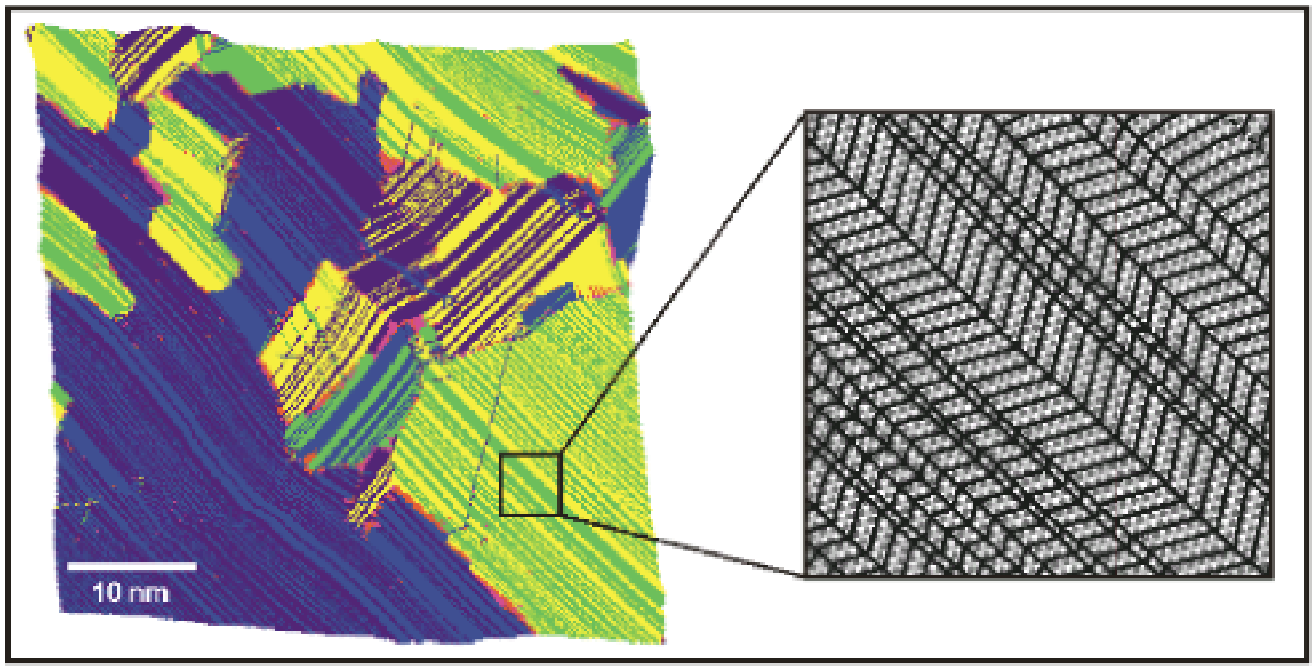
MD simulations study of microstructure formation during martensitic transformations



By Oliver Kastner, GFZ Potsdam, Germany

with contributions by
Graeme Ackland / U. Edinburgh UK
Gunther Eggeler / U. Bochum, Germany
Roni Shneck / U. Beer-Sheva, Israel
Wolf Weiss / WIAS Berlin, Germany

Scope

Reference to shape memory alloys (SMA): Physical situation

Method: MD simulations (very briefly)

Lennard-Jones crystals in 2D:

Thermo-mechanical properties: Small crystal assemblies

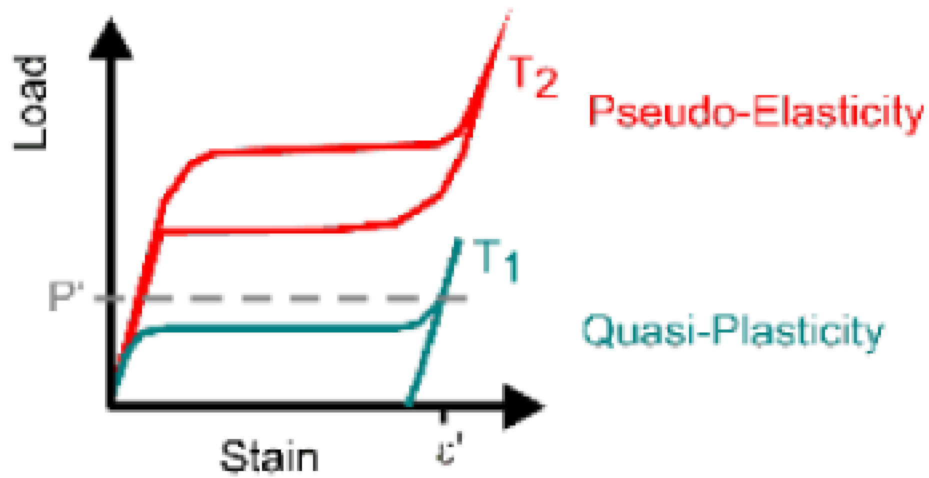
Microstructure formation in extended crystals

