Island morphology at early stages of MBE growth on bcc(110) surface

Dmytro Goykolov and Miroslav Kotrla

(theoretical dpt., Institute of Physics, AS CR)

Outline

Common EU-NSF Project MagDot

Objectives of the project & subproblems investigated in Prague

Early stages MBE growth on bcc(110) surface

- Metropolis vs. kinetic Monte Carlo method
- Model of MBE growth on bcc(110) surface
- Results for island density and island shape
- Dependence on strain
- Conclusion & Outlook

MAGDOT

Common EU-NSF Project

Acronym: MAGDOT
Start: 1/1/2006
End: 12/31/2009

Bridging Atomistic to Continuum - Multiscale Investigation of Self-Assembling Magnetic Dots during Epitaxial Growth

EU

Technical University, Dresden

A. Voigt

Helsinki University of Technology

T. Ala-Nissila

CNRS, Grenoble

O. Fruchart

Intitute of Physics, AS Prague

M. Kotrla

USA

University of Michigan

K. Thornton

Northwestern University

P. Voohees

University of California, Davis

M. Asta

University of California, Irvine

J. Lowengrub

Objectives and methods

- study of self-assembly of nanoscale metalic islands during homo- and heteroepitaxy applicable for high density magnetic storage materials from a computational point of view
- development and utilization of a set of computational research tools spanning different length and time scales from atomistic to continuum

- First principles electronic density-function theory
- Monte Carlo for atomistic modeling of structure and growth
- Kinetic rate equations - tens of nanometers
- Step flow models - mesoscopic description
- Phase field method - coarse-grained scale, based on free energy functional

Participation of IPASCR in MagDot

MagDot Participant No.6

atomistic modeling of initial stages of growth – submonolayer growth

kinetic Monte Carlo (KMC)

Involved people:

- Miroslav Kotrla – Principal Investigator
- Martin Mašín – researcher
- Dmytro Goykolov – postdoc since October 2007
- Ondřej Maršálek – undergraduate student MFF UK

  only in begining (development of WWW pages) SimNANO Wiki

External:

Sebastian Weber – University of Wuezburg

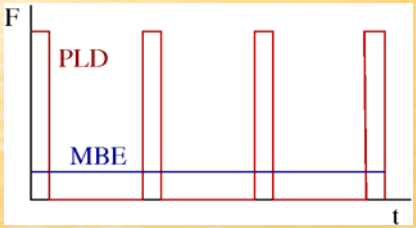
Subproblems investigated in our group

- simulation of MBE island growth on bcc(110) surface
- interplay between chemical interaction and strain caused by misfit
- kinetics of pulsed laser deposition (PLD) method

Subproblems investigated in our group

- simulation of MBE island growth on bcc(110) surface
- interplay between chemical interaction and strain caused by misfit — off-lattice MC
- kinetics of pulsed laser deposition (PLD) method

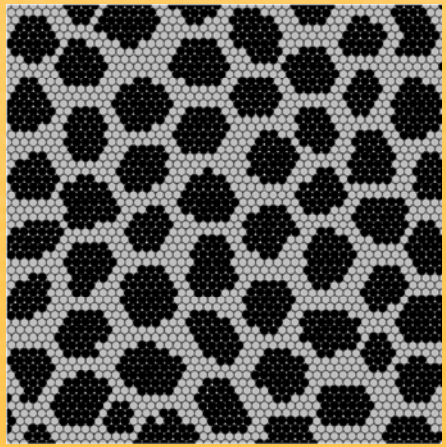
the following talk



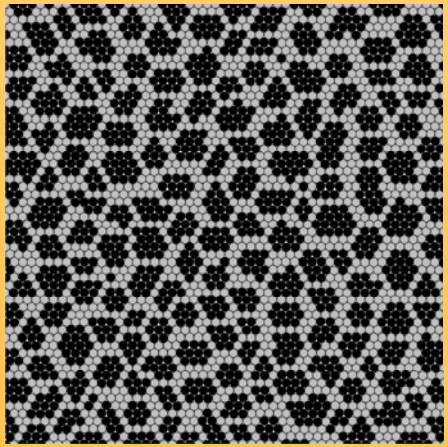
very different time scales

work in progress

misfit 5 %



misfit 7 %



phase separation regime

S. Weber et all: J. Phys.: Cond. Matt. **20** (2008), **2654004**

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Metropolis Monte Carlo method overview

Algorithm

Choose site at random

Generate random number ρ

Perform jump if:

$$\rho < \rho_M$$

Otherwise — ignore this site and choose another one.

Drawbacks

Some of the events are ignored — especially at low temperatures.

Consequently: long computational times

Kinetic Monte Carlo (N-fold way algorithm)

Introduced by Bortz, Kalos and Lebowitz (1975) as a method to speed up MC simulation .

