Inducing chemical ordering and enhancing magnetic anisotropy in FePt and FePd by ion irradiation – an atomistic computer simulation study

Outline:

- Motivation
- $L1_0$ superstructure – domain boundary energetics and kinetics
- Ion irradiation of disordered FePd (FePt) layers
- Irradiation of disordered FePd layers with DSRO
- Irradiation of FePd (FePt) nanoclusters
- Conclusion

Collaboration:

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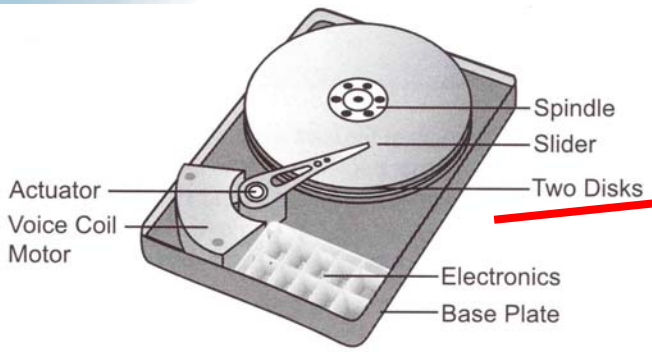
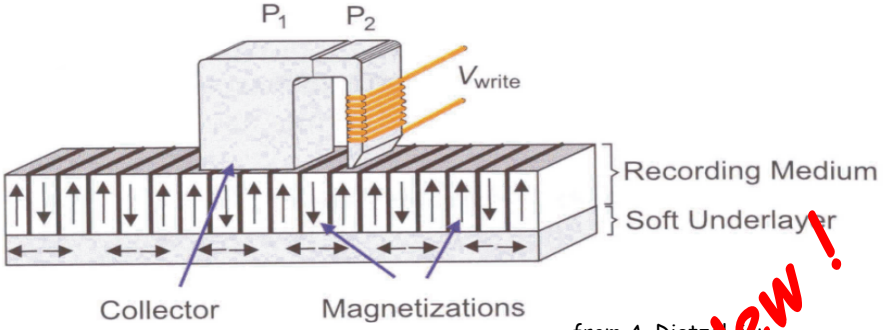
Motivation for studies of FePd / FePt: Magnetic recording (remains Moore's law valid ?)

The paramagnetic limit is a roadblock for a traditional increase of HD memory



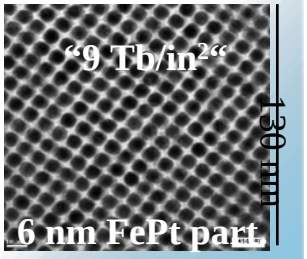


from A. Dietzel, IMI Nanoelectronics & Information Technology

New !

- achieve high packaging density
- circumvent superparamagnetism
- boost magnetic coercivity
- large anisotropy
- allow low-T processing
- ...

- vertical recording
- patterned media

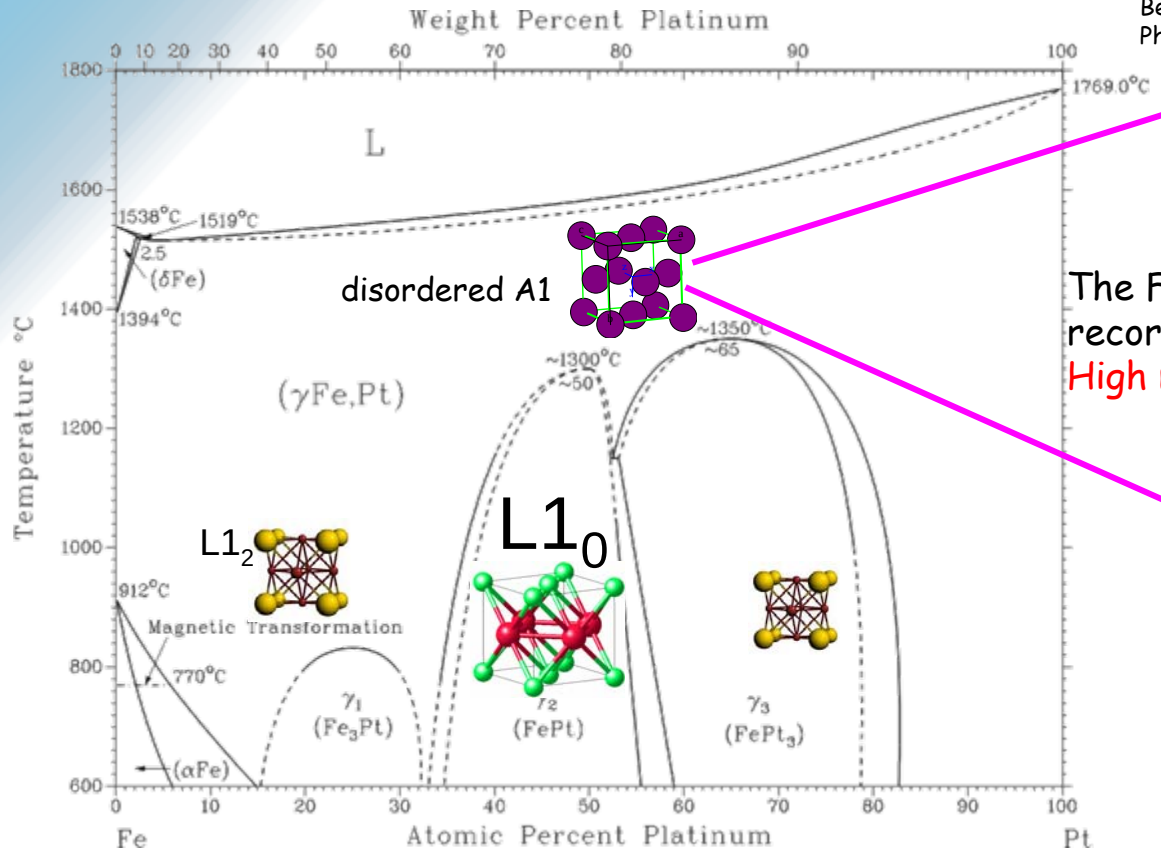


New highly anisotropic recording materials
→ **processing of FePd, FePt, CoPt, ...**

Bernas, Attane, Heinig et al., Phys. Rev. Lett. 91 (2003)

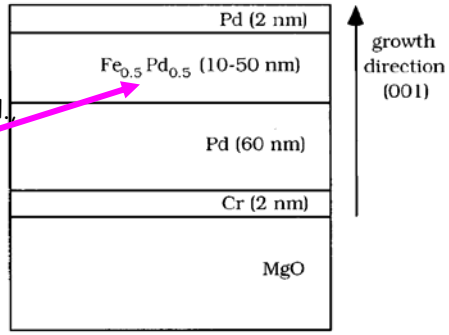
The Fe-Pt phase, its preparation:

- FePt forms in cubic fcc (A1) structure as synthesized
- Post-deposition annealing required to form $L1_0$ order

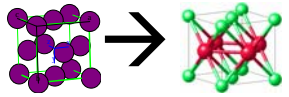


Gehanno et al.,
JAP 84 (1998) 2316

Bernas, Attane, Heinig et al.,
Phys.Rev.Letters 91 (2003)



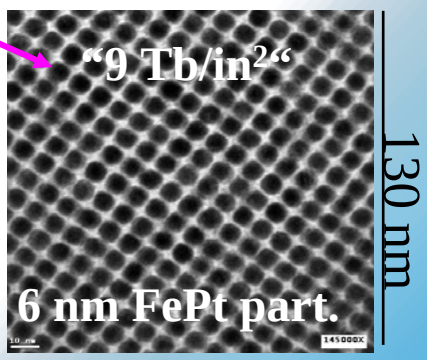
The FePt phases prepared for magnetic recording are initially disordered.
High magnetic anisotropy due to $L1_0$ structure



?

Self-org. magn. array assembly of FePt NCs on TEM Grid (0.1 mm scale)

Seagate



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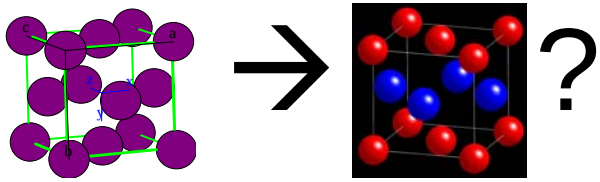
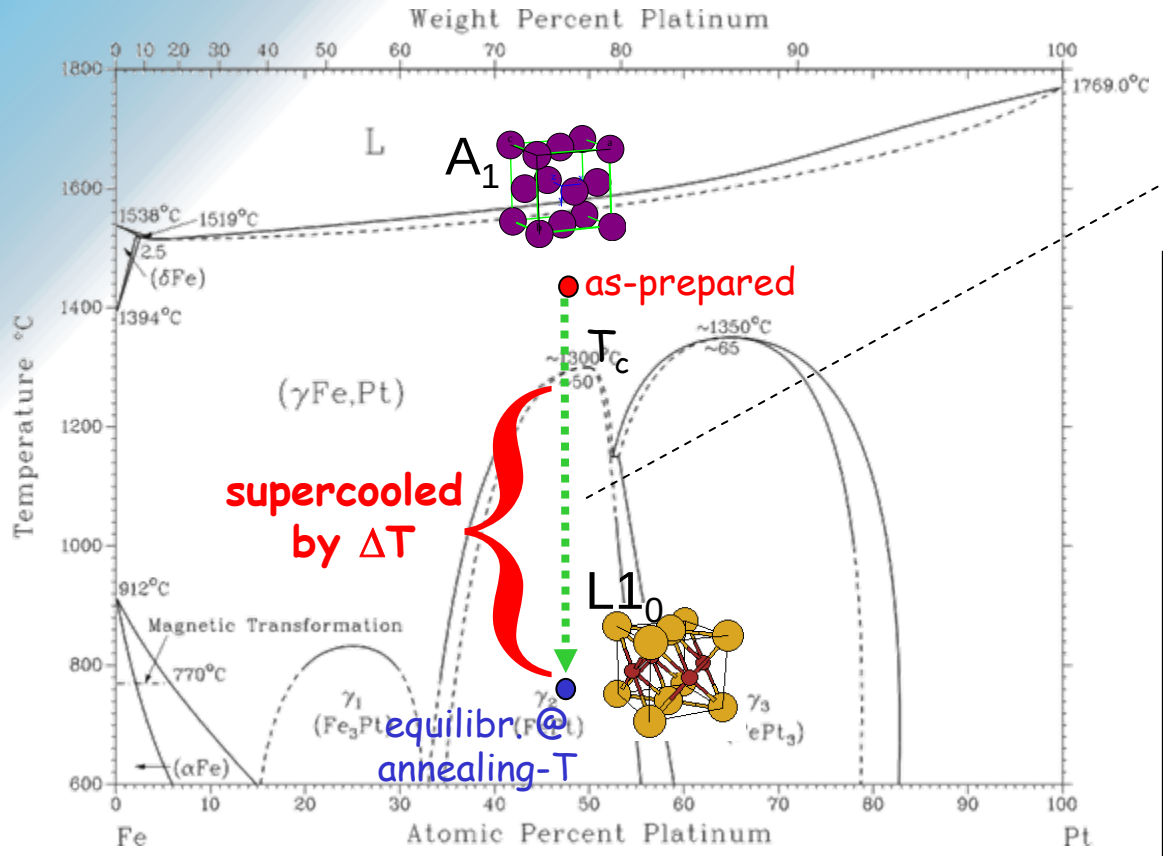
Institute of Ion-Beam Physics and Materials Research

