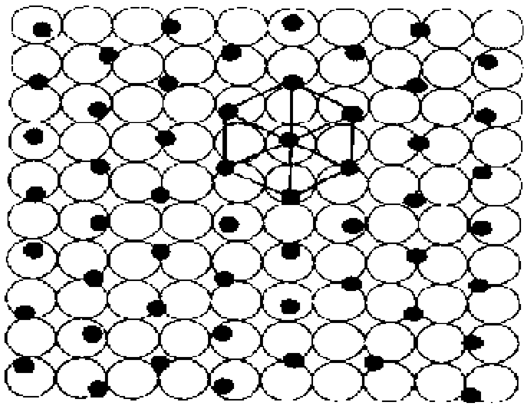
• square-lattice pinning potential U(r)

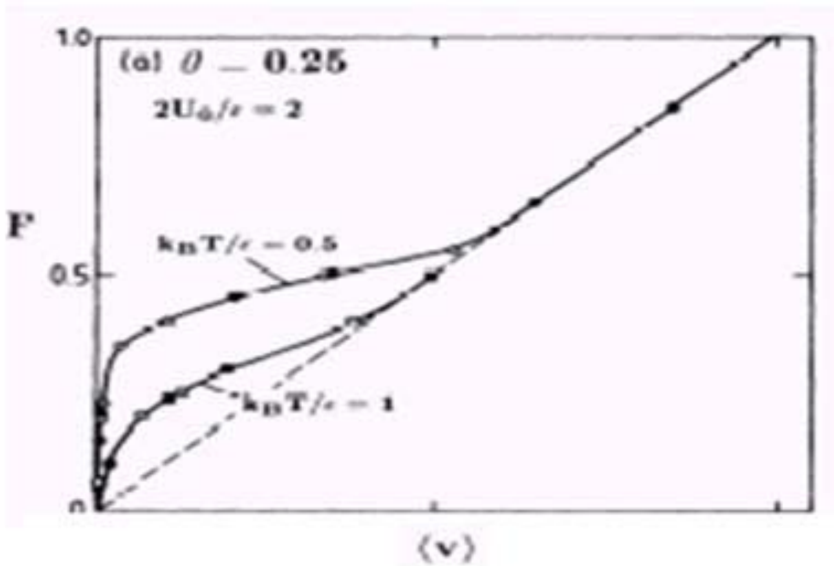
• Langevin dynamics

$$m\frac{d^2 r_i}{dt^2} + m\eta\frac{dr_i}{dt} = -\frac{\partial V}{\partial r_i} - \frac{\partial U}{\partial r_i} + F + f_i$$

$$< f_i(t) f_j(t') >= 2m\eta k_B T \delta_{i,j}\delta(t-t')$$

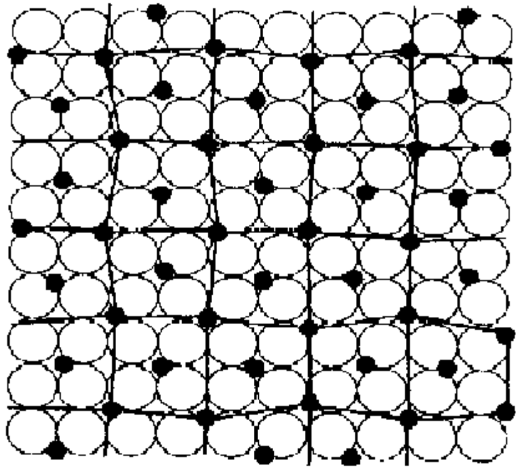
incommensurate





Dynamic melting and freezing

Persson, J.Chem.Phys.103,3449 (1995)