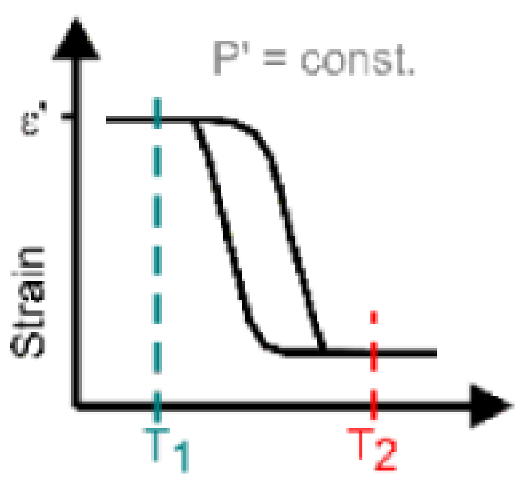
Microstructure evolution and hysteresis

Nucleation of martensite

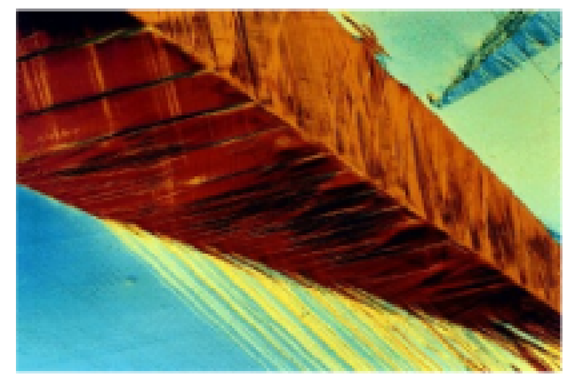
SMA macro and micro phenomena

Tensile tests

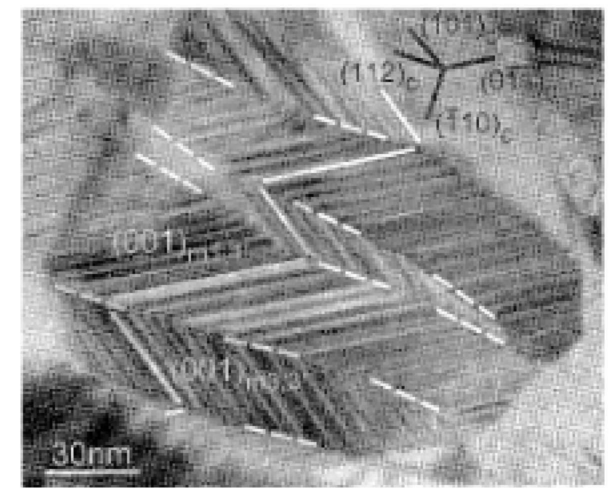




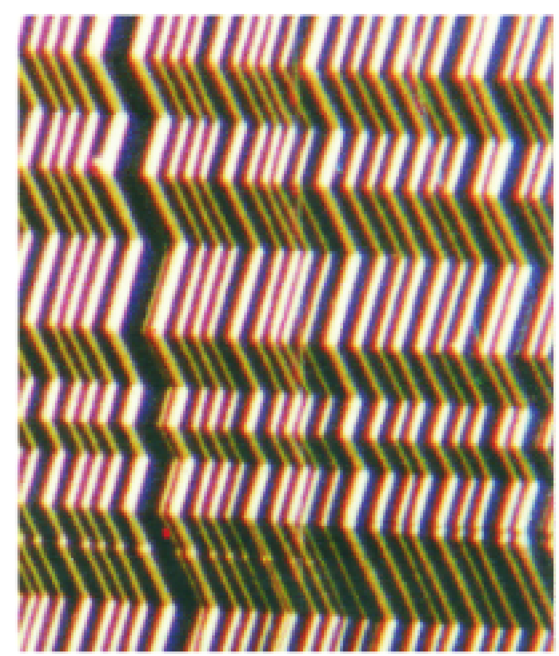
Morphology



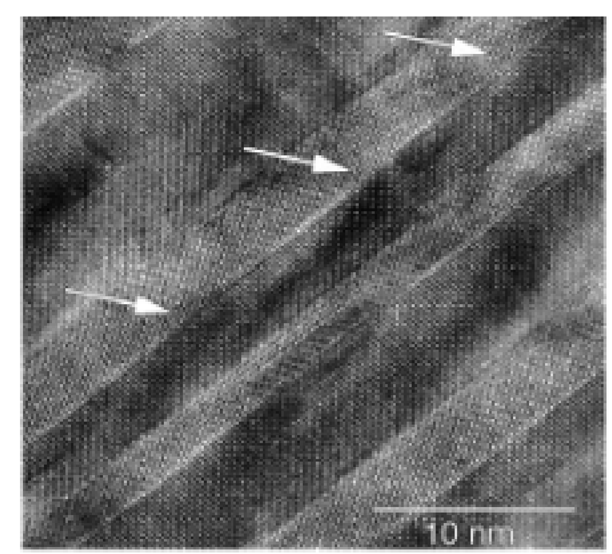
Martensite growth in CuAlNi 1cm-scale, Tan & Xu, 1990



"Herringbone" shaped martensite lamellae in NiTi. Waitz 2005

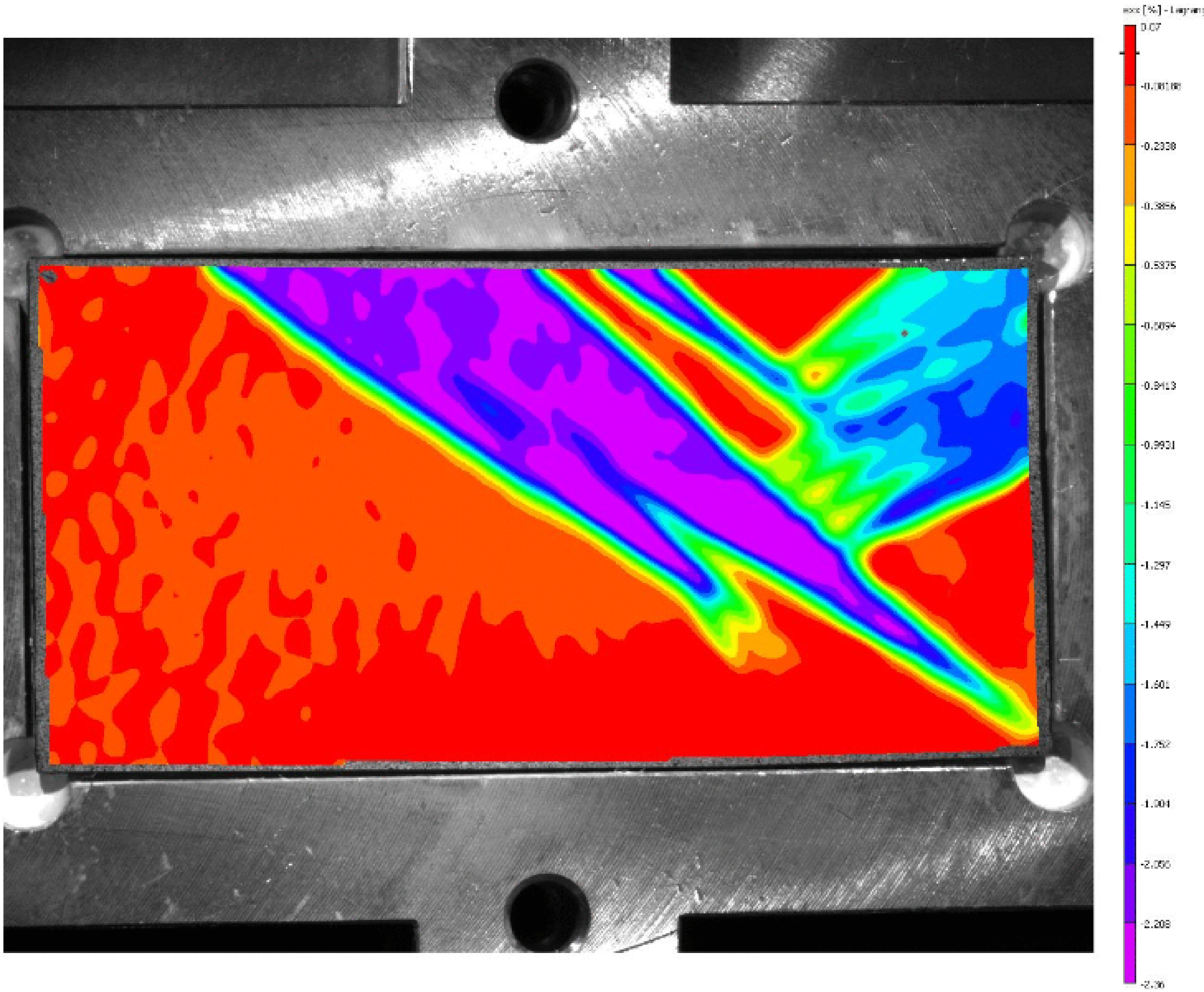


Martensite twins in CuAlNi 0.1 mm-scale, Tan & Xu, 1990



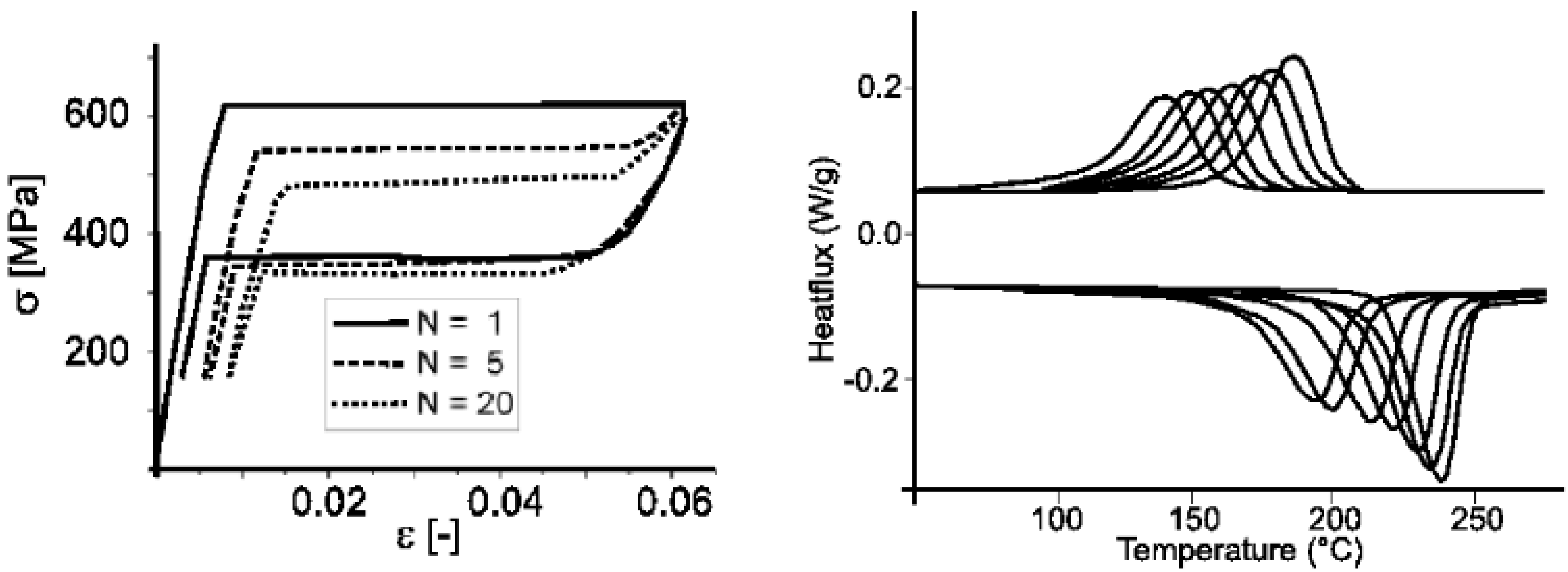
Nano-Twins in NiAl Boullay et al. 2003

T-induced MT in a CuAlNi plate (digital image correlation)