The $L1_0$ ordering kinetics of FePt

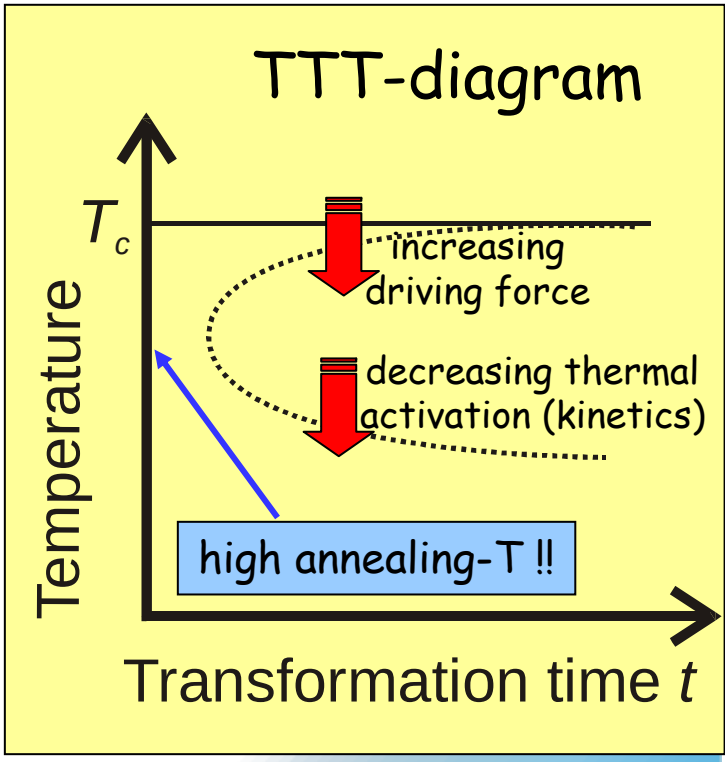
Post-synthesis annealing-T is a compromise between
(a) desired internal $L1_0$ ordering, (b) unfavorable coalescence





in a 1st approximation, the ***driving force*** *for $L1_0$ ordering is*

$$\frac{\Delta H}{V_m}\frac{\Delta T}{T_c}$$

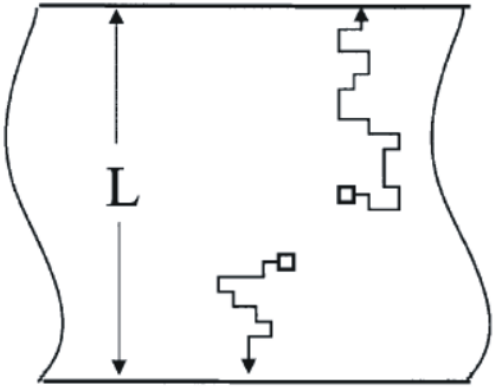


How can we lower the A1→L1$_0$ Transformation-T ?
Ion irradiation !

Bernas, Attane, Heinig et al., PRL91 (2003)
Gehanno et al., JAP 84 (1998) 2316

Assumptions:

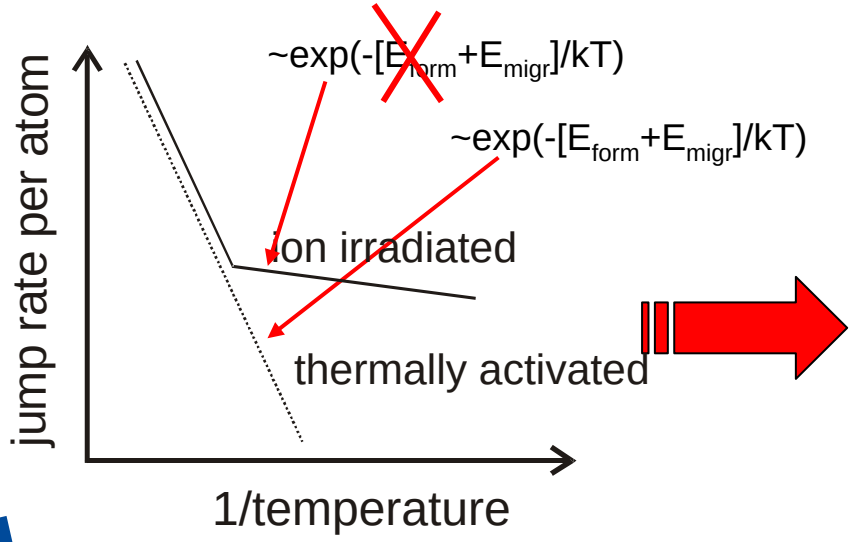
- chemical ordering by migrating vacancies
- vacancy in metals migrate fast, even at RT
- concentration at RT is low due to high formation energy
- **non-thermal vacancy formation by ion irradition**

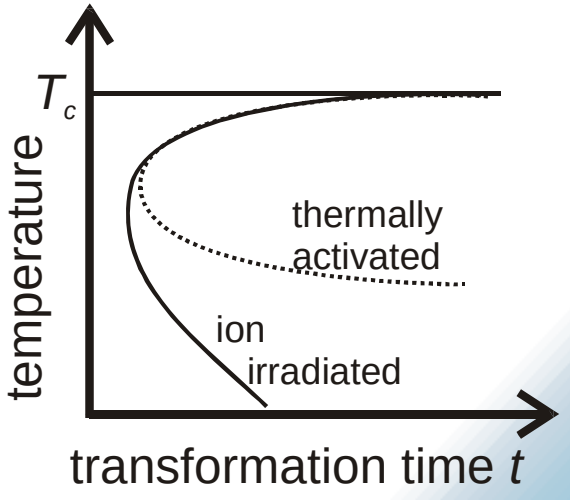


$L \sim \sqrt{Dt}$
$t \sim L^2/D$
(~ no. jumps)

L↑ →better ordering

→ vacancy sinks determine ordering efficiency





Ordering by ion irradiation : Kinetic Monte Carlo simulation

kMC simulation:

→ up to 16 million lattice atoms

→ pairwise interactions (can be more general)

→ kinetics due to individual vacancies

→ periodic boundary cdns in (x,y) plane ;

→ surface & interface are sinks

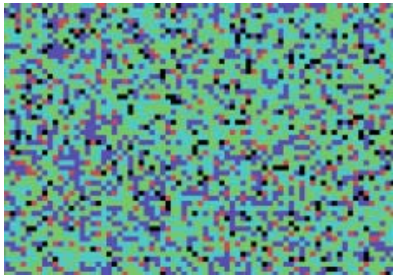
→ energy barriers deduced from bond strengths

$$E^B_{Fe-Fe} \approx E^B_{Pd-Pd} < E^B_{Fe-Pd}$$

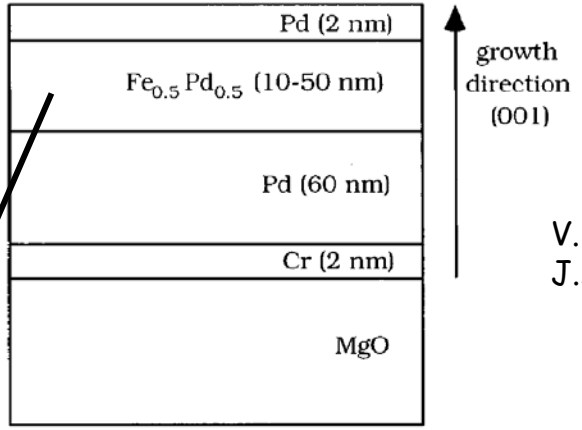
→ vacancy jump probabilities

$$\Gamma \propto \exp\left(-\left[\sum_{final} E^B_{X-Y} - \sum_{initial} E^B_{X-Y}\right] / k_B T\right)$$

as-deposited layers

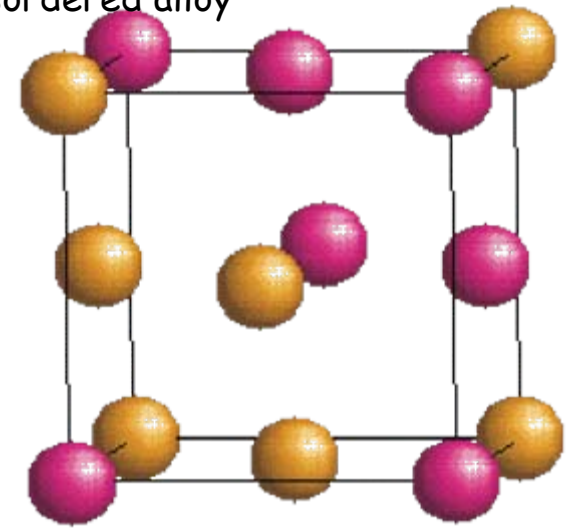


add moving vacancies



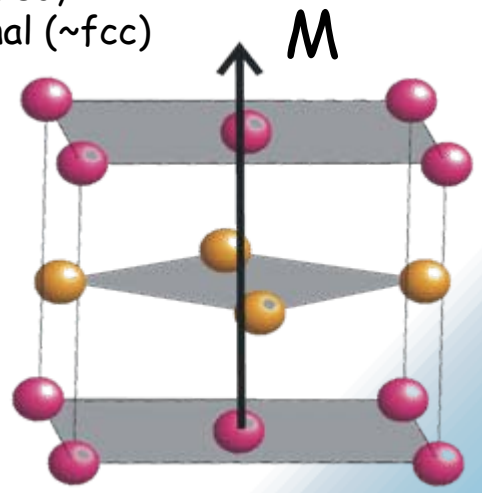
V. Gehanno et al.,
J.Appl.Phys., 84 (1998) 2316

aligned fcc structure,
but chemically
disordered alloy



920 K

$L1_0$ ordered,
tetragonal (~fcc)



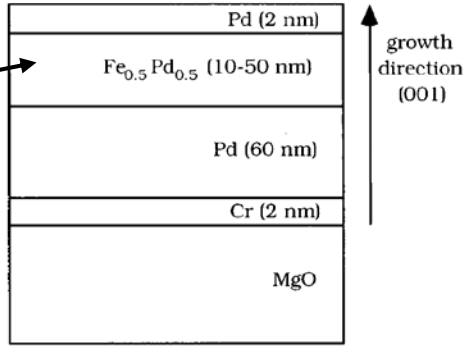
Can T_c be lower?
Control of ordering?