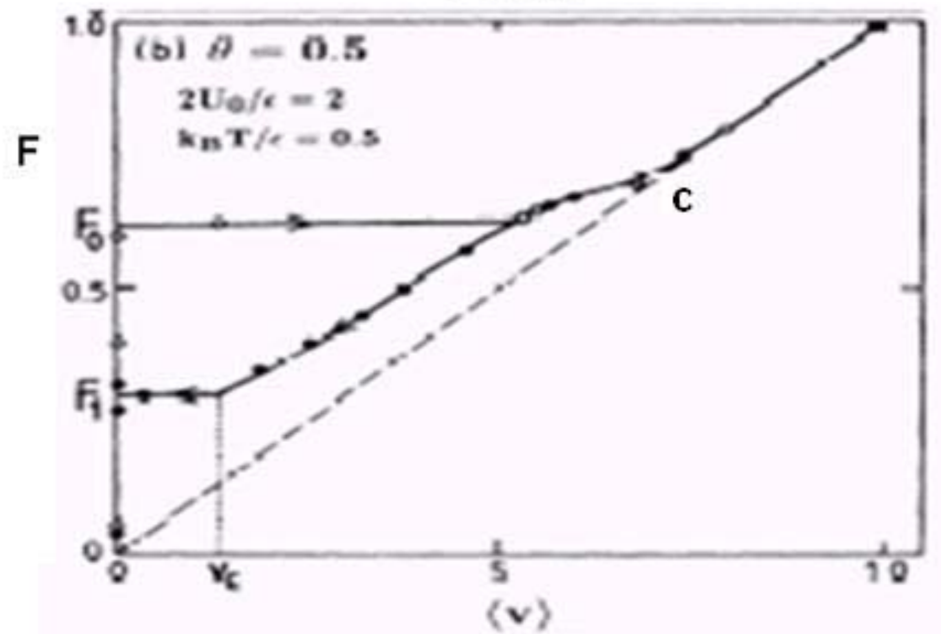


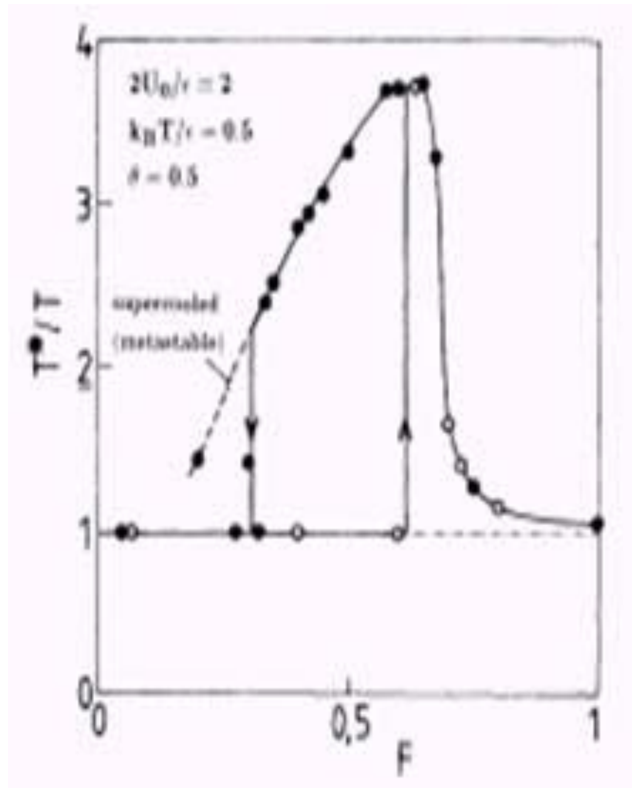
commensurate

Effective temperature

$$kT^{*} = m(<v^{2}> - <v>^{2})$$

T<Tm





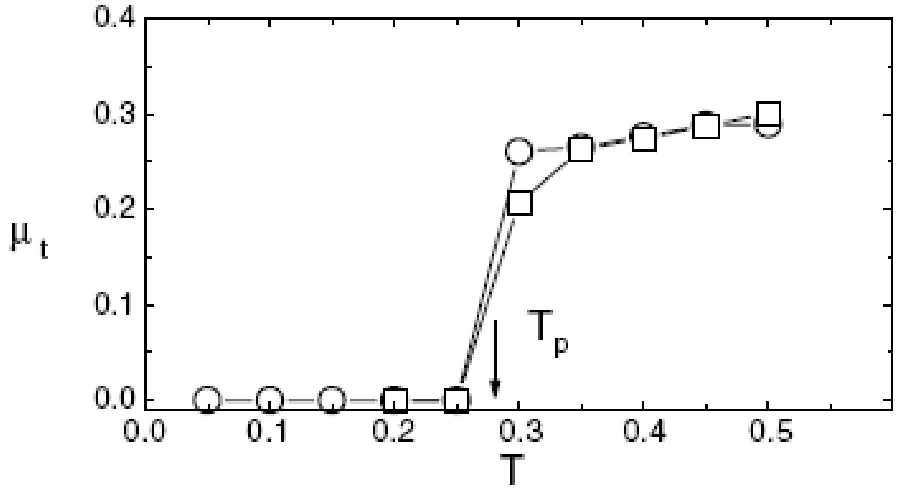
Transverse pinning

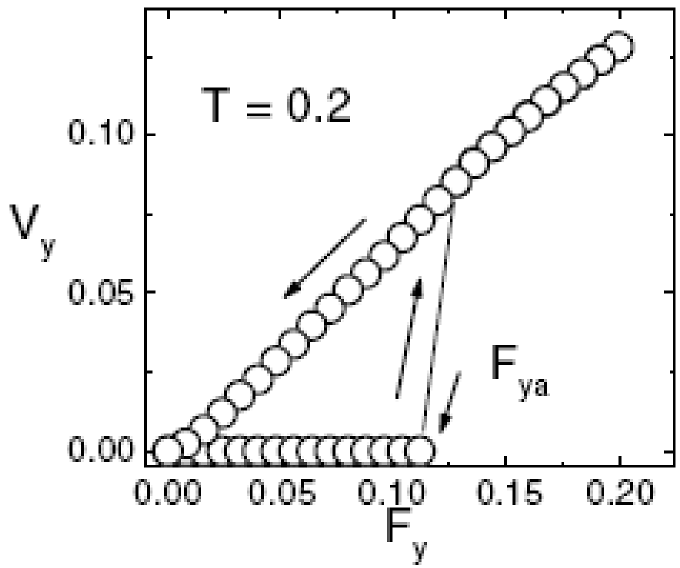
Granato, Ying, PRL85, 5368 (2000)

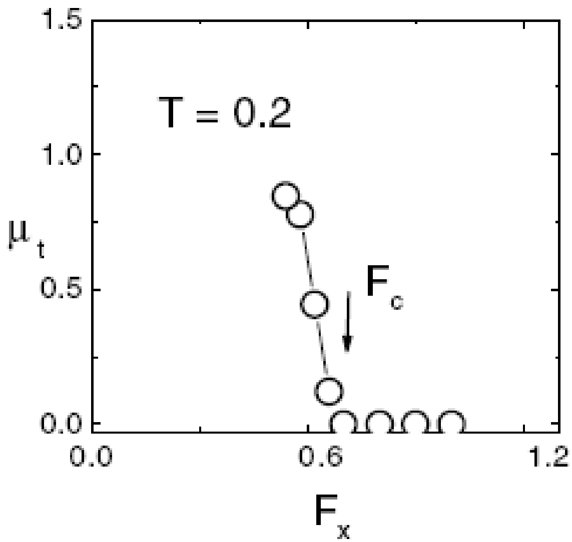
- Response to additional transverse force in the sliding state

F >> F_c

$$\mu_t = Lim_{f_y \to 0} \frac{V_y}{f_y}$$







Phase-field modelling

- instead of particles, represent the system by continuous fields
- describe solid, liquid and gas phases
- choose a free-energy that is a functional of the fields
- the dynamics of the fields should minimize the free-energy functional:

simplest free-energy functional

$$F[\psi(x)] = \int d\vec{x}\, [\frac{\lambda}{2}(\nabla \psi(x))^2 + \frac{r}{2}\psi^2 + \frac{u}{4}\psi^4]$$

- non conserved field Ginzburg-Landau Allen-Cahn equation

$$\frac{\partial \psi(x)}{\partial t} = -\gamma \frac{\partial F[\psi]}{\partial \psi(x)}$$

- conserved field Cahn-Hilliard equation

$$\frac{\partial \psi(x)}{\partial t} = \gamma \nabla^2 \frac{\partial F[\psi]}{\partial \psi(x)}$$

Phase-field-crystal modelling

Elder, Katakowski, Haataja, Grant, PRL. 88, 245701 (2002)