Main idea of BKL algorithm: **avoid discarded moves**

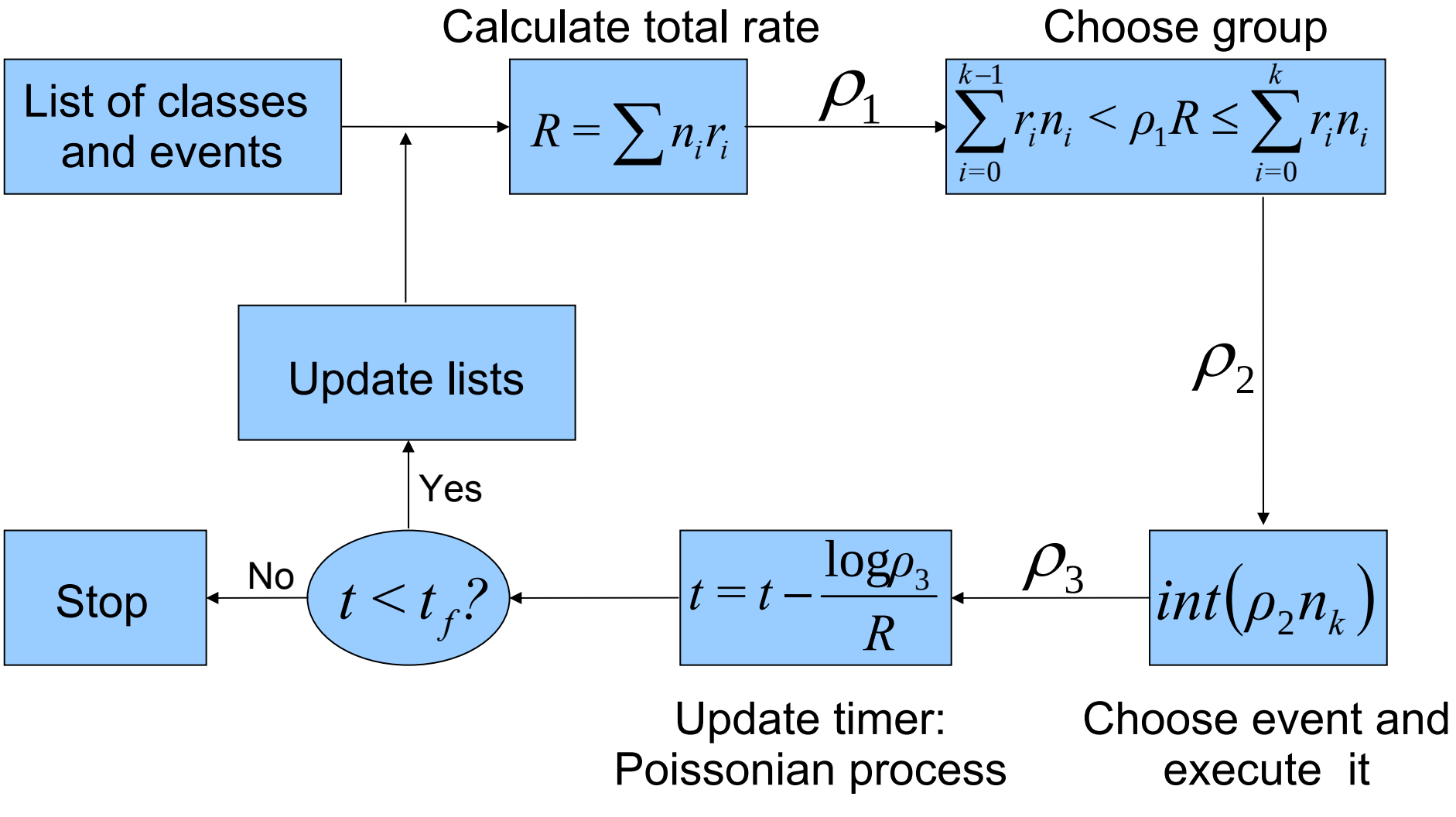
Example: 1D Ising chain

Six classes of environments

1. Choose environment class
2. Randomly choose spin to flip
3. Execute event

A. B. Bortz, M. H. Kalos and J. L. Lebowitz, J. Comp. Phys. 17, 10 (1975)

Details of KMC Algorithm



Applications: **Surface diffusion**; **Surface growth**; Vacancy diffusion in alloys; Coarsening of domain evolution; Defect mobility and clustering in ion or neutron irradiated solids…

Advantages of KMC

Event is performed at every step – no waist of time

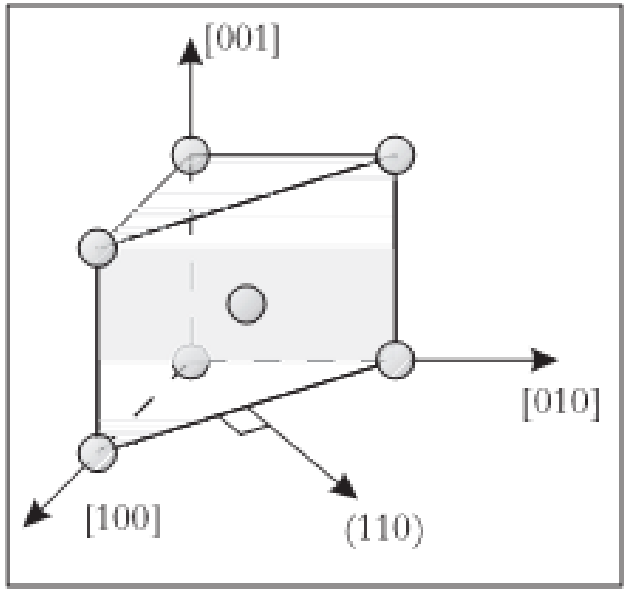
More efficient in terms of simulation time