=Pd

=Fe

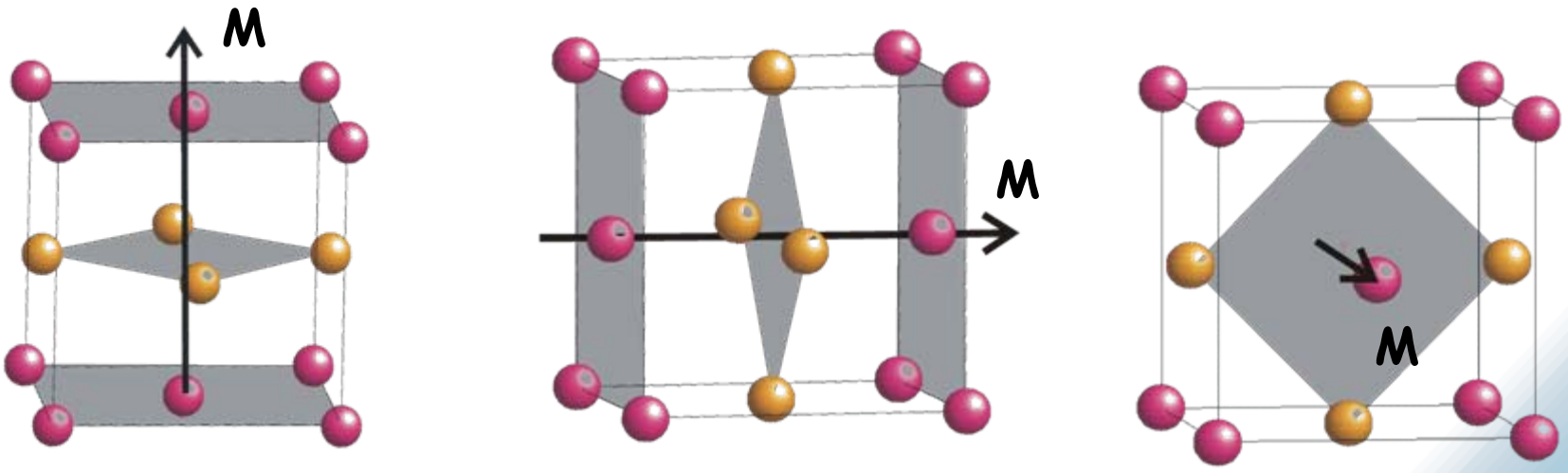
FePd layer is monocrystalline (or has (001) texture),

But the c-axis of the $L1_0$ structure is not fixed
(→ multi-domain structure)

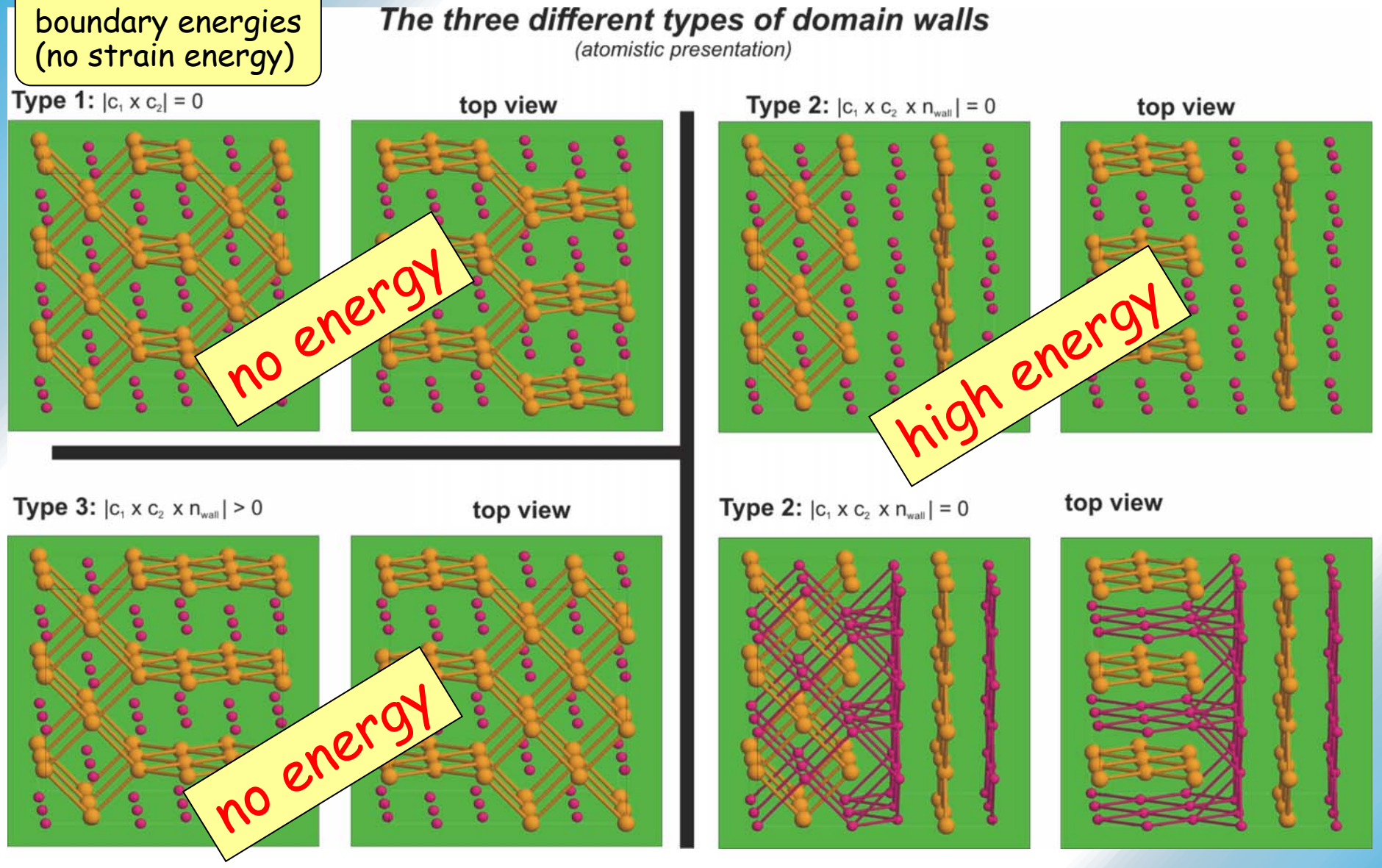


aims: - align $L1_0$ domains (c-axis), i.e. maximize anisotropy

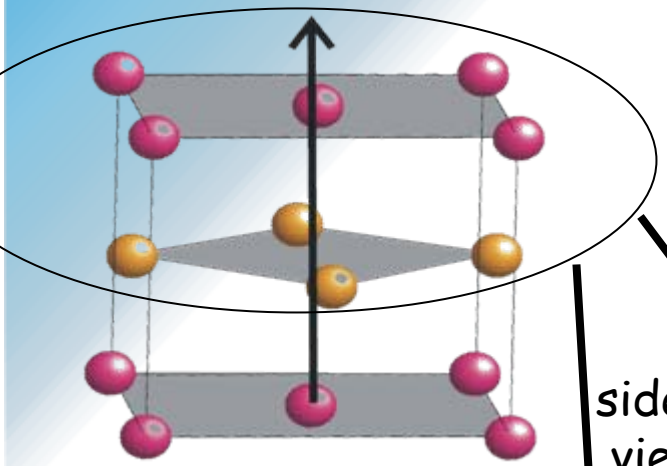
- lower phase transition T



Chemical domain boundary energies (no strain energy)



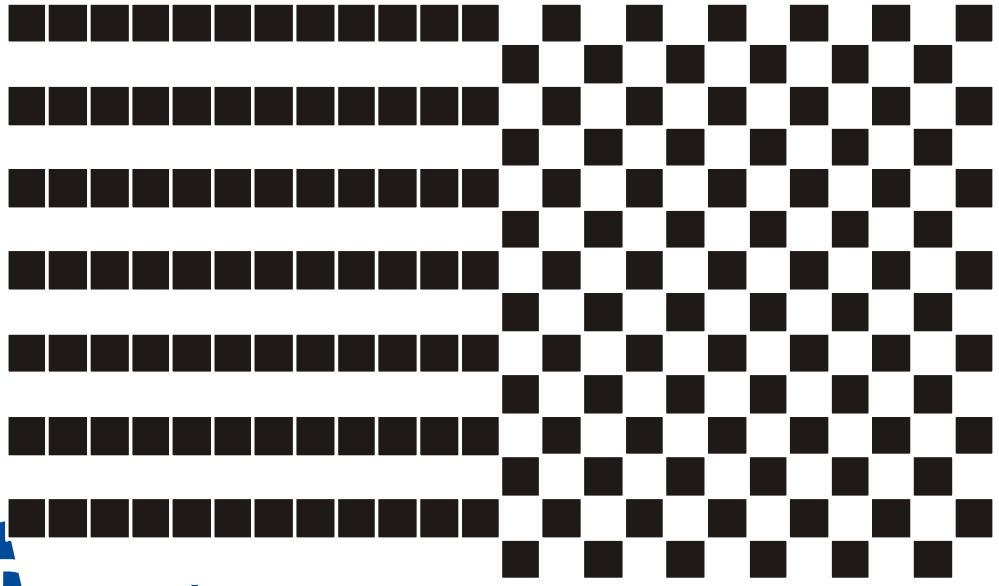
Imaging technique in this presentation:

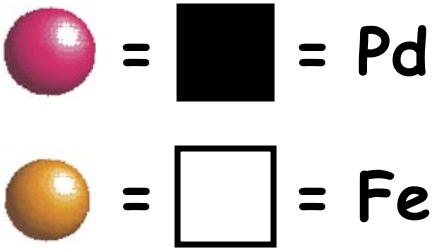


- cutting 2 atomic planes out of the 3D lattice
- show Pd atoms only, suppress Fe atoms

side view

top view





The three different types of domain walls

(schematic presentation)