- continuous phase field retaining some information on atomic scale

$$F[\psi] = \int d\vec{x}[\frac{1}{2}\psi(\vec{x})(r+\lambda(\nabla^2+k_o{}^2)^2)\psi(\vec{x})+\frac{u}{4}\psi(\vec{x})^4]$$

$$\frac{\partial\psi(x)}{\partial t} = \gamma\,\nabla^2\,\frac{\partial F[\psi]}{\partial\psi(x)}$$

- freee-energy minimized by a periodic pattern : a phase-field crystal
- allows for elasticity, multiple crystal orientations, dislocations , etc.
- dynamics on diffusive times scales

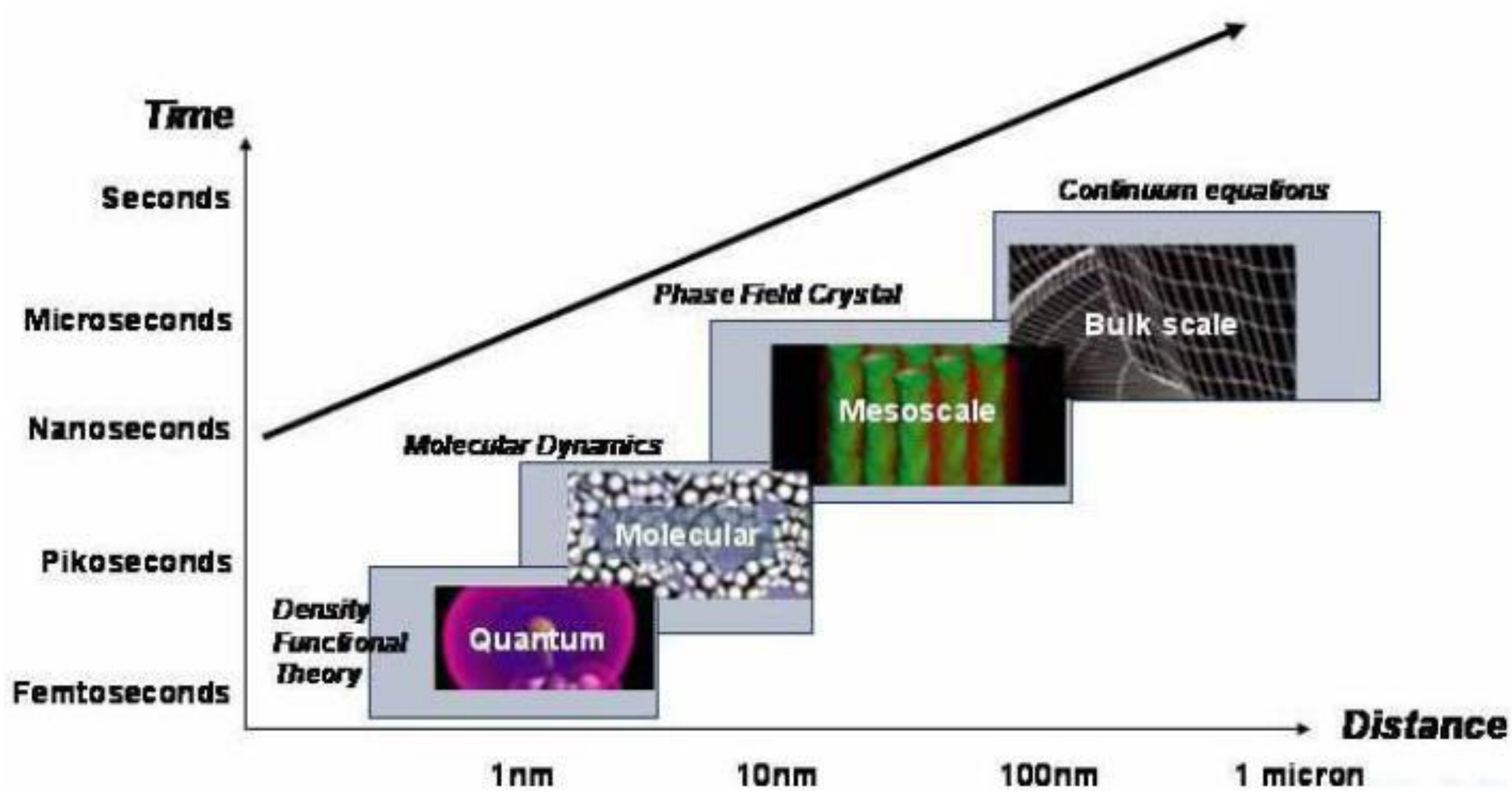
- can be derived from classical density functional theory of freezing (DFT)
- phase field can be identified as deviations of the density from the uniform liquid:

$$\psi(\vec{x}) = (\rho(\vec{x})-\rho_l)/\rho_l$$

Elder, Provatas, Berry,
P. Stefanovic, Grant, PRB 75, 064107 (2007).

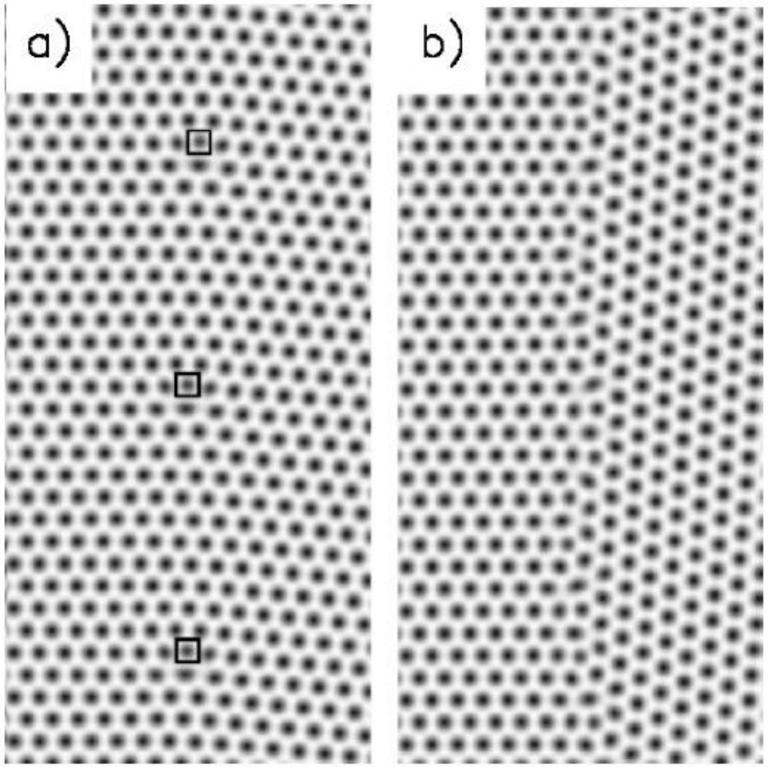
Time and length scales

- phase-field crystal modelling provides a bridge between atomistic and continuous length scales