Courtesy A. Musolff, BAM and A. Schaefer, RUB

Functional fatigue of SMA on mechanical and thermal cycling

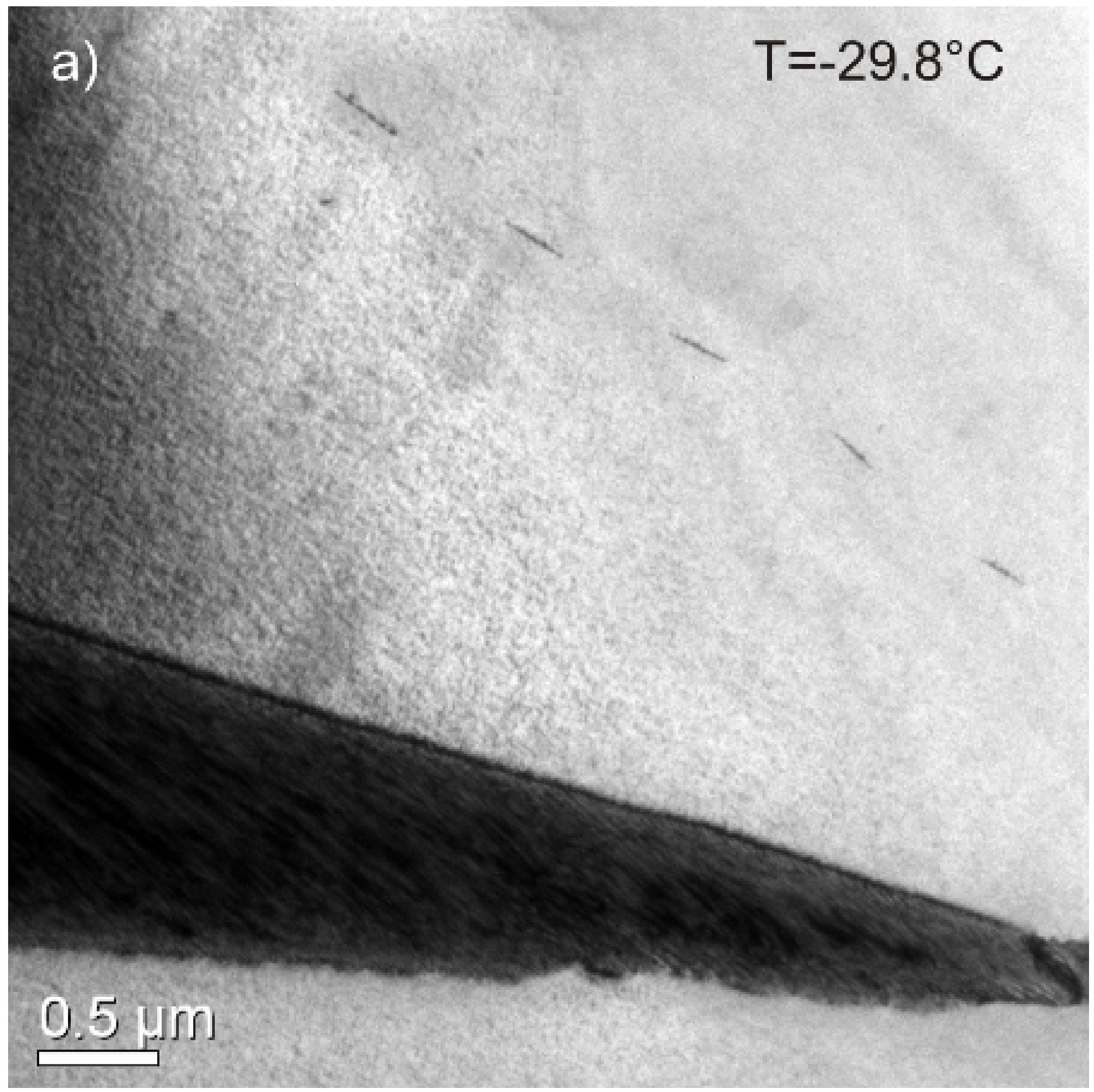


Courtesy J. Frenzel and M. Wagner, Ruhr-University Bochum

... is related to the evolution of microstructure!

In-situ TEM thermal cycling of Ni50.4Ti49.6

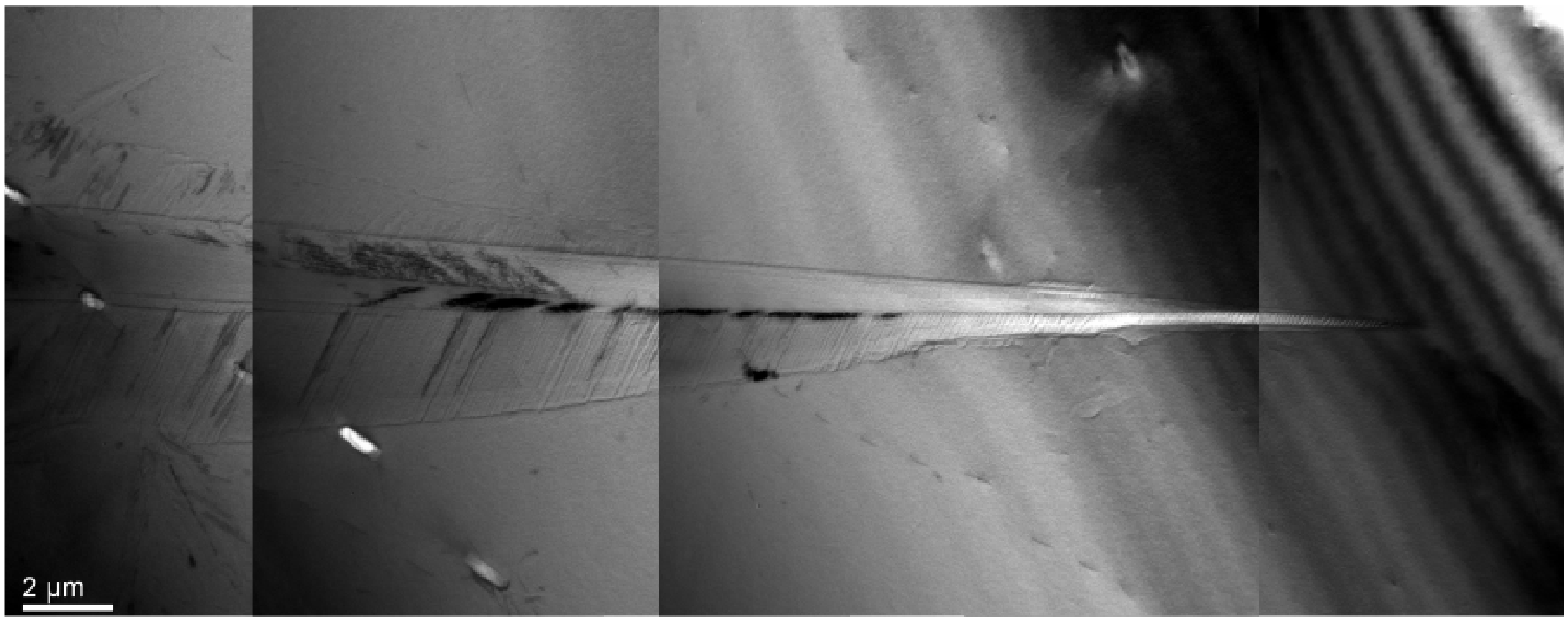
Martensite wedge growth upon cooling



Courtesy T. Simon and Ch. Somsen, Ruhr-University Bochum

In-situ TEM thermal cycling of Ni50.4Ti49.6

Same locus after reverse transformation: Dislocation mark



Courtesy T. Simon and Ch. Somsen, Ruhr-University Bochum

MD simulation method

MD method in a nutshell

Aim: Calculation of the phase space trajectories $\{\mathbf{x}_\alpha, \dot{\mathbf{x}}_\alpha\}$ *for an ensemble of* $\alpha = 1 \ldots N$ *atoms*