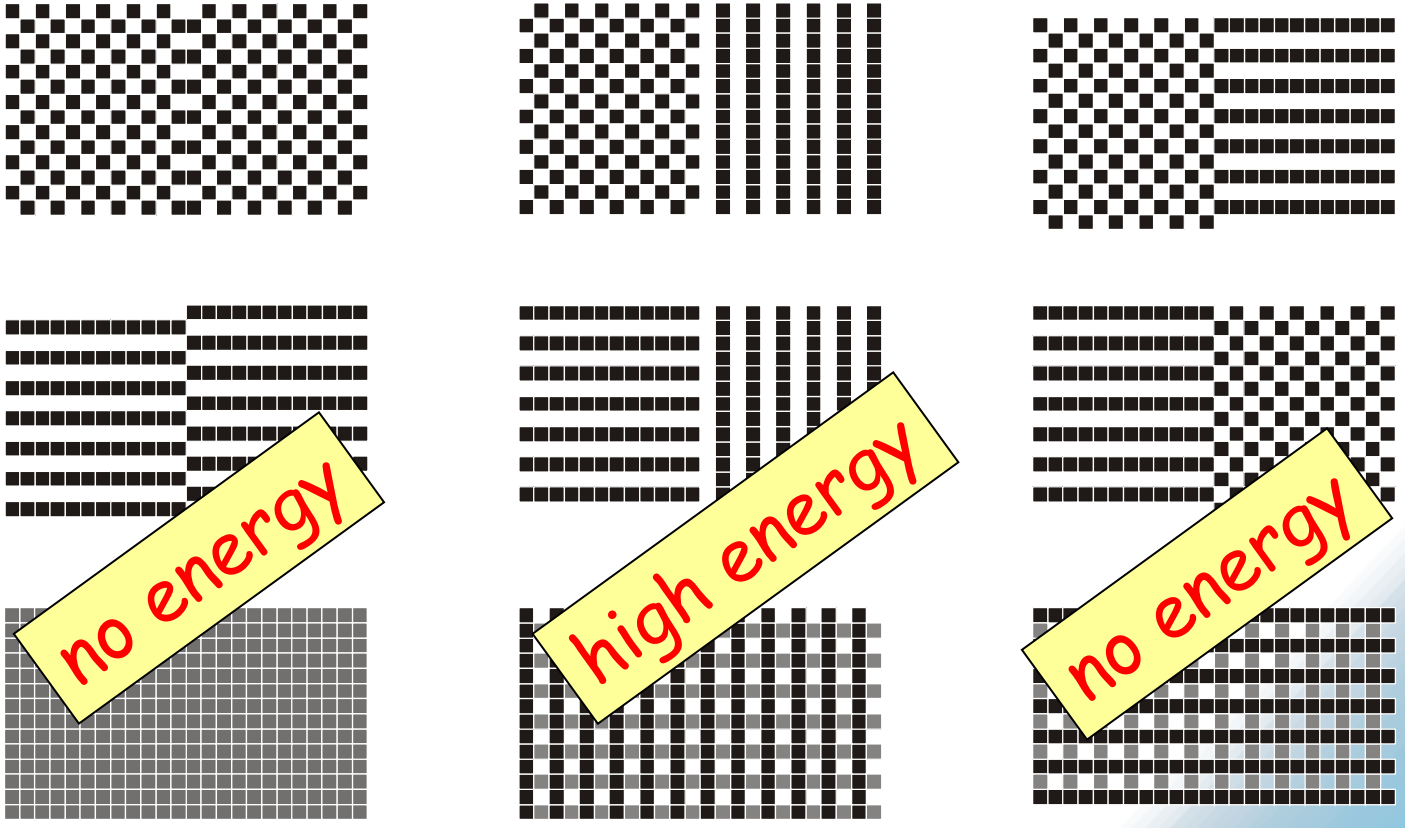
Type 1:
$|c_1 \times c_2| = 0$

Type 2:
$|c_1 \times c_2 \times n_{wall}| = 0$

Type 3:
$|c_1 \times c_2 \times n_{wall}| > 0$

top view

side view



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The atomistic simulation program package

impurity profiles (TRIM, TRIDYN, Ge wetting layer)

boundary conditions: (interfaces, system size, ...)

thermodynamic data base: (T, D, C_{sol}, bond strengths, capture radius, ...)

Input

kinetic 3D lattice Monte Carlo simulation

diffusion, phase separation, reactions, ...

Output

Bit Field (atom's coordinates)

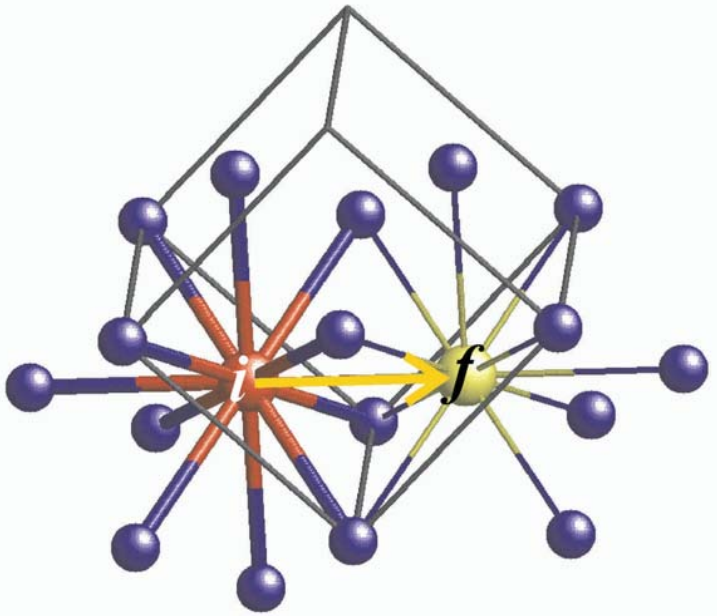
qualitative results

system's evolution path

- visualized by sequences of snapshots
- visualized by computer animations
-

quantitative results

- impurity concentration profiles,
- clusters position, size, density, shape, size distribution
- distribution of tunneling distances
- width of dunuded zone,
- planar cluster spacing (distribution of nearest neighbors)



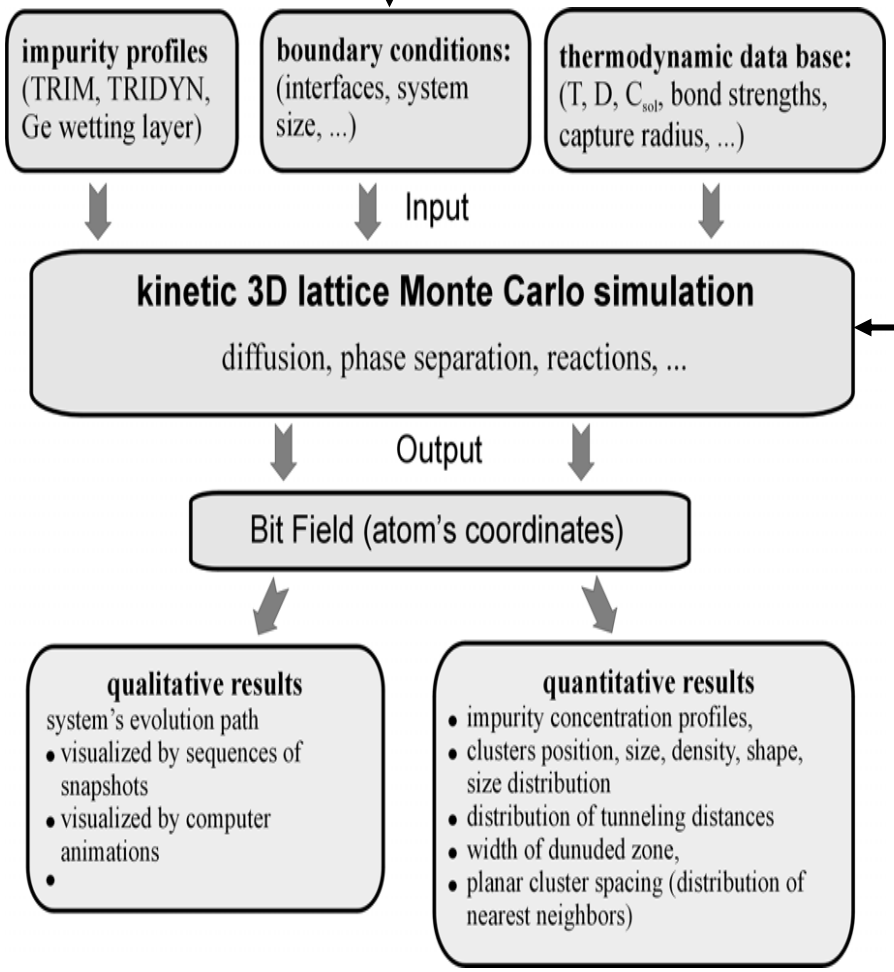
The jump configuration in an fcc lattice.

The red atom on the lattice site *i* attempts to jump to the empty lattice site *f*.

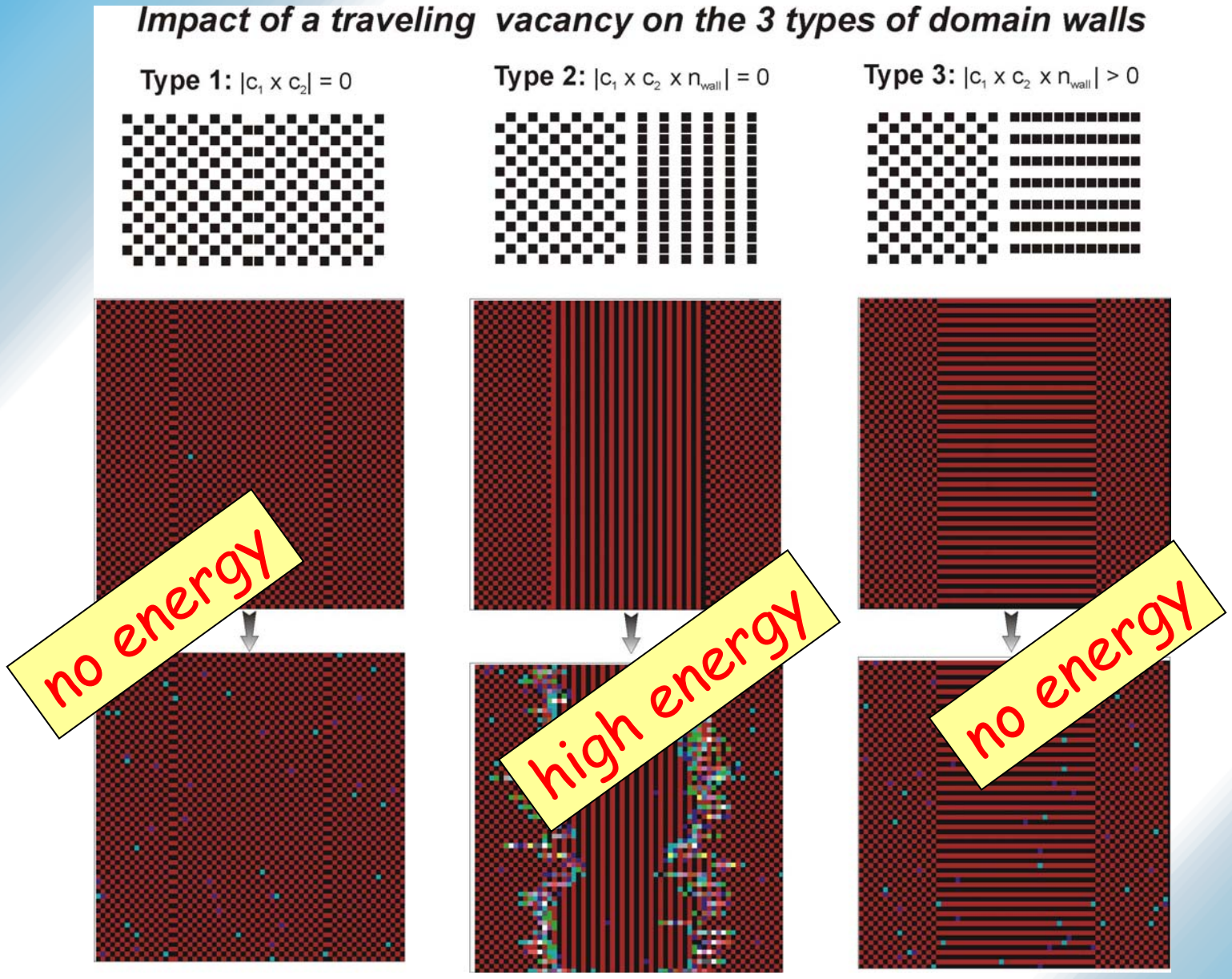
FePd layer properties (DSRO) according to Gehanno et al., J.Appl.Phys. 84 (1998) 2316

vacancy introduction according to ion irradiation conditions

Bond strength for FePd calculated from data of Barmak, Appl.Phys.Lett. **80** (2002)55222 , T=500K



Random walk of the vacancy up to its annihilation at the surface/interface → new vacancy


Impact of a traveling vacancy on the 3 types of domain walls
Type 1: |c1 x c2| = 0
Type 2: |c1 x c2 x nwall| = 0
Type 3: |c1 x c2 x nwall| > 0
no energy
high energy
no energy

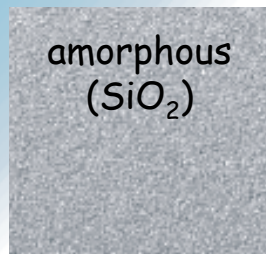
What means a well-ordered highly-anisotropic magnetic media (FePt) ?