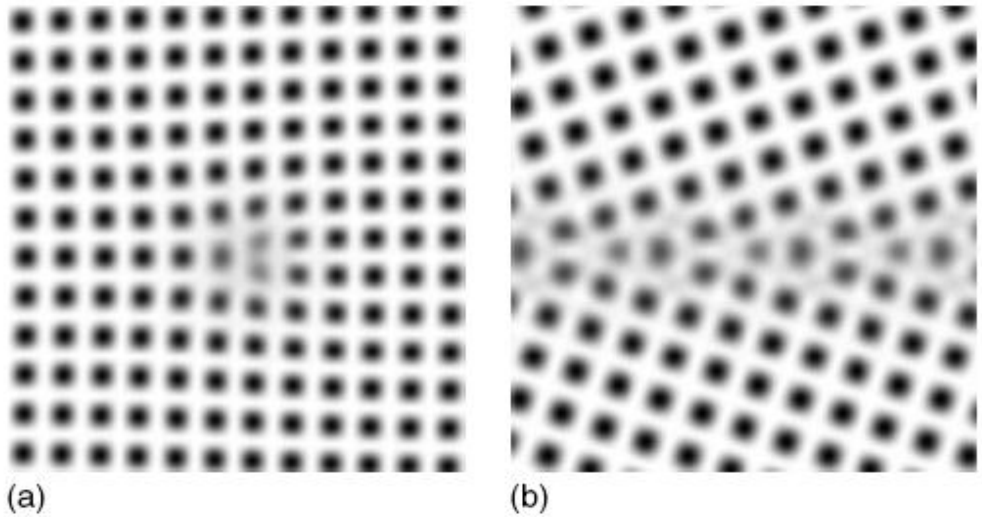
Examples of defects in the phase-field crystal
Grain boundaries

two dimensions
hexagonal



Elder, Grant, PRE 70, 051605 (2004).

three dimensions
bcc



Jaatinen, Achim, Elder, Ala-Nissila, PRE 80, 031602 (2009)

Phase-field-crystal model for an adsorbed monolayer

Achim, Karttunen, Elder, Granato, Ala-Nissila, Ying, PRE 74, 021104 (2006);

- add a pinning potential V(x,y)

$$F = \int d\vec{x}[\frac{1}{2}\psi(r+(\nabla^2+1)^2)\psi + \frac{1}{4}\psi^4 + V\psi]$$

- conserved dynamical equations

$$\frac{\partial\psi}{\partial\tau} = \nabla^2\{[r+(1+\nabla^2)^2]\psi + \psi^3 + V\}$$

- for V(x,y)=0 , the minimum correspond to hexagonal lattice $k_h \approx 1$

- lattice constant mismatch

$$\delta_m = (k_h - k_s)/k_h$$

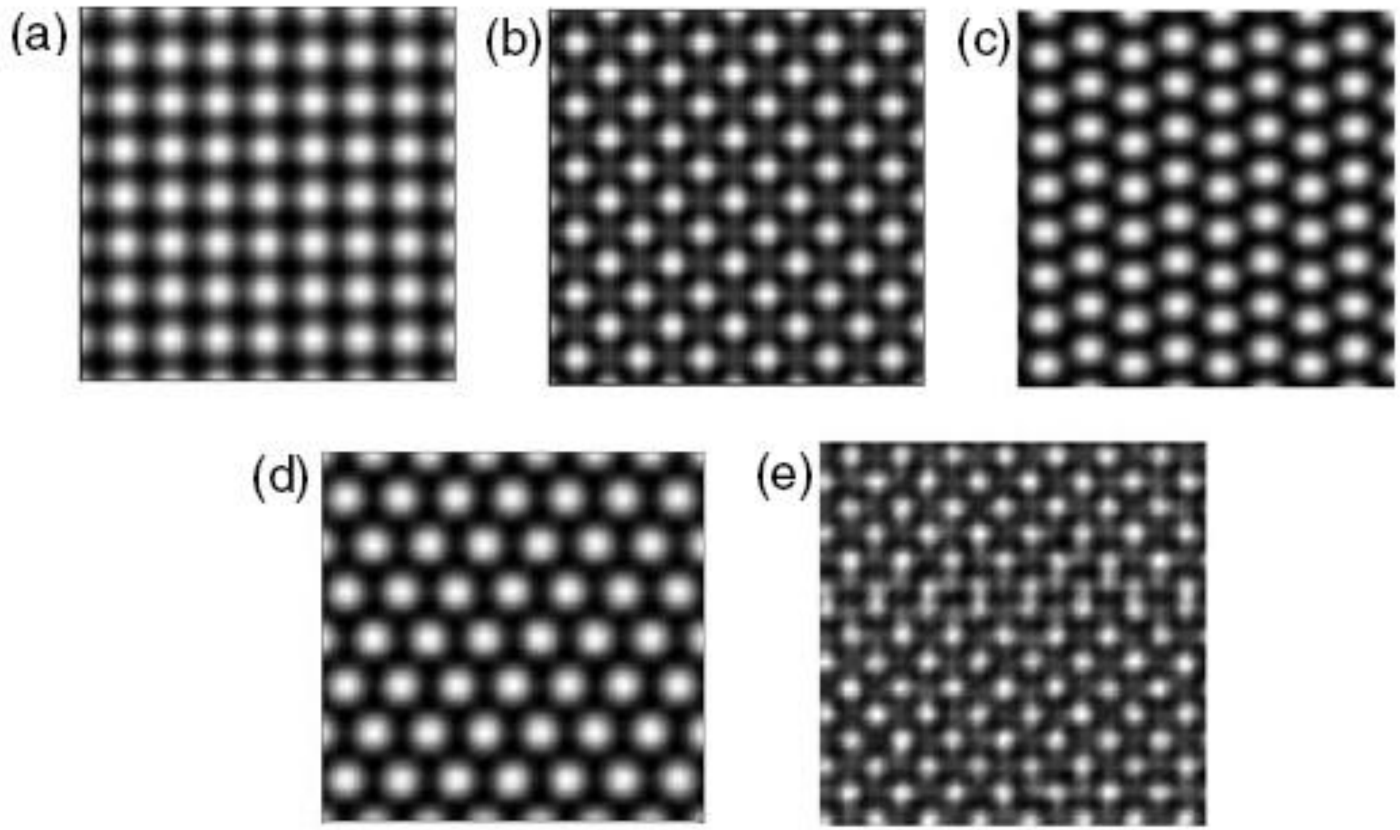
Fundamental requirements to model adsorbed layers