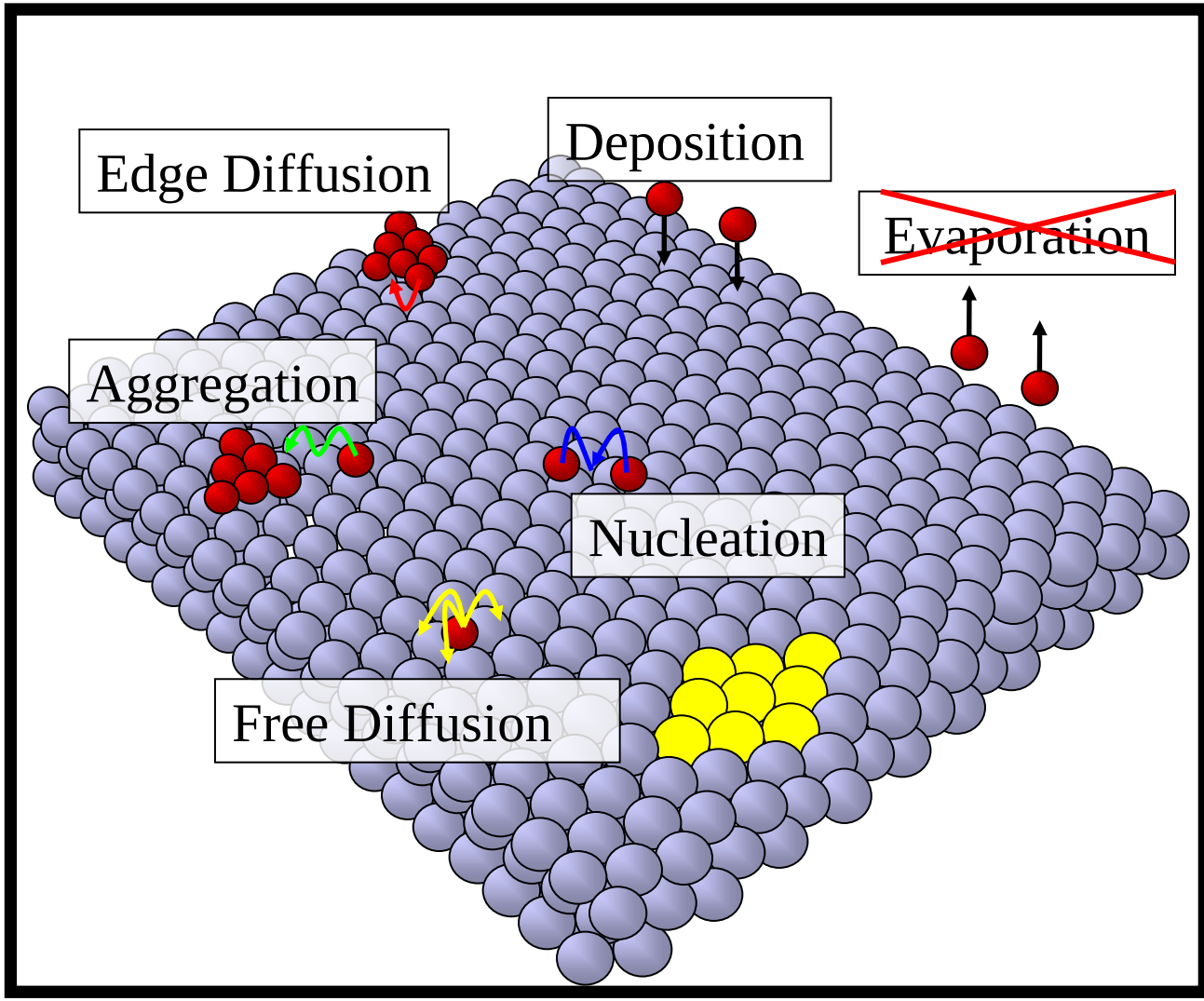
Disadvantages of KMC

- One need to know all possible events (and reactions) in the system prior to starting the simulation
- Main difficulties: organizing the list of events and search algorithms while choosing event group and particular event.

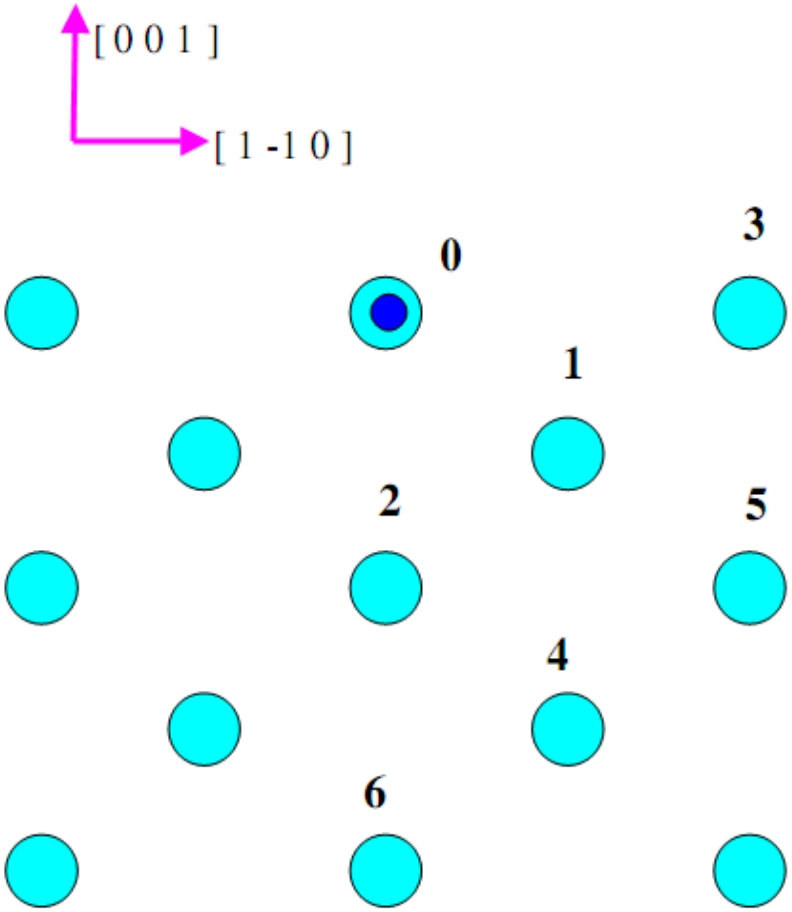
MBE on bcc(110): – Solid-on-Solid model

bcc(110) surface





Diffusion Barriers



Diffusion barriers include:

- free diffusion barrier E_d ;
- interaction with the 1st, 2nd, … nearest neighbors at the initial and final position

$$E_n, E_{2n}, E_{3n} \ldots$$

- effect of strain;

Interaction Energies: Material-Dependent Parameters

From the experiments: only E_d and ν_0 . Interaction with the neighbors – varying parameters.

P.O Jubert et. al. Surface Science 522 (2003) 8.

Theoretical calculations: spin-polarized electronic density functional theory, generalized-gradient approximation

neighbor :	nearest	second	third	fouth	fifth	sixth
E_b (eV) :	−0.3389	−0.0717	–0.07885	0.01005	0.004125	−0.007475

M. Asta, to be published.

Diffusion Barriers Calculations: Bond-counting Scheme.

$$E = E_d + (n_1 - \mu m_1)E_n + (n_2 - \mu m_2)E_{2n} + (n_3 - \mu m_3)E_{3n}$$

Event Rates:

- Deposition:

$$\tau = \frac{1}{Fa^2}$$

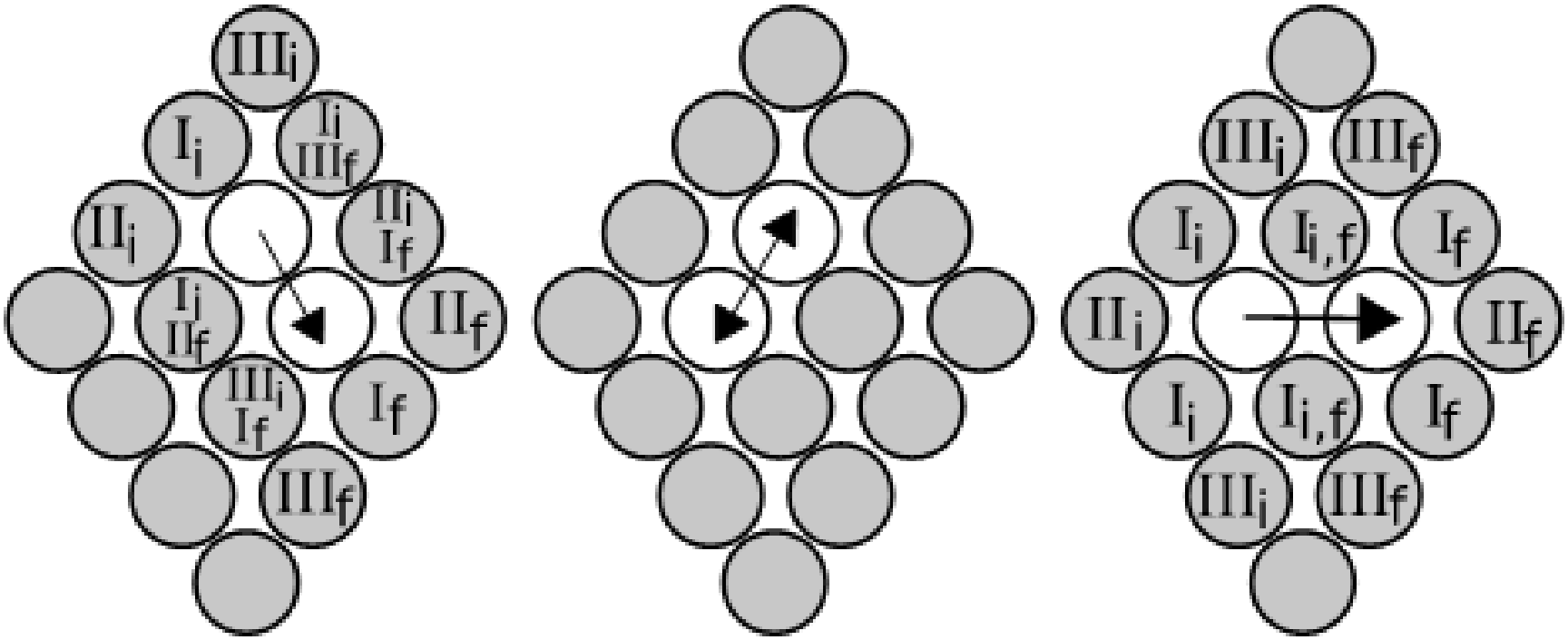
- Diffusion:

$$r_i = \nu_0 e^{-E_i / k_B T}$$

Limitations:

- No strain: homoepitaxial system
- No Ehrlich-Schwoebel barrier:
  - diffusion up the step edge is forbidden;
  - diffusion down the step edge is a regular diffusion event;
- No exchange diffusion
- No interlayer transport

List of All Possible Events



First and second nearest neighbors: 2^8 = **256**

Three combinations for the final and initial position each due to the 3rd neighbors: **2304**

Two independent directions: **4608**

Total number of events: **4609**

Binning KMC Algorithm[1,2]

Calculate global rate of all events:

$$R = N\tau + \sum_{\alpha=1}^{M} N_\alpha r_\alpha$$

Individual probabilities of events:

$$P(\tau) = \frac{N\tau}{R}$$ deposition event

$$P(r_\alpha) = \frac{N_\alpha r_\alpha}{R}$$ diffusion event α

[1] P. A. Maksym, Semicond. Sci. Technol. 3, 594 (1988)
[2] N. Haider, S. A. Khaddaj, M. R. Wilby and D. D. Vvedensky, Comput. Phys. 9, 85 (1995)

Cumulative probability table:

$$C_\alpha = \sum_{j=1}^{\alpha} P(r_j),\ \alpha = 1,\ldots,M$$ diffusion event probabilities

$$C_{M+1} = C_M + P(\tau)$$ deposition event probability

Choose particular event and execute it:

$$C_{\alpha-1} < \rho \le C_\alpha$$ diffusion event α is chosen

$$C_M < \rho \le C_{M+1}$$ deposition event is chosen

Update simulation timer:

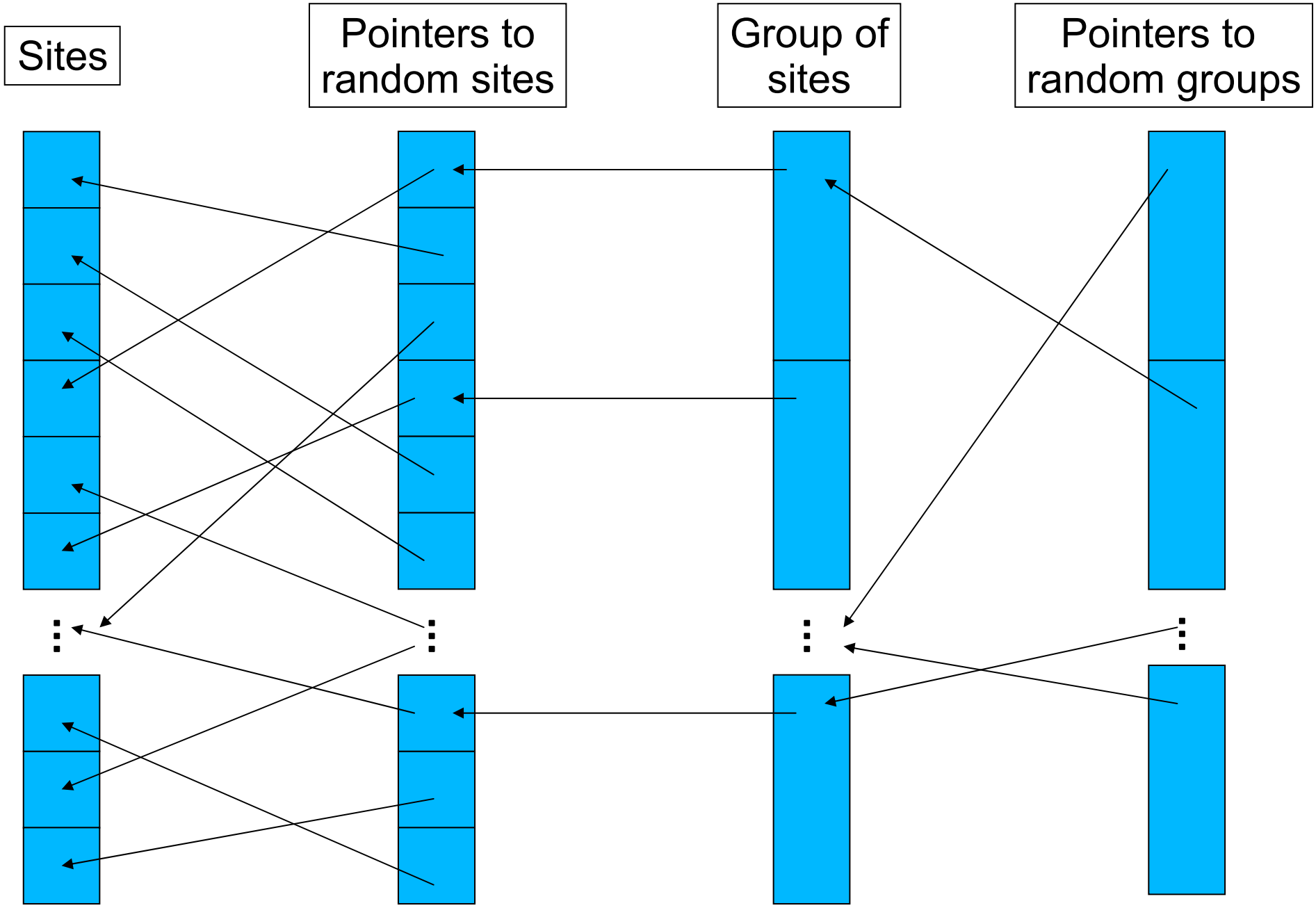
$$t = t - \frac{\log\rho_2}{R}$$

Technical details of the algorithm

2D array `lattice[x][y]` to store height (number of deposited atoms) at each lattice site: map it to 1D array with indexes `i=x+y*`L_x.

Deposition: site is chosen at random

Diffusion: to prevent events with high hopping rates dominate the simulation, create several additional structures for the representation of the lattice array.


Sites
Pointers to random sites
Group of sites
Pointers to random groups

Fe Islands in Fe/Mo(110) Grown by Molecular Beam Epitaxy

M. Bode et al.
PRL **92** (2004) 067201.

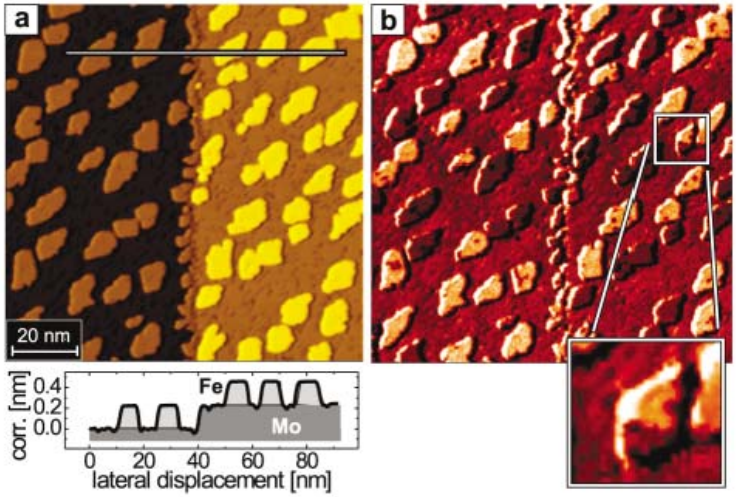
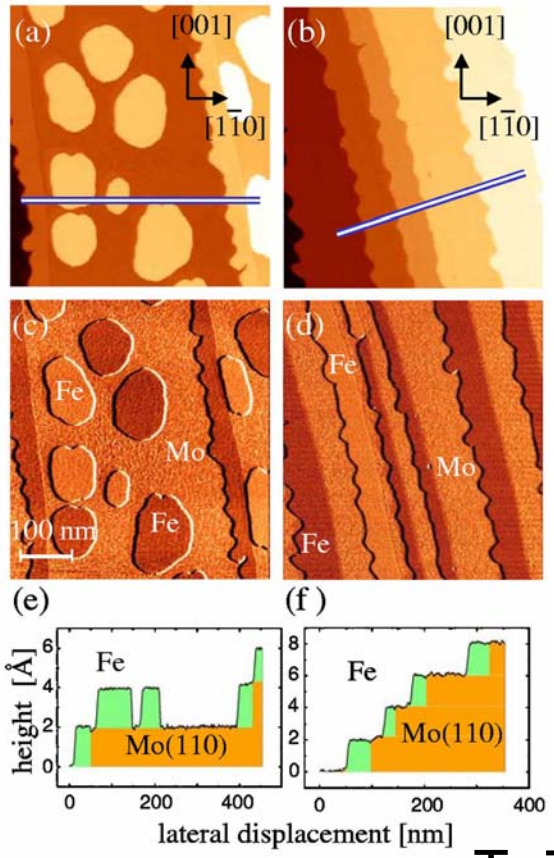