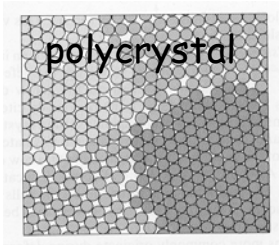
atomic structure

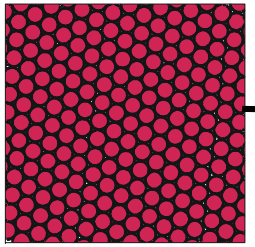
chemical disorder

chemical order (no LRO)

chemical order (LRO)

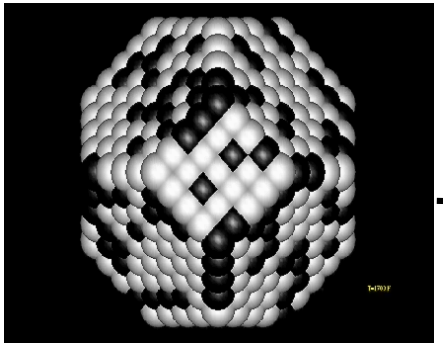






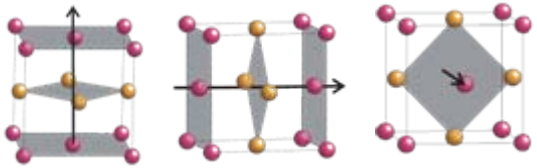
monocrystal

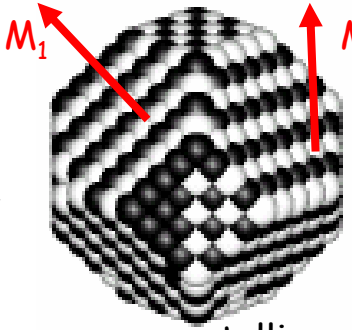
Bo Yang, ECI-Conf.



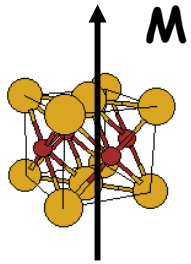
monocrystalline & disordered

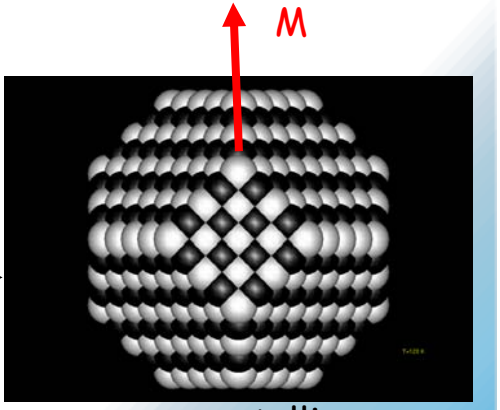
3 ***variants*** of $L1_0$





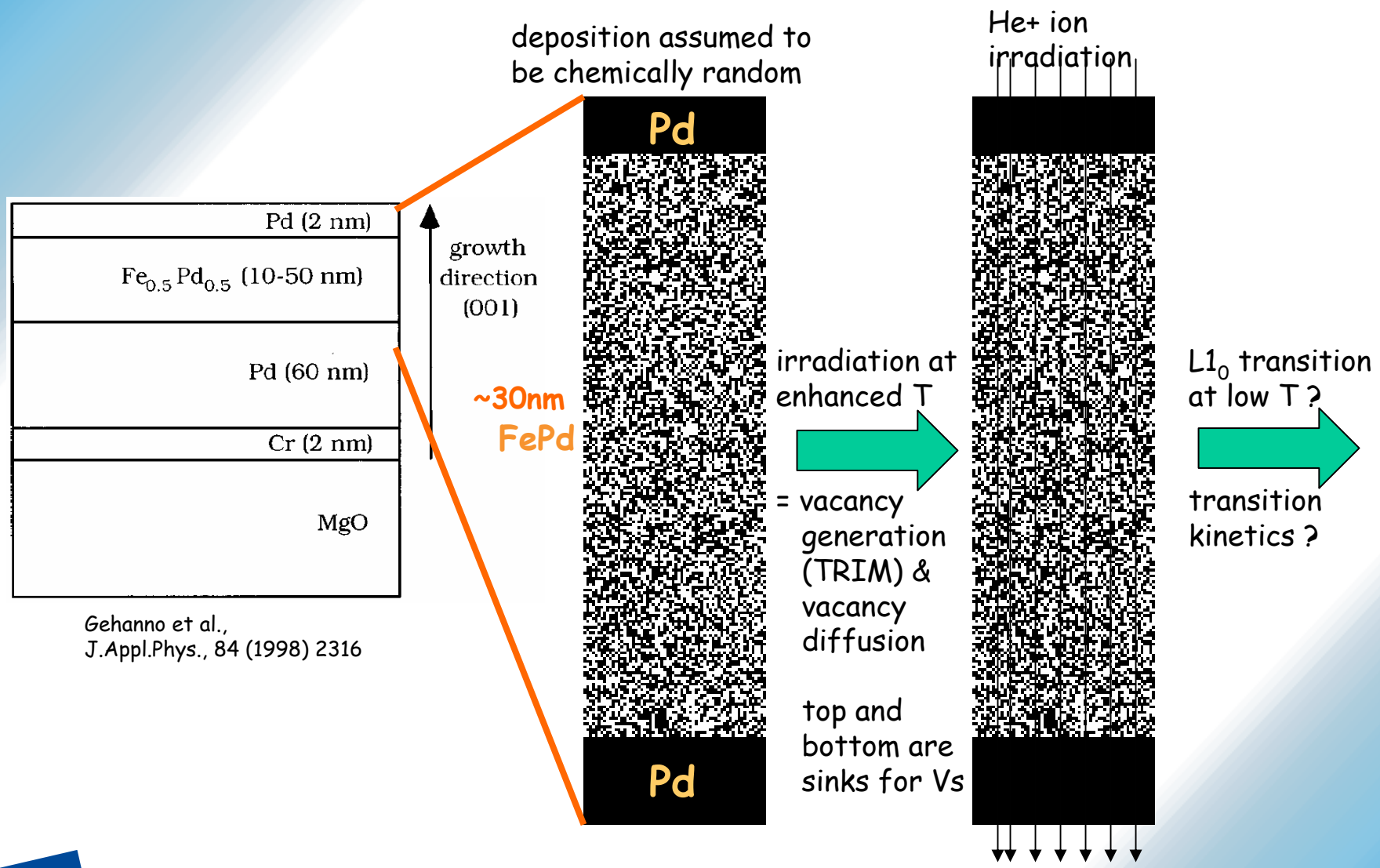
monocrystalline & $L1_0$ ordered & multi-variant





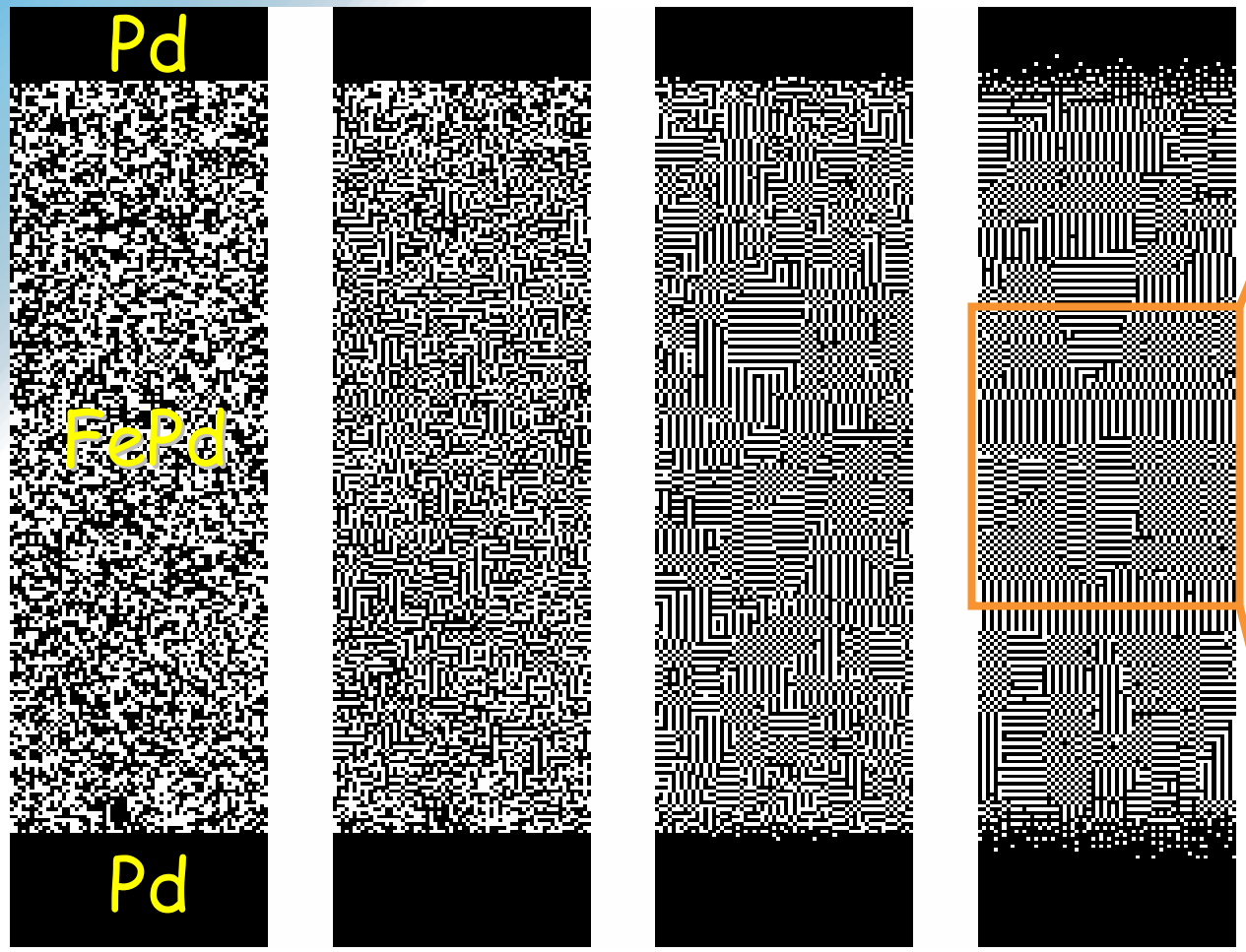
monocrystalline & ordered & single-variant

Scheme of the computer experiment



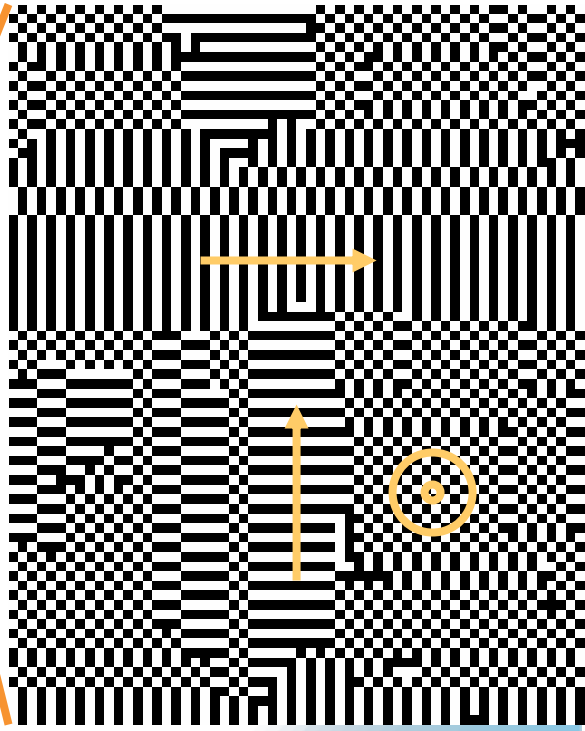
Gehanno et al.,
J.Appl.Phys., 84 (1998) 2316