- commensurability effects
- depining by thermal fluctuations
- force-induced depinning

Minimum free-energy structures

- square-lattice pinning potential $V(x,y) = V_0[\cos(k_s x) + \cos(k_s y)],$

(1 x 1) c(2 x 2) (2 x 1)

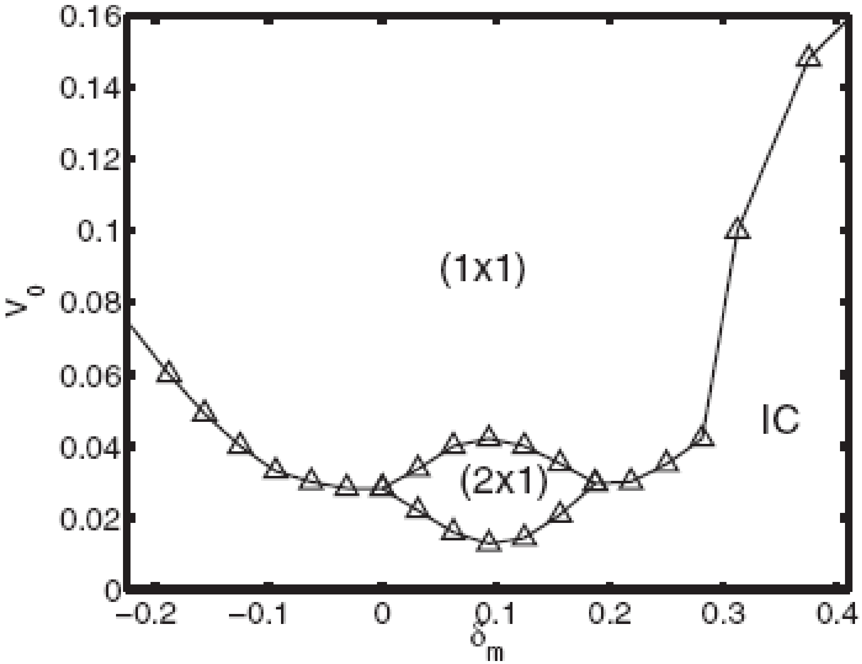


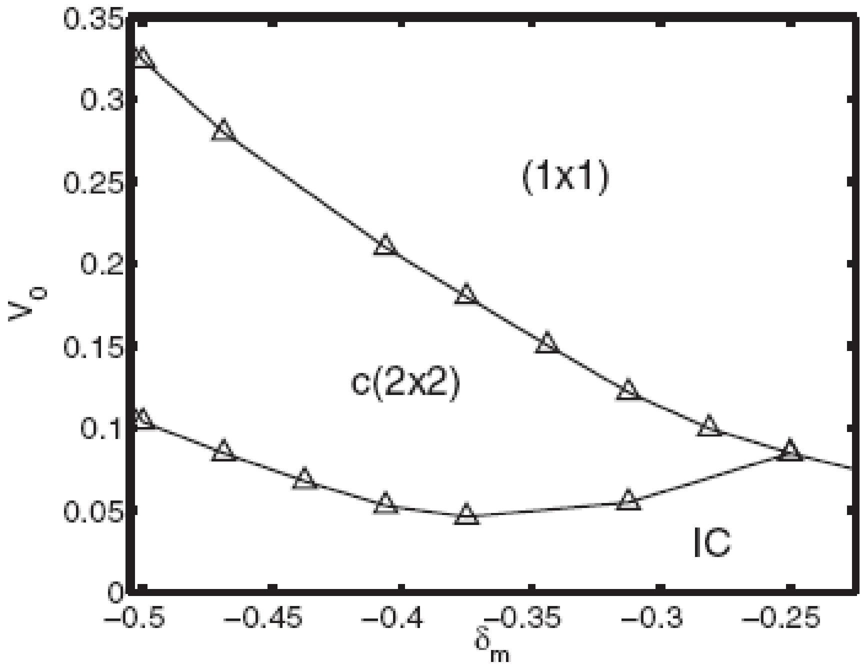
Hexagonal IC IC with domain walls near c(2 x 2)

Potential-misfit phase diagram

near (1 x 1) phase

near c(2 x 2) phase





Thermal fluctuations

Ramos, Granato, Achim, Ying, Elder, Ala-Nissila, PRE 78, 031109 (2008);

- to go beyond mean-field approximation
  regard free-energy functional as an effective Hamiltonian

$$H_{PFC} = \int d\vec{x}[\frac{1}{2}\psi(r+(\nabla^2+1)^2)\psi + \frac{1}{4}\psi^4 + V\psi]$$