Classical approach:

- *Atoms considered as masspoints,*
- *Continous energy*

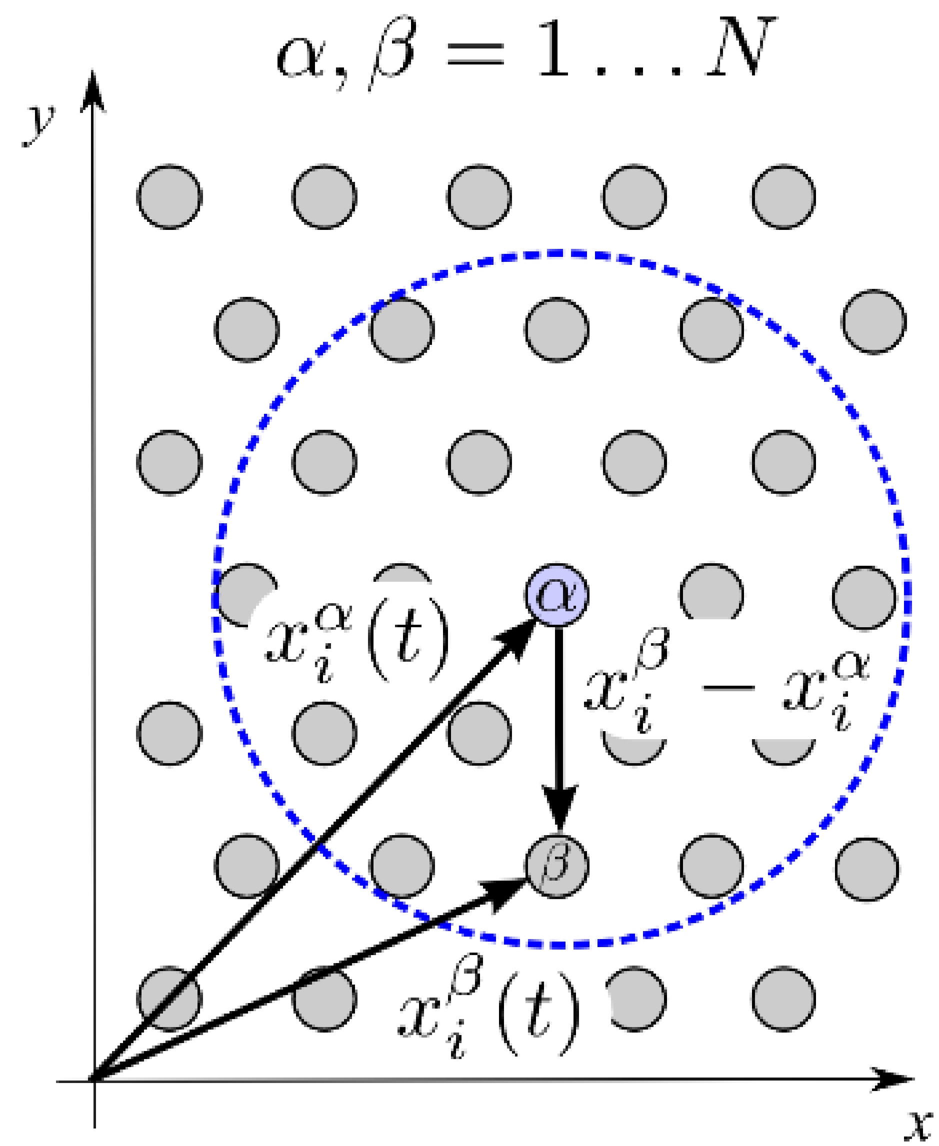
Newtonian Equations of Motion:

$$m_\alpha \ddot{\mathbf{x}}_\alpha = \mathbf{f}_\alpha$$

$\mathbf{f}_\alpha = -\nabla_\alpha V_\alpha^{\mathrm{int}}$ *interaction force acting on* α

Required:

- *Potential interaction energy*
  Pairpotentials: L-J, Toda, Morse
  Many-body potentials: EAM, DFT-based, BOP
- *Initial conditions*



Interaction neighbourhood

Numerical computation is required. *Solution: Thermodynamic process*

Direct quantities: Potential & kinetic energy

Potential energy of individual atoms

$$V_\alpha^{\mathrm{int}} = \sum_{\beta \in r_c} \Phi_{\alpha\beta}(r_{\beta\alpha(t)})$$

Kinetic energy:

- *of interaction neighbourhood's mass centre* $\mathbf{x}_S$

$$E_S^{\mathrm{kin}} = {}^{\mathrm{m_S}}/_{2}\mathbf{v}_S^2$$

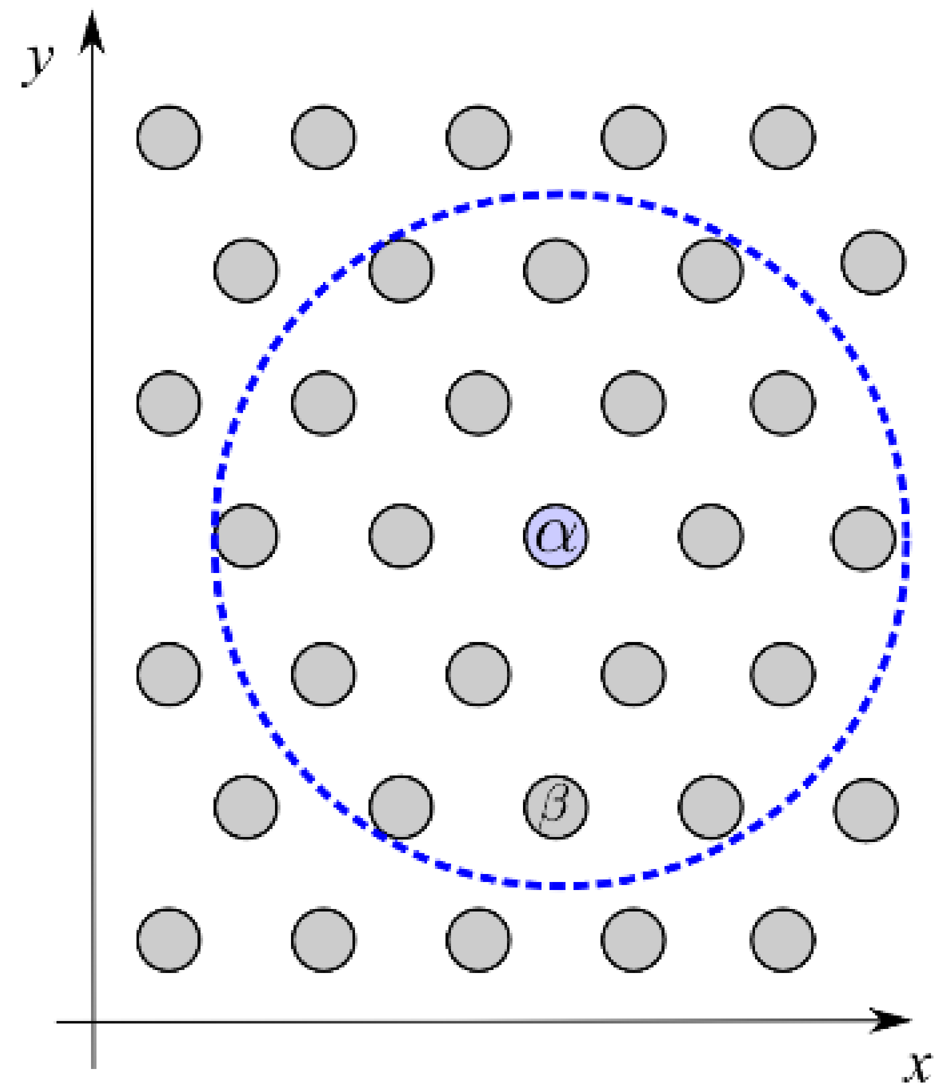
with $\mathbf{v}_S = \sum_{\beta \in r_c} {}^{\mathrm{m}_\beta}/_{\mathrm{m_S}} \dot{\mathbf{x}}_\beta$