He^+ irradiation at 500 K → $L1_0$ transition



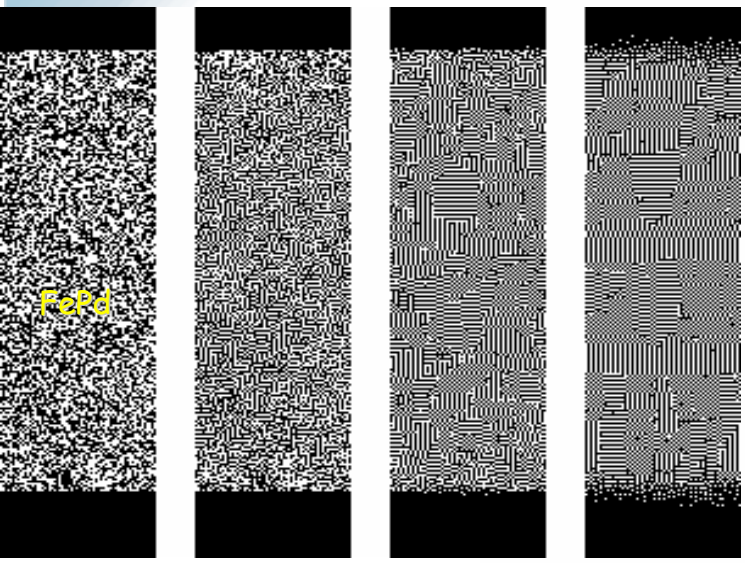
0 dpa | 4E-4 dpa | 0.004dpa | 0.04 dpa

$L1_0$ phase of FePd with different superstructure domains

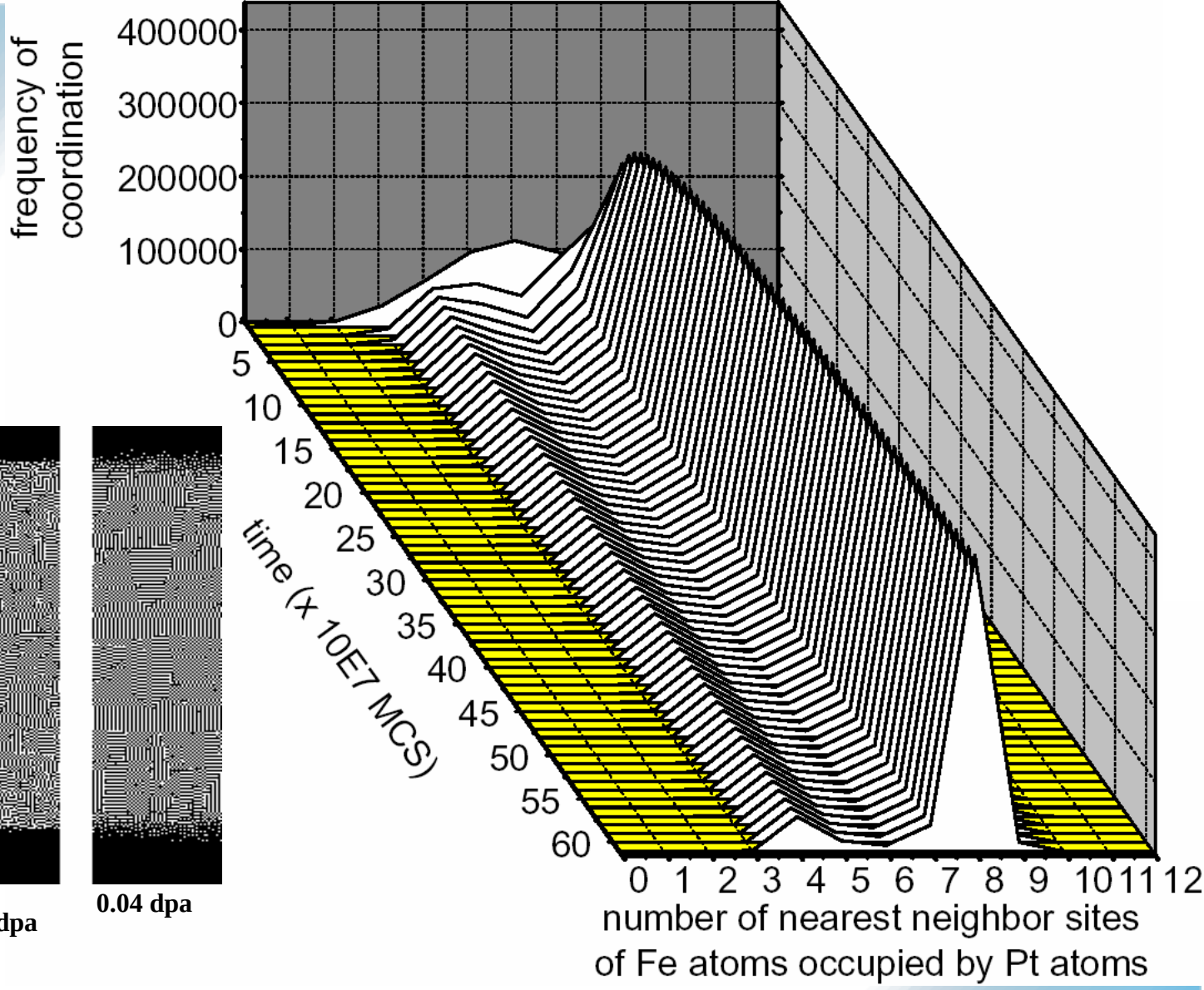


arrows indicate the strong magnetic direction of the $L1_0$ domains

atom's coordination

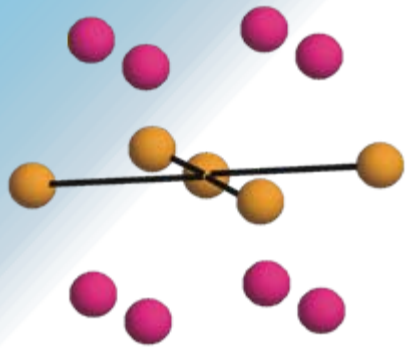


0 dpa 4E-4 dpa 0.004dpa 0.04 dpa



DSRO

Experiment: Atoms in the deposited layer have some Directional Short Range Order (DSRO)
$DSRO_{in\text{-}plane}$=0.82; $DSRO_{out\text{-}plane}$=0.37

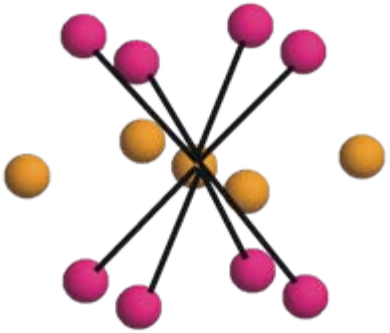


$DSRO_{in\text{-}plane}$:

probability that in-plane nearest neighbors of a Fe atom are occudied by Fe atoms

random alloy:
$DSRO_{in\text{-}plane}$ = 0.5
$DSRO_{out\text{-}plane}$ = 0.5

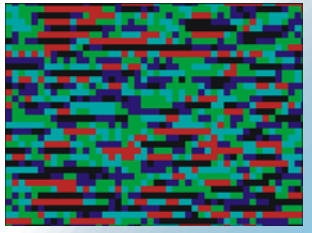
perfect ordering:
$DSRO_{in\text{-}plane}$ = 1.0
$DSRO_{out\text{-}plane}$ = 0



$DSRO_{out\text{-}plane}$:

probability that out-of-plane nearest neighbors of a Fe atom are occudied by Fe atoms

Exp.: initial values
$DSRO_{in\text{-}plane}$ = 0.82
$DSRO_{out\text{-}plane}$ = 0.37



$$P_{setting}^{Pd} = \left[a + \frac{1}{2}\sin\left(\frac{\pi}{4}\left(N_{in-plane}^{Pd} - 2\right)\right)\right]\left[a + \frac{1}{2}\sin\left(\frac{\pi}{4}\left(2 - N_{in-plane}^{Fe}\right)\right)\right]\sqrt{b + \sin\left(\frac{\pi}{2}\left(4N_{out-of-plane}^{Fe} - 1\right)\right)}$$

a=0.515
b=1.2

Forschungszentrum Dresden Rossendorf

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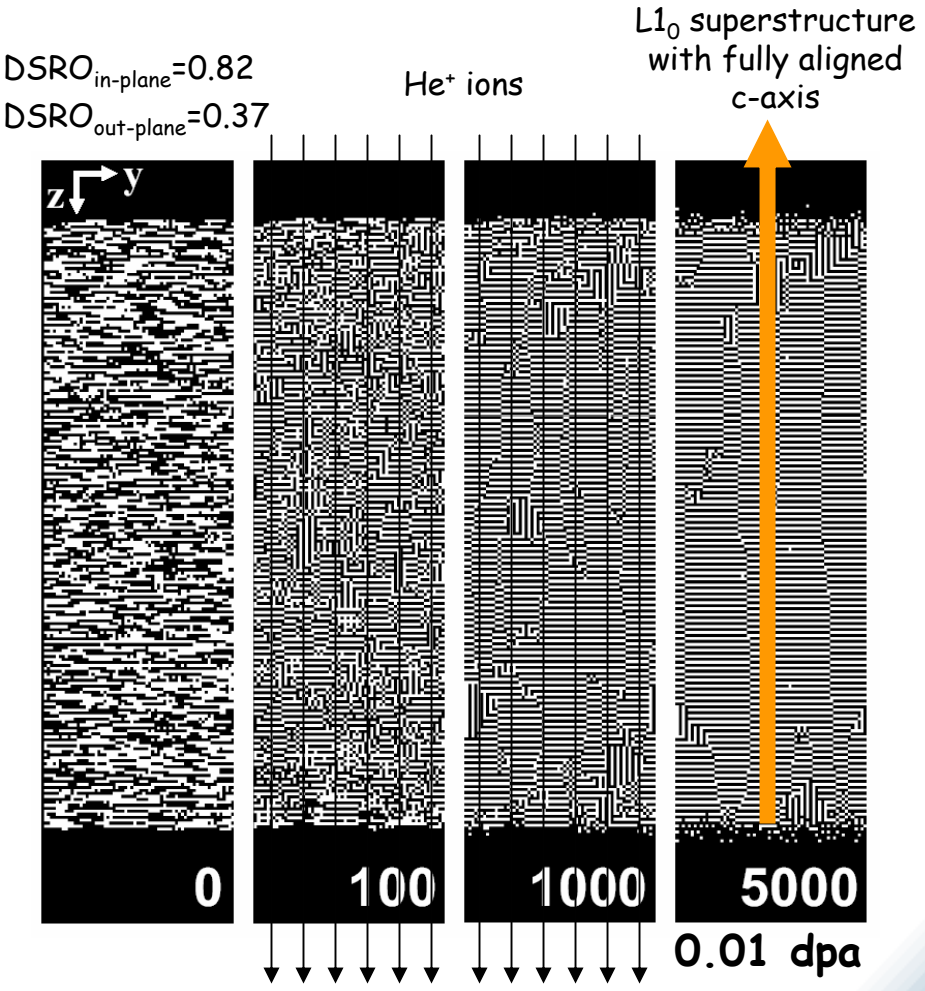
Ordering Intermetallic Alloys by Ion Irradiation