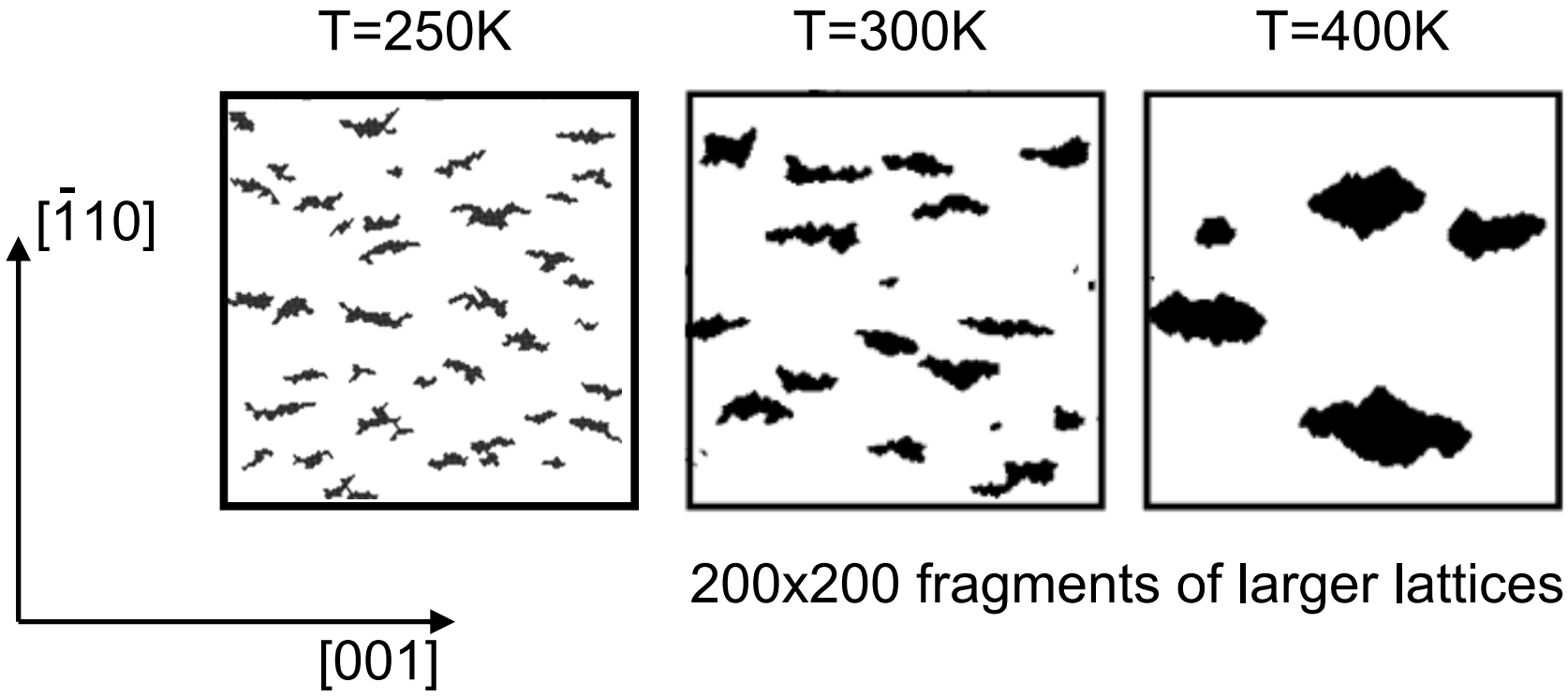
FIG. 1 (color). (a) Topographic STM image and (b) the simultaneously measured out-of-plane sensitive magnetic dI/dU signal of two Mo(110) terraces decorated with Fe islands (overall coverage 0.25 ML). The line section (lower panel) reveals that the substrate's step edge and the islands are of monatomic height (≈ 2 Å). During image recording one island switches from dark to bright (inset). Measurement parameters are $T = 13$ K, $U = 90$ mV, and $I = 1$ nA.

J. Prokop et al.
PRB **73** (2006) 014428.



T=700K

Island Morphology

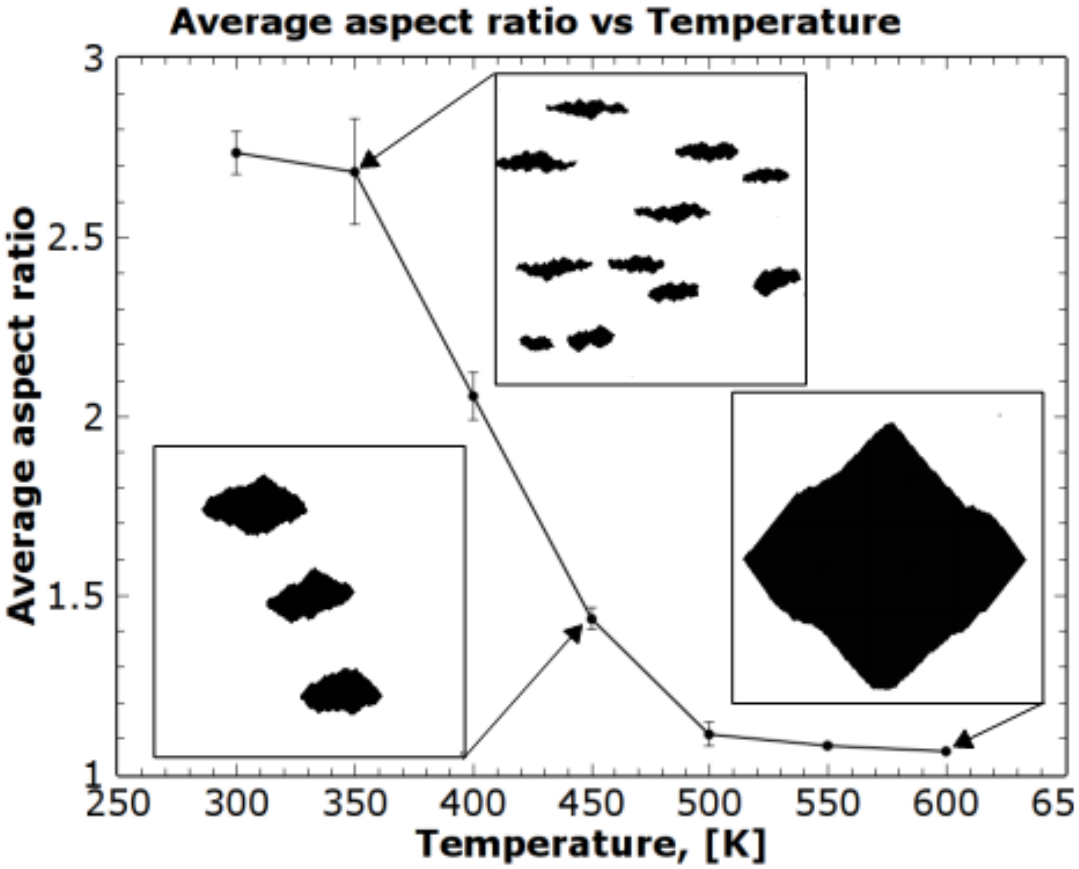


200x200 fragments of larger lattices

Anisotropic diffusion: no diffusion along [001] direction

Modified interaction energies: no interaction with the 3rd neighbors, different interaction with 2nd neighbor: $E_{2n} = 0.1eV$