- *of devitoric fluctuations about* $\mathbf{x}_S$

$$E_\alpha^{\mathrm{kin}} = {}^{\mathrm{m}_\alpha}/_{2}\left(\dot{\mathbf{x}}_\alpha - \mathbf{v_S}\right)^2$$

Temperature:

$$\frac{f}{2} k_B T = \frac{1}{N_C} \sum_{\beta \in r_c} \frac{m_\beta}{2} \left(\dot{\mathbf{x}}_\alpha - \mathbf{v_S}\right)^2$$



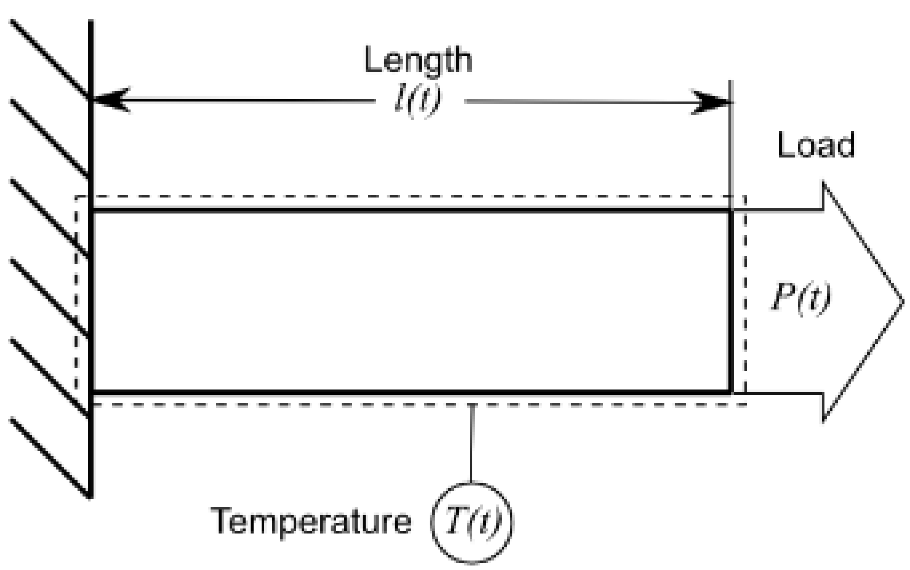
Interaction neighbourhood

Indirect quantity: Free energy

Two approaches:

Macroscopic approach:
Integration of MD-measured load-strain isotherms P(l, T) using Gibbs' Equation

$$F(T,l) = F_0(T,l_0) + \int_{l_0}^{l} P(T,\hat{l})\, d\hat{l}$$



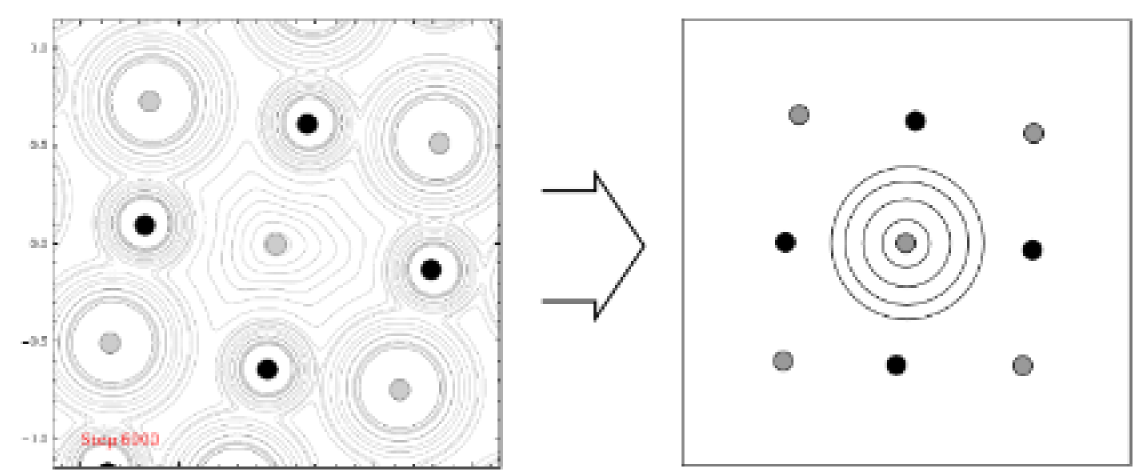
Finite-sized crystals, fully-unharmonic

Microscopic approach:
Statistical mechanics: Partition function
Analytic evaluation possible in the harmonic limit.

Mean atomic internal energy

$$\frac{F}{N} \approx \varepsilon_0 + k_B T - T\, k_B \left\{ \ln T + \ln \frac{2\pi k_B T}{\lambda} \right\} + C(T)$$

Mean atomic entropie



Infinite, perfect crystals, harmonic limit

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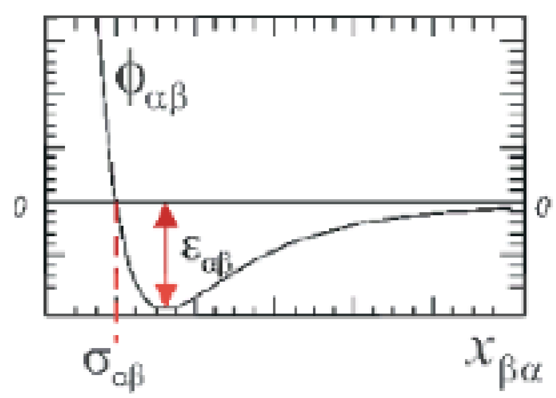
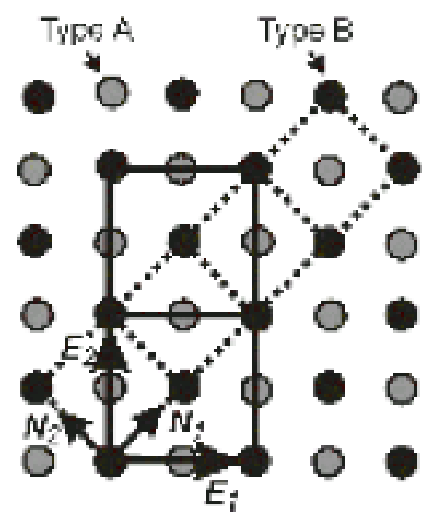
2D Lennard-Jones crystals

Binary Lennard-Jones crystals in 2D

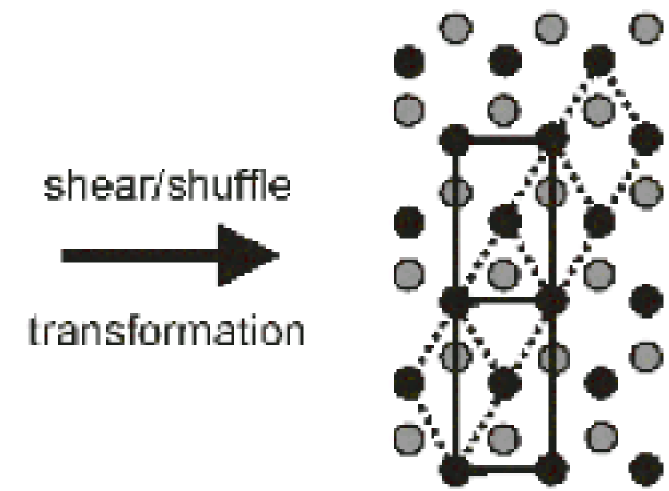
Generic L-J pair potential



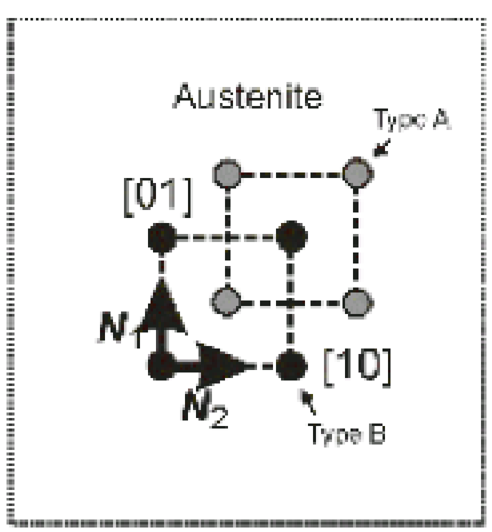
"High-T stable austenite"