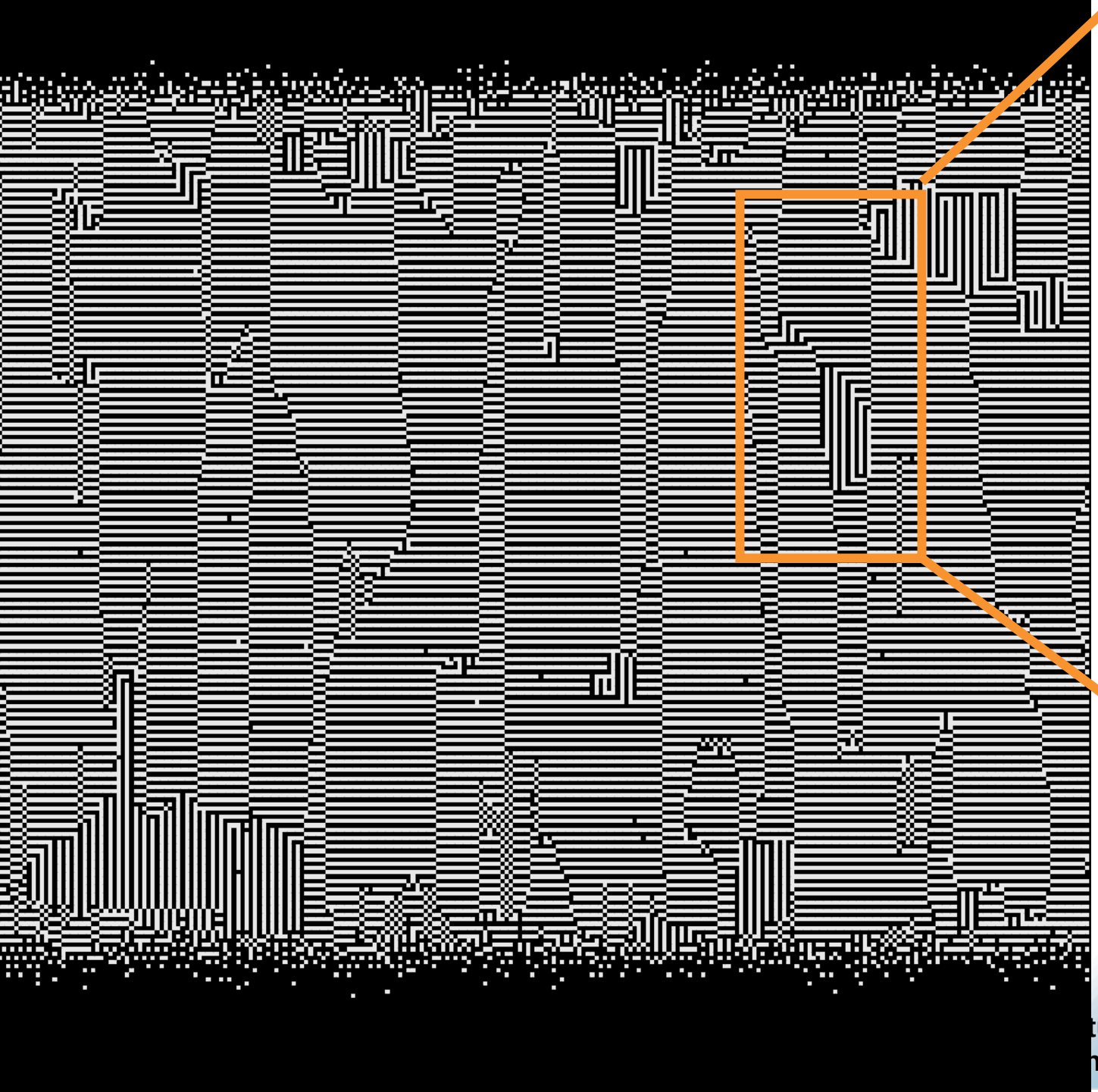
Bernas, Attane, Heinig et al., Phys. Rev. Lett. 91 (2003)

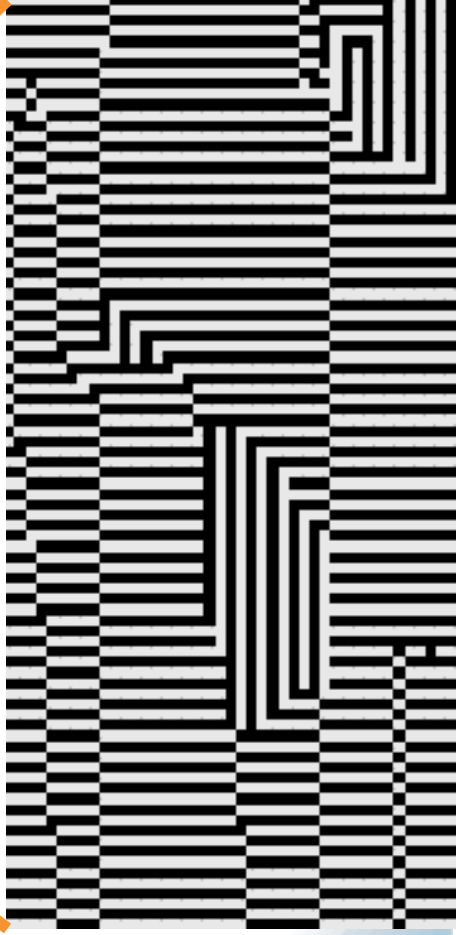
ca. 30 nm FePd sandwiched between Pd;

DSRO due to the deposition process

Small symmetry breaking during deposition results in global symmetry breaking by irradiation







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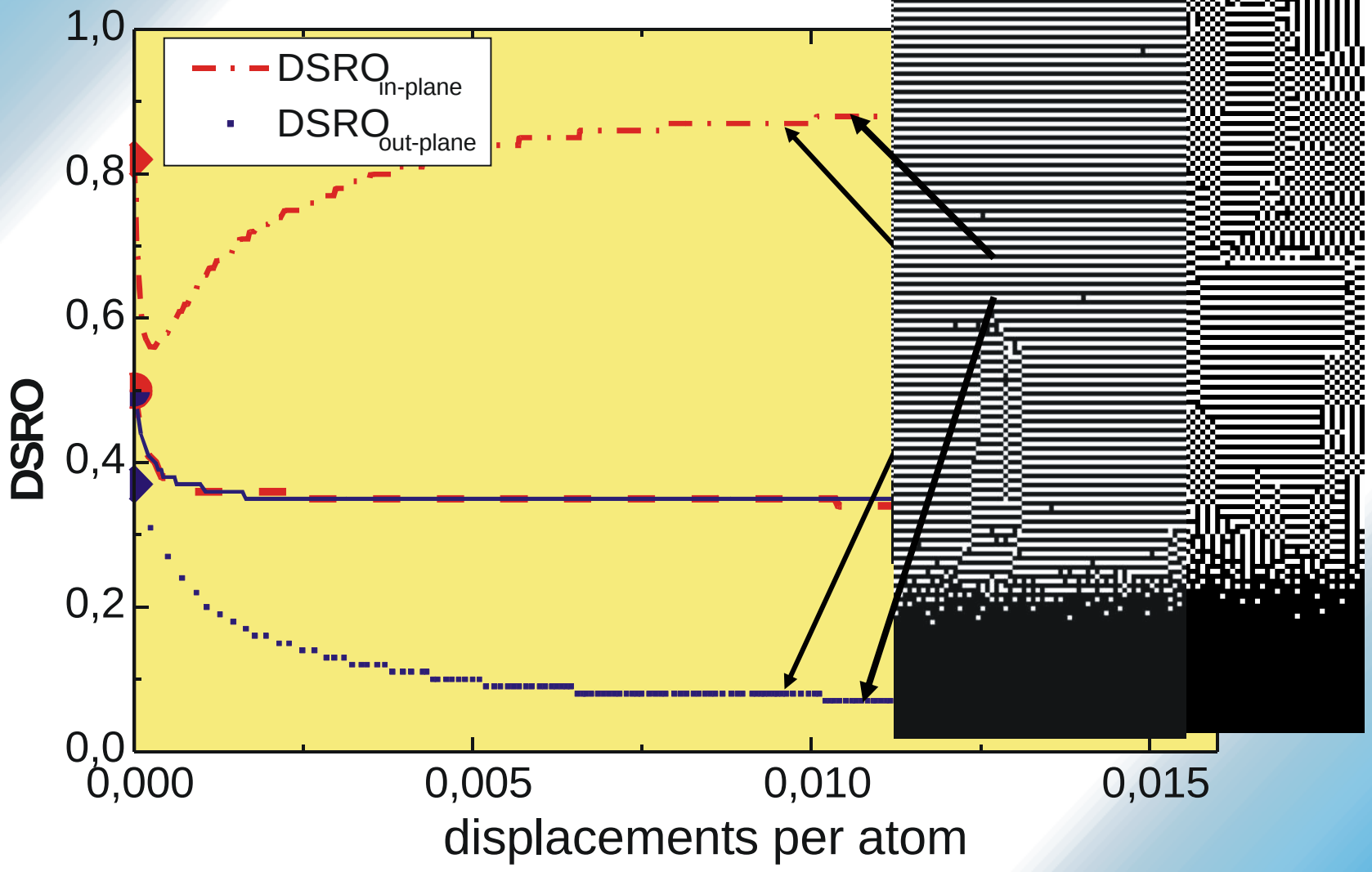
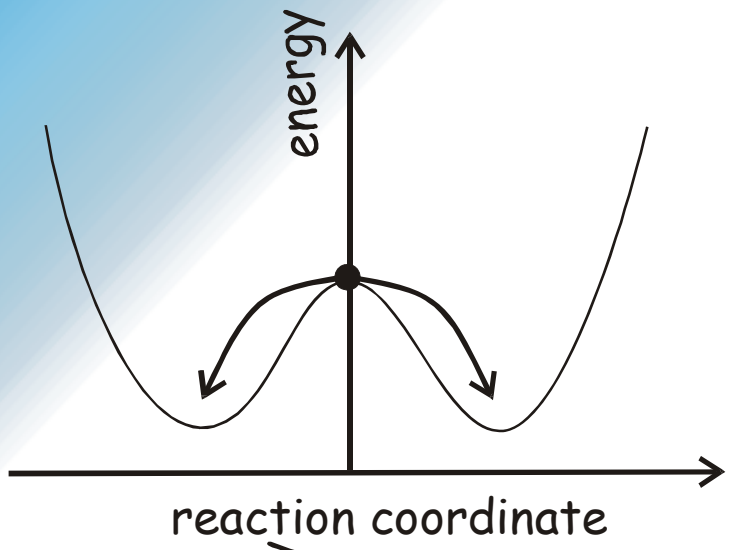
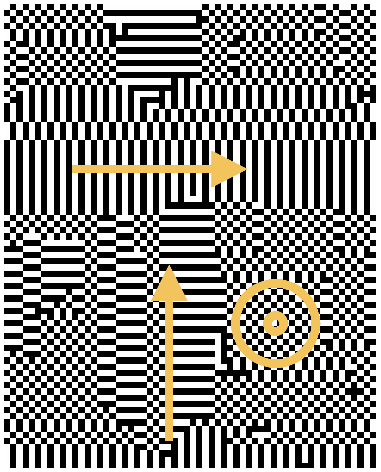
Evolution of DSRO during ion irradiation