- fluctuations are taken into account by the partition function:

$$Z = \int \delta\psi \, e^{-H_{PFC}[\psi]/kT}$$

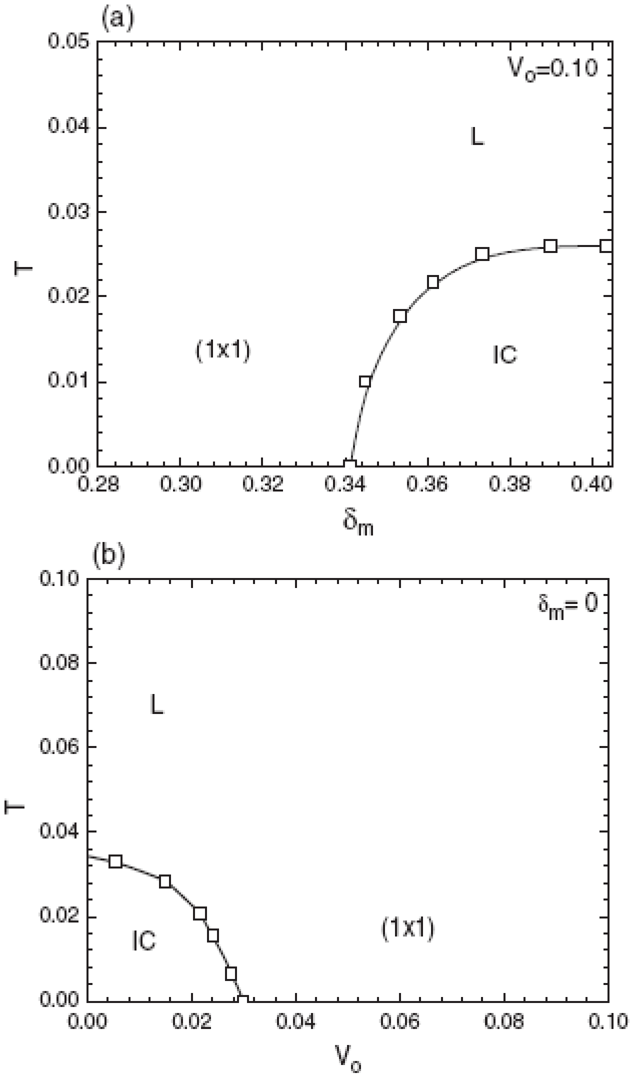
- equilibrium behavior obtained by:
  - Langevin dynamics: $\frac{\partial\psi(\vec{x})}{\partial t} = \gamma\nabla^2 \frac{\partial H_{PFC}}{\partial\psi(\vec{x})} + \zeta(\vec{x},t)$

$$< \zeta_i(\vec{x},t)\zeta_j(\vec{x}',t') >= 2\,\gamma\, k_B T\nabla^2\delta(\vec{x}-\vec{x}')\delta(t-t')$$

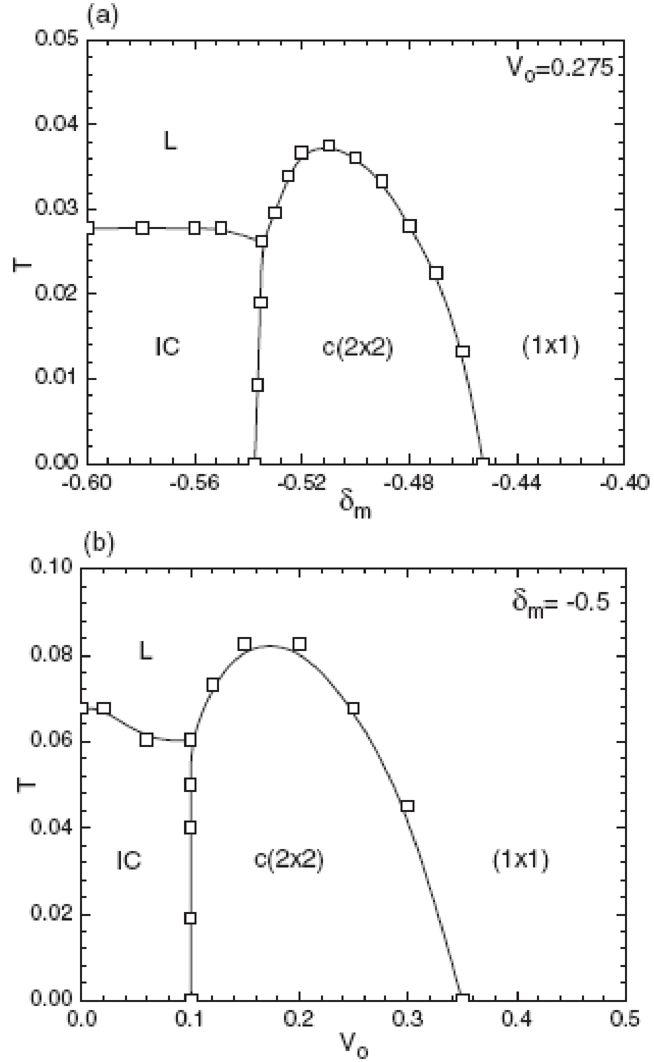
  - Monte Carlo method: Metropolis , Parallel tempering