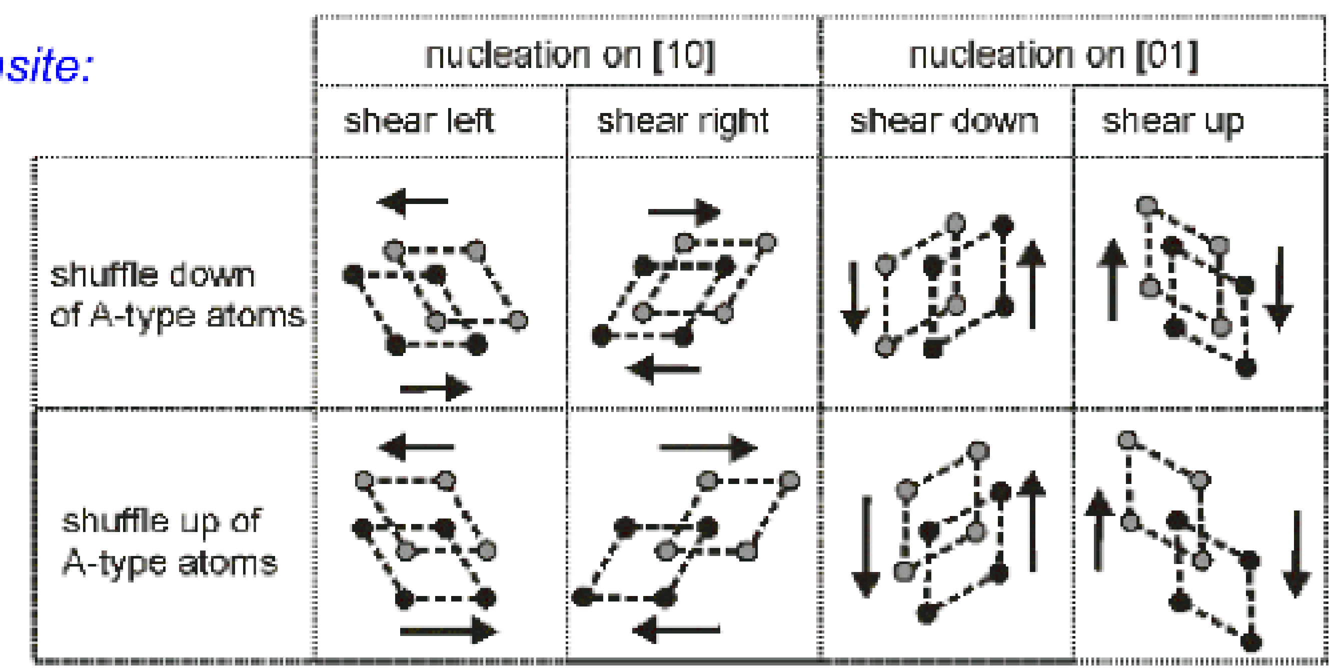


Low-T stable martensite



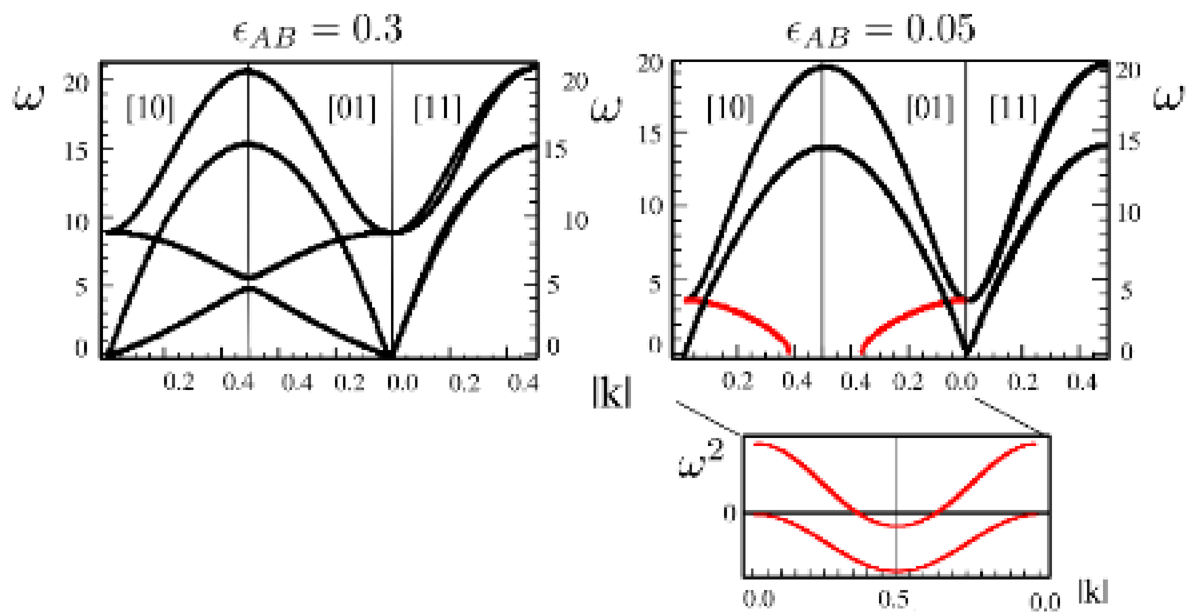
8 Variants of martensite:





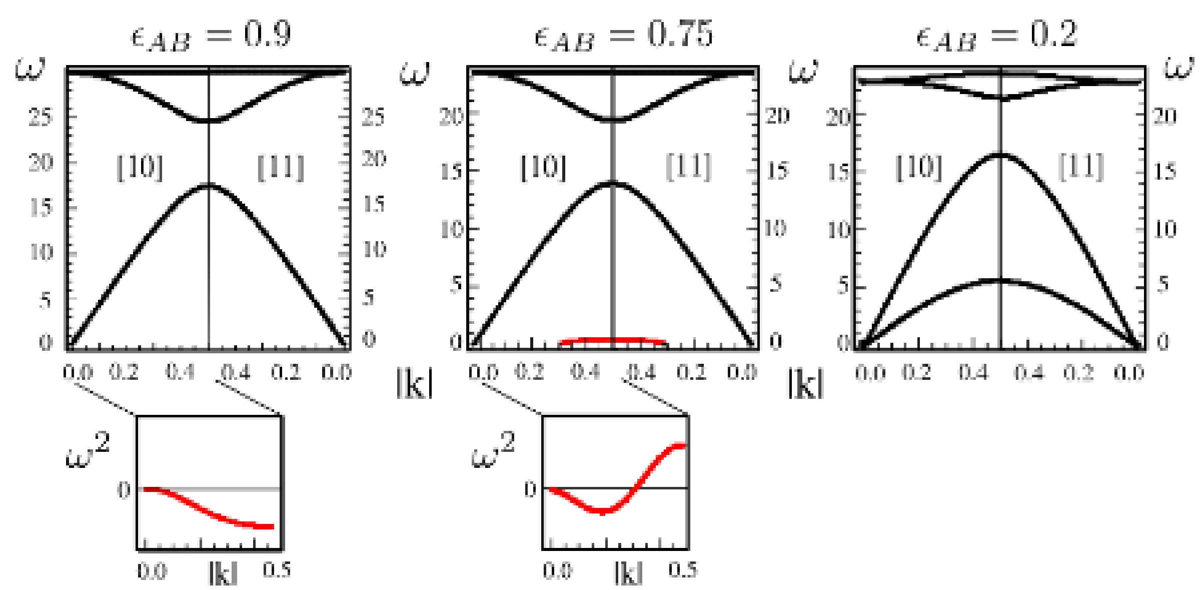
Mechanical stability

Austenite



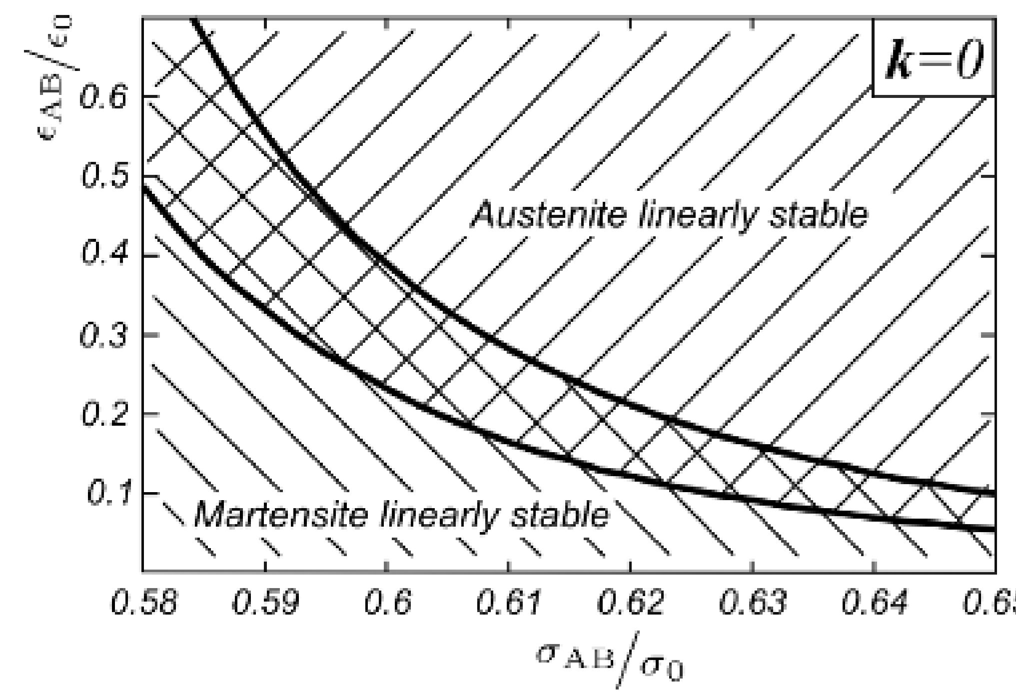
decreasing I-parameter ε_{AB}

(all remaining constant)



Martensite

"Phonon Stability map"



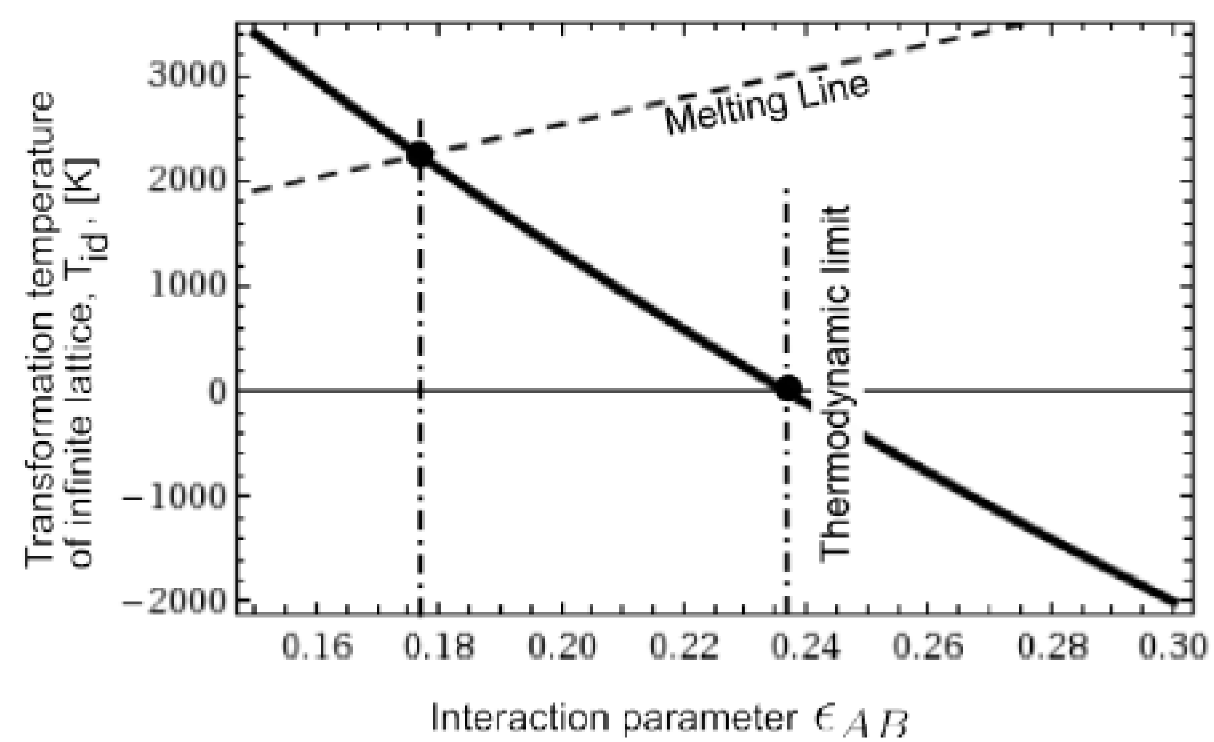
Thermodynamic stability

At equilibrium:

$$f_{\mathrm{aust}}(T) \;=\; f_{\mathrm{mart}}(T)$$

$$e_{\mathrm{aust}} - k_B T \ln \frac{2\pi k_B T}{\lambda_{\mathrm{aust}}} \;=\; e_{\mathrm{mart}} - k_B T \ln \frac{2\pi k_B T}{\lambda_{\mathrm{mart}}}$$

$$T_E \;=\; \frac{e_{\mathrm{aust}} - e_{\mathrm{mart}}}{k_B \ln \lambda_{\mathrm{mart}} / \lambda_{\mathrm{aust}}}$$