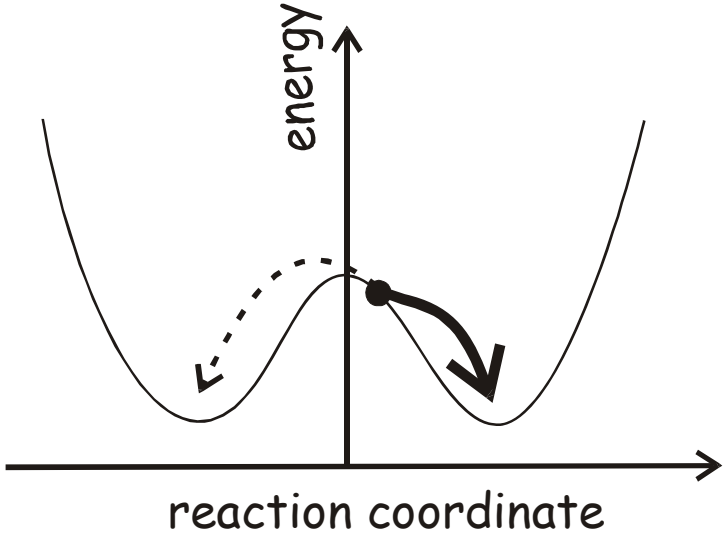


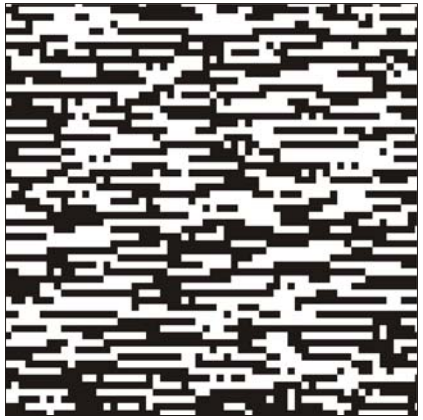
Small symmetry breaking results in long range order



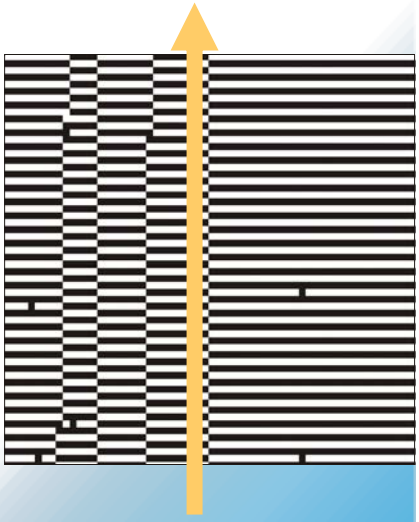
irradiation





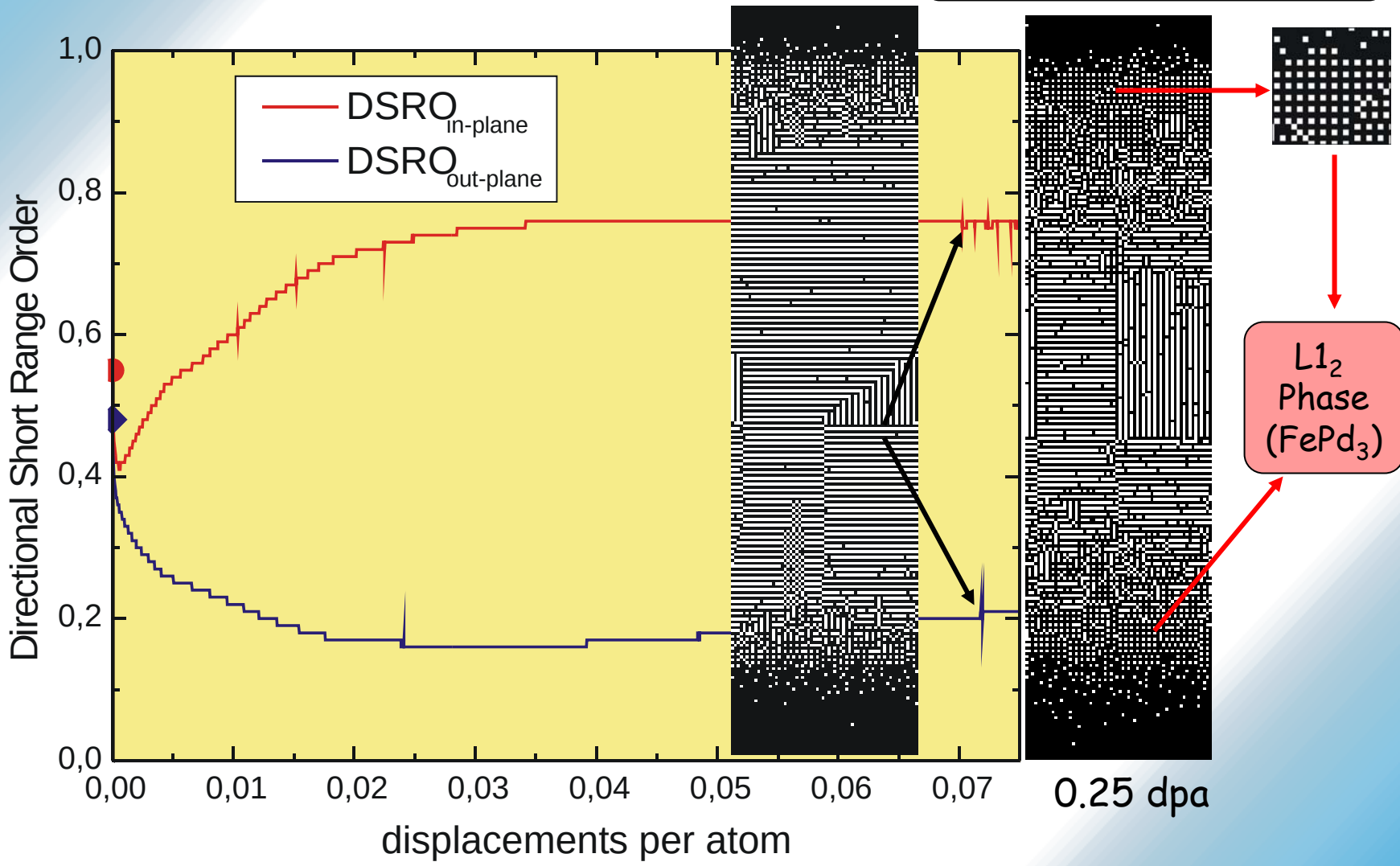


irradiation



Small initial DSRO: $DSRO_{in\text{-}plane}=0.55$ $DSRO_{out\text{-}plane}=0.48$ → long range order ?

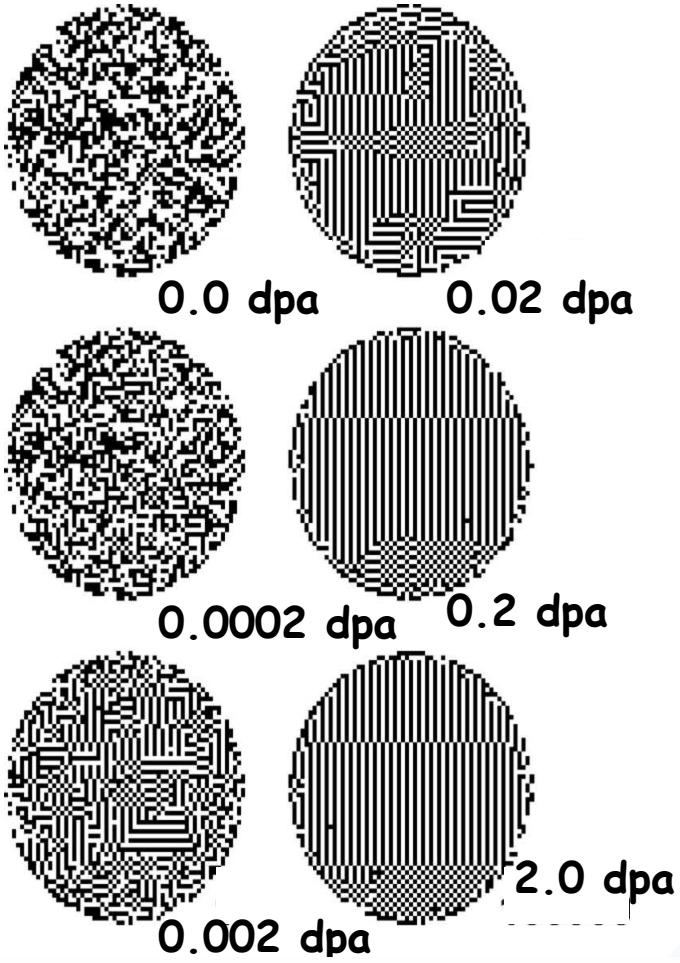
Yes,
but higher fluence needed

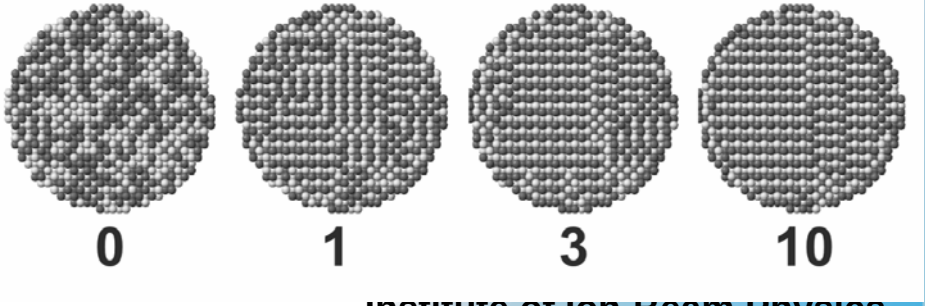


FePd nanoparticles

$L1_0$ transition of passivated FePd nanoparticle with R~6nm under He^+ ion irradiation @ 500 K

- Due to the small particle size, particle tend to become monodomain particles
- However, non-energetic domain boundaries lead to incomplete c-axis alignment even at high fluences
- Thus, also for nanoparticles an initial DSRO is desired to get full c-axis alignment.
- The smaller the particles the more dpa's are needed to achieve full $L1_0$ order (compare the dpa of the 2 simulations





Conclusion

- He^+ irradiation lowers the $L1_0$ transition T_c considerably
- We predict that the collisional vacancy formation lowers T_c
- Initial DSRO (coming from deposition) evolves to long range order by irradiation
- Kinetic Monte Carlo simulations predicts this process, the agreement with experimental results is even quantitative
- It is predicted that even a small DSRO (= broken symmetry) might lead to substantial c-axis alignment
- First results for FePd nanoparticles predict tendency of monodomain superstructure formation