Temperature phase diagram

near (1 x 1) phase



near c(2 x 2) phase

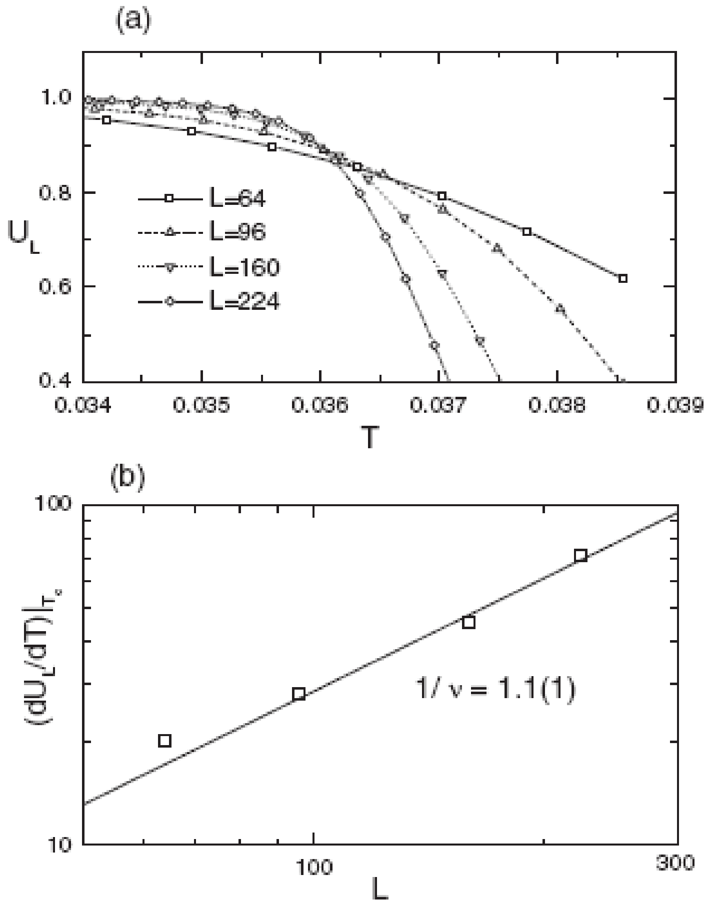


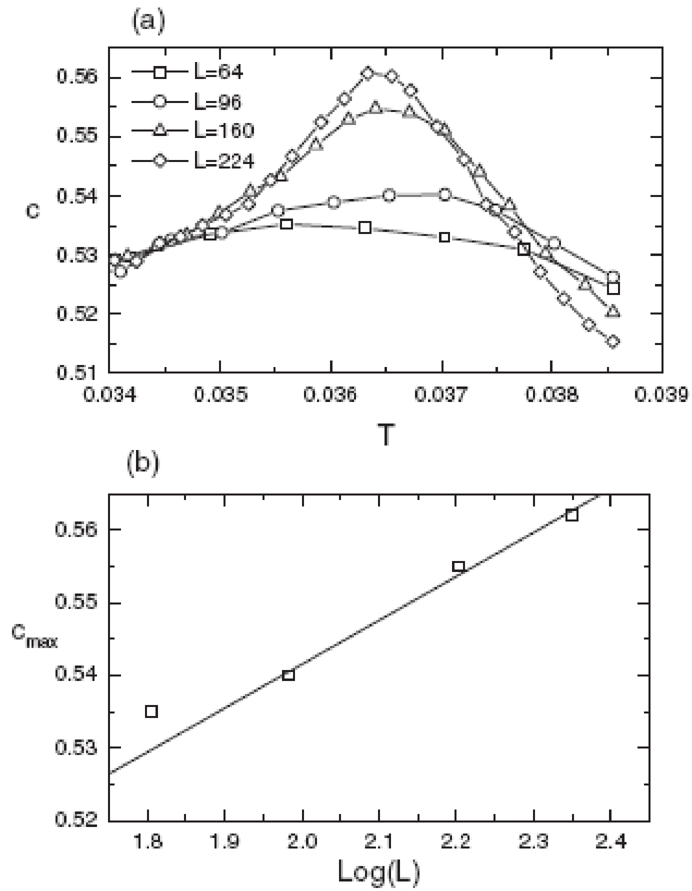
Scaling analysis
c(2x2) melting

Specific heat $\quad C_{\max} \propto L^{\alpha/\nu}$

Binder ratio

$$U_L = 2 - \frac{<|\rho_{k_0}|^4>}{(<|\rho_{k_0}|^2>)^2}$$





$$\frac{\partial U_L(T_c)}{\partial T} \propto L^{1/\nu}$$

• results consistent with Ising universality class

Velocity response at zero temperature force-induced depinning

Achim, Ramos, Karttunen, Elder, Granato, Ala-Nissila, Ying, PRE79, 011606 (2009);

$$H_{PFC} = \int d\vec{x}[\frac{1}{2}\psi(r+(\nabla^2+1)^2)\psi + \frac{1}{4}\psi^4 + V\psi]$$

- add a convective gradient term proportional to external force in the dynamical equations:

$$\frac{\partial\psi(\vec{x})}{\partial t} = \nabla^2 \frac{\partial H_{PFC}}{\partial\psi(\vec{x})} + \vec{f}\cdot\vec{\nabla}\psi(\vec{x})$$

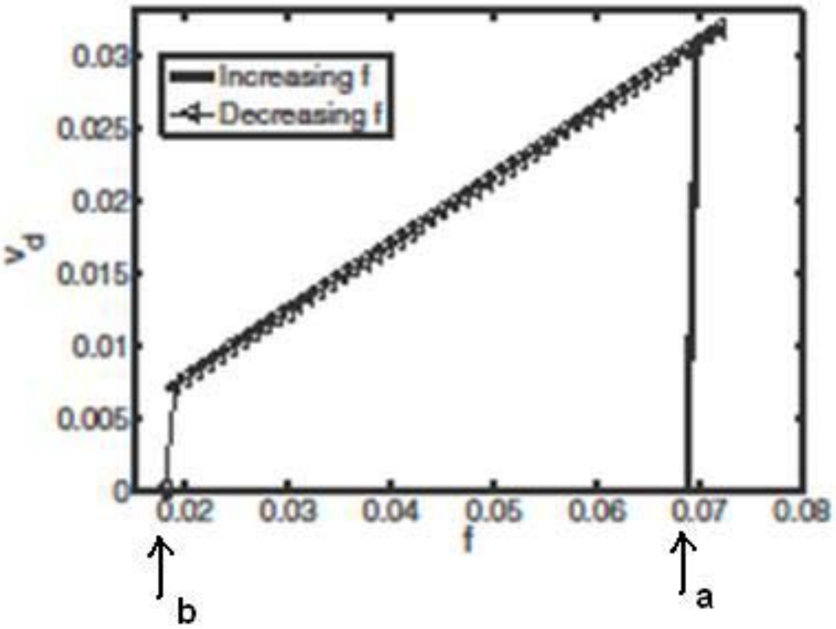
- velocity measurements:

  - from the phase field $\quad V = << |\frac{\partial\psi}{\partial t}|>_x / <|\frac{\partial\psi}{\partial x}|>_x >_t$