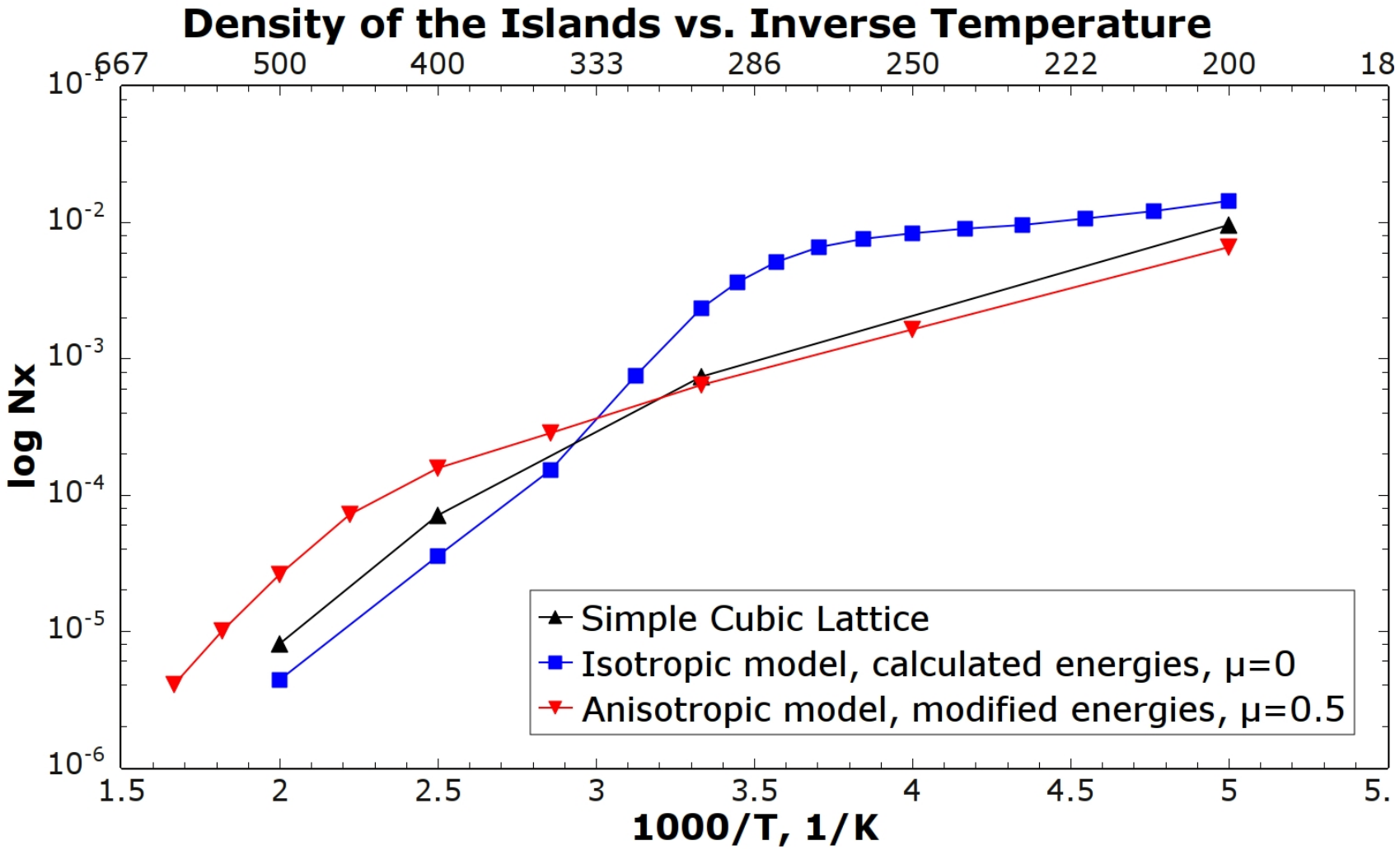
Average aspect ratio (a.a.r.): average ratio of the island dimensions in the directions $[\bar{1}10]$ and [001] for each island averaged over all atomic islands in the system.



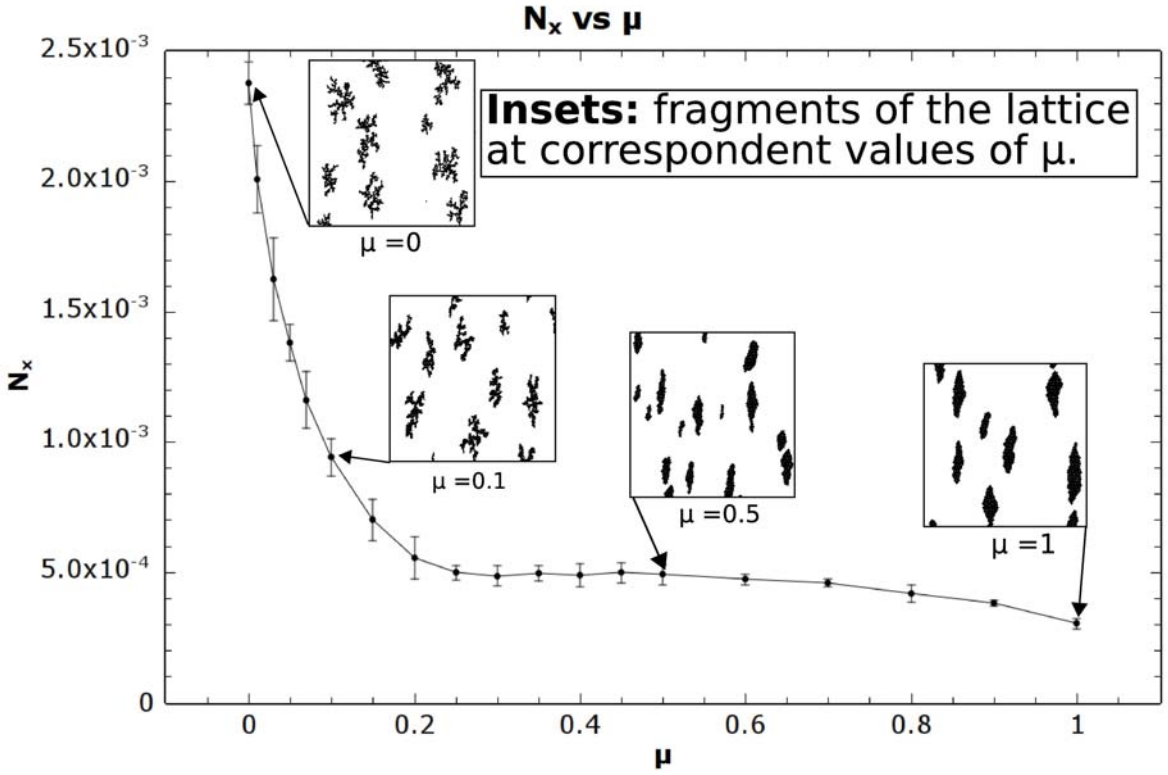
Islands are becoming Larger and more compact with smoother edges.