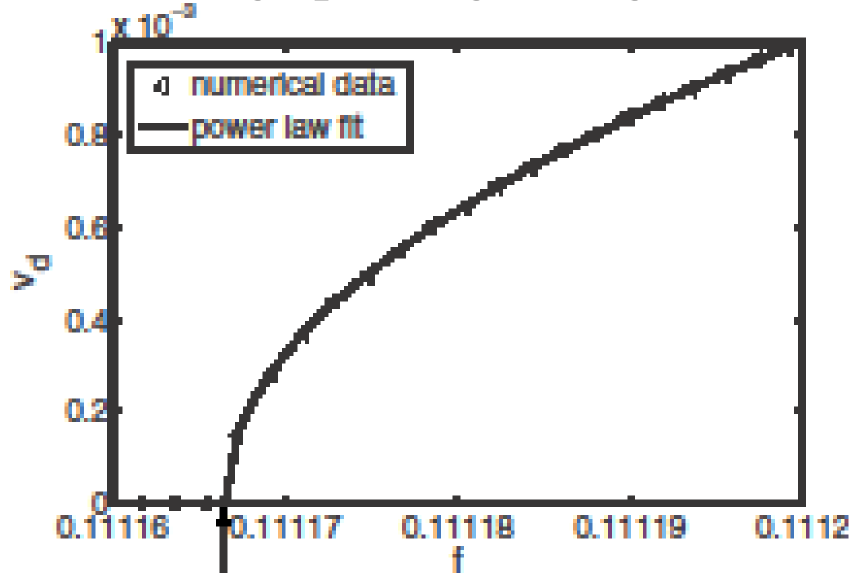
  * from the local maxima positions $\quad \vec{v}_d = < \frac{1}{N_p}\sum_{i=1}^{N_p}\vec{v}_i(t) >$

Velocity response at T=0

Small pinning strength



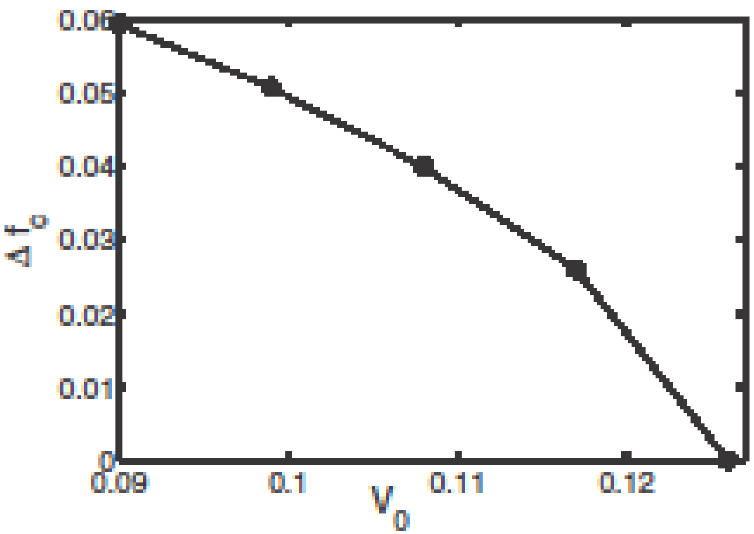
Large pinning strength



$$v_d \propto (f - f_c)^{\xi}$$

$$\xi = 0.50(3)$$

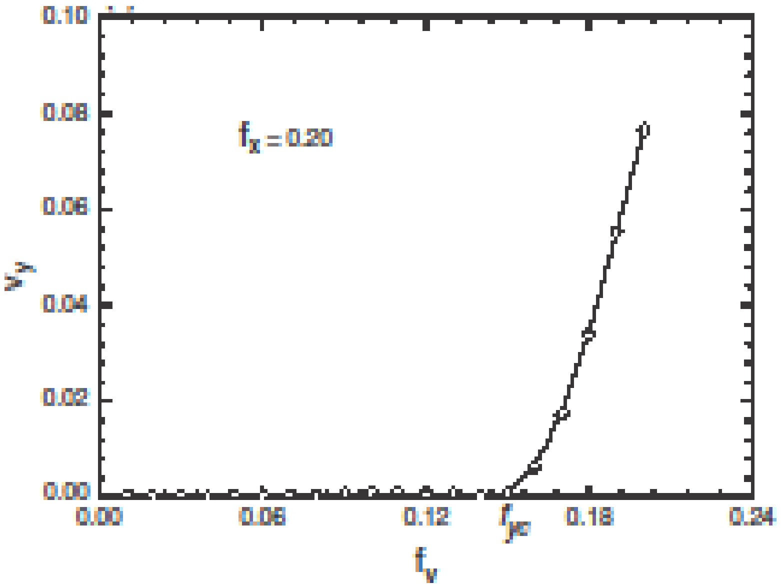
Different critical forces



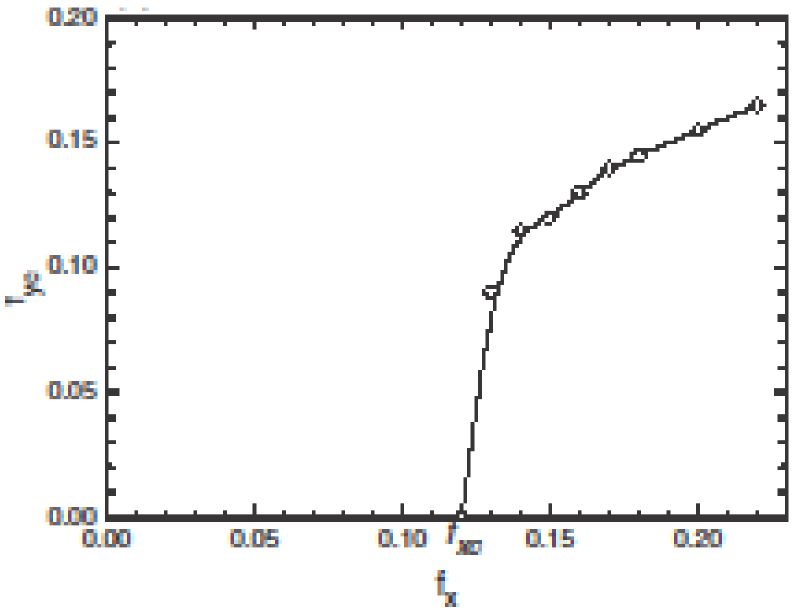
$$\Delta f_c = f_a - f_b$$

Transverse response at large velocity

transverse velocity response



critical transverse force



velocity from peak positions

$$\vec{v}_d = < \frac{1}{N_p} \sum_{i=1}^{N_p} \vec{v}_i(t) >$$

Conclusions

- PFC model provides a density field description of adsorbed layers: commensurability effects, thermal depinning , force depinning and inertial effects .
- velocity response to an external force at low T, shows hysteresis with dynamical melting and freezing transitions at distinct critical values.
- main features of the nonlinear response are similar to the results obtained for atomistic models.
- dynamical melting and freezing mechanisms appear to be different
- It should be possible to describe realistic adsorbed layer systems by adjusting the parameters of the model.