For high T – a.a.r. is saturated

Island Density. Arrhenius Plot.



Island Density vs. μ



Isotropic model

Calculated interaction energies.

Density saturates.

a.a.r. decreases

Effect of Strain.

Additional term in the diffusion barrier:

$$E = E - \alpha E_e$$

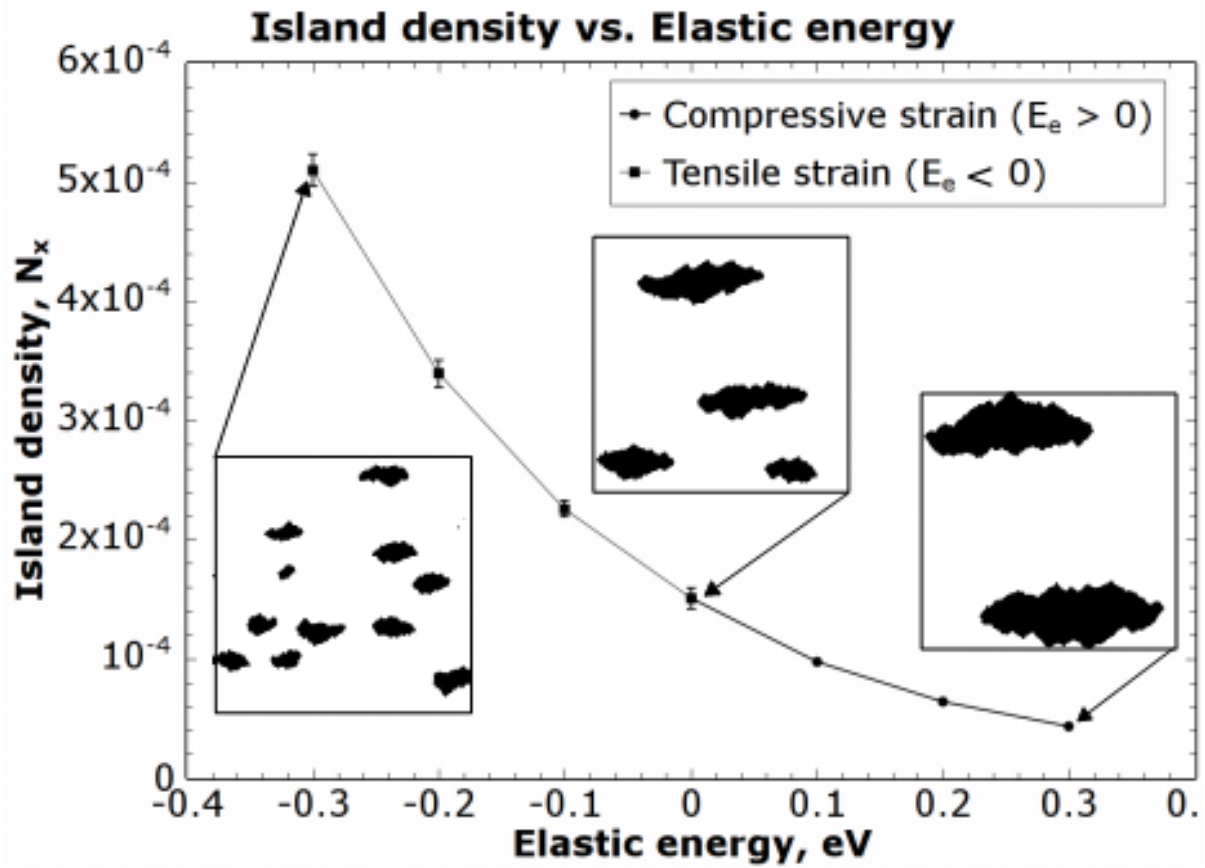
α – coefficient of the elastic relaxation, which depends on the number of occupied neighbors.

$\alpha = 0.4, 0.25, 0.1, 0.03, 0$ for 0, 1, 2, 3 and 4 neighbors

E_e – elastic energy of the unit cell

N. Grandjean and J. Massies, J. Crystal Growth, 134, 51 (1993)

Island Density vs. Elastic Energy



T=400K

Island shape do not change significantly: a.a.r. slowly changes from 1.8 to 2.1.

Island size becomes larger.

Conclusions

International EU-NSF Project “MagDot” and its goals were introduced

Growth model and KMC algorithm for MBE on bcc(110) was developed

Island morphology in submonolayer regime was investigated:

- dependence of island shape and density on substrate temperature
- dependence of island density on the strength of influence of the final position configuration
- heteroepitaxial system – effect of strain

Outlook

Obtain island configurations at higher temperatures

Adjust values of diffusion barriers

Obtain realistic values of strain parameters specifically for Fe/Mo(110)

Simulations were performed on the cluster **DAVID** dedicated for the material research.

ACKNOWLEDGEMENTS:
This work work was supported by joint funding under EU STRP 016447 MagDot and NSF DMR Award No. 0502737, and by Project AV0Z 10100520 of ASCR.