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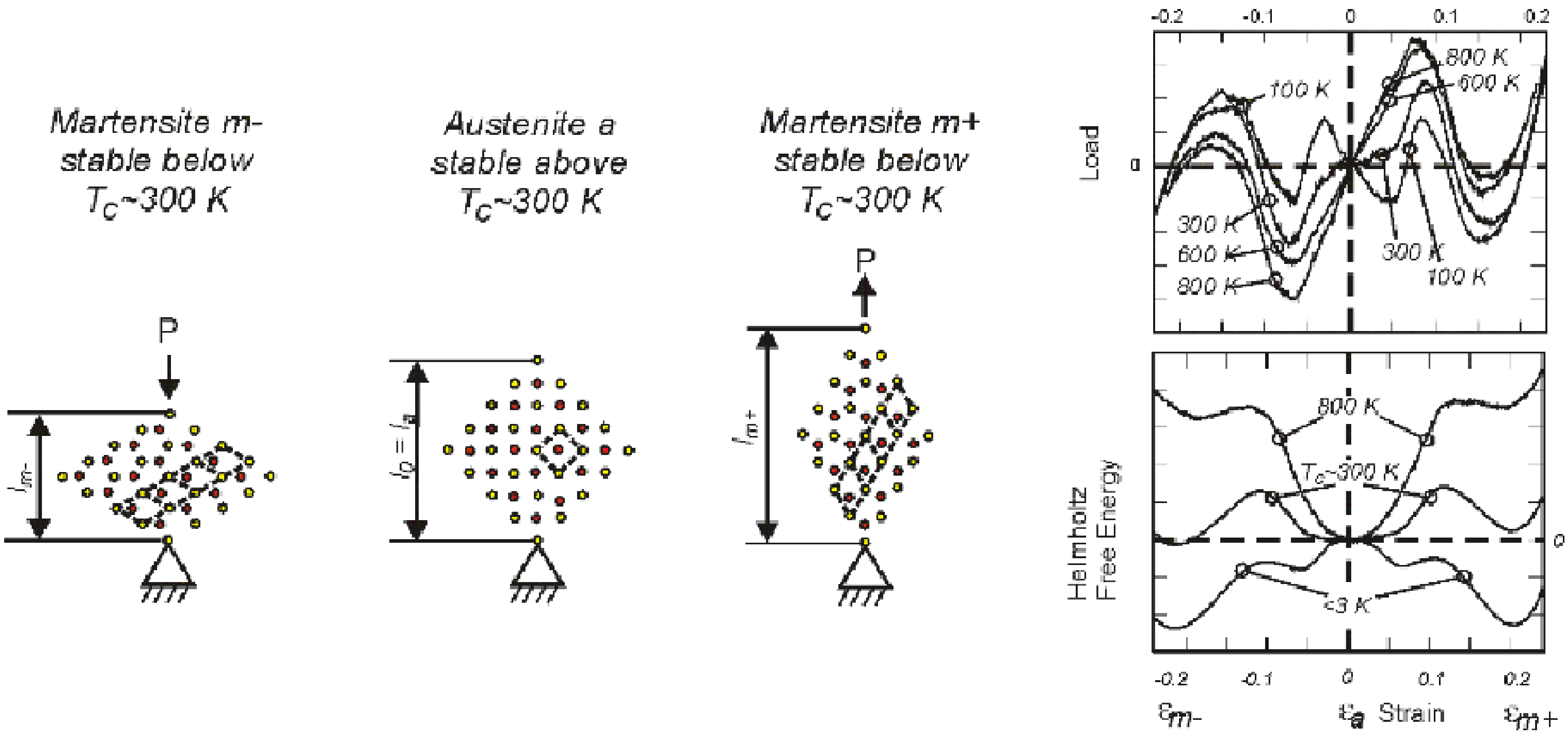
Properties of small assemblies

Thermodynamics of a small 41-atomic system



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Microstructure formation in extended crystals

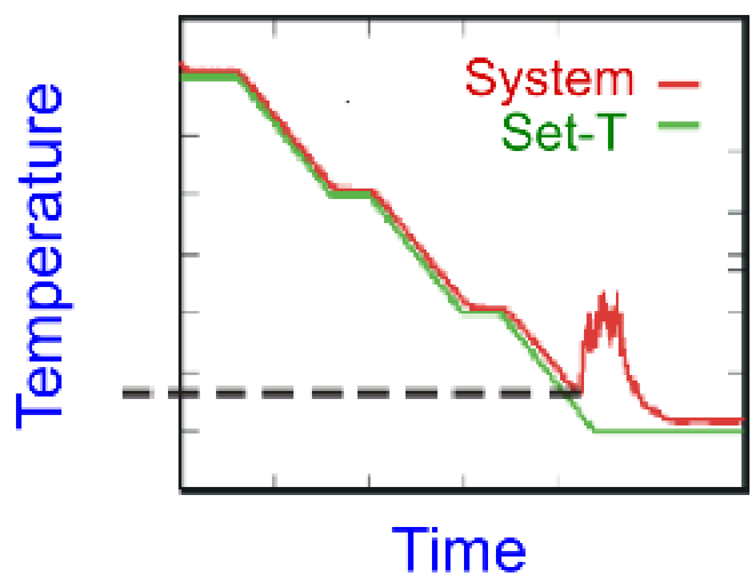
Nucleation and growth of MT in a 2D bar

10,000 atom bar

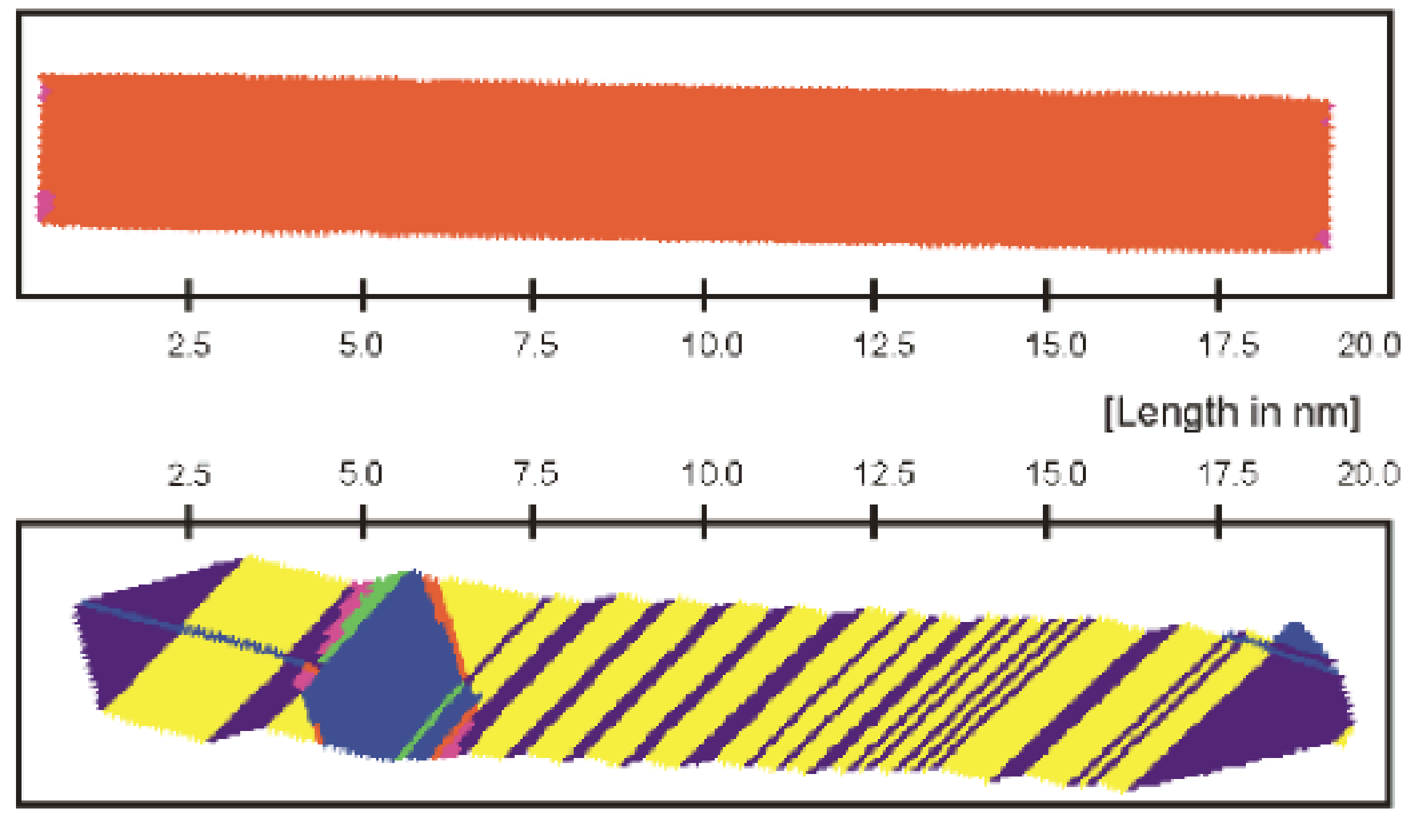
Thermostat

Free Surface

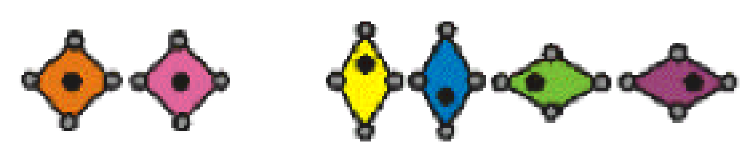
Parallel Computation



Initial configuration: Austenite at 400 K



Martensitic twin structure at 100 K



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Bar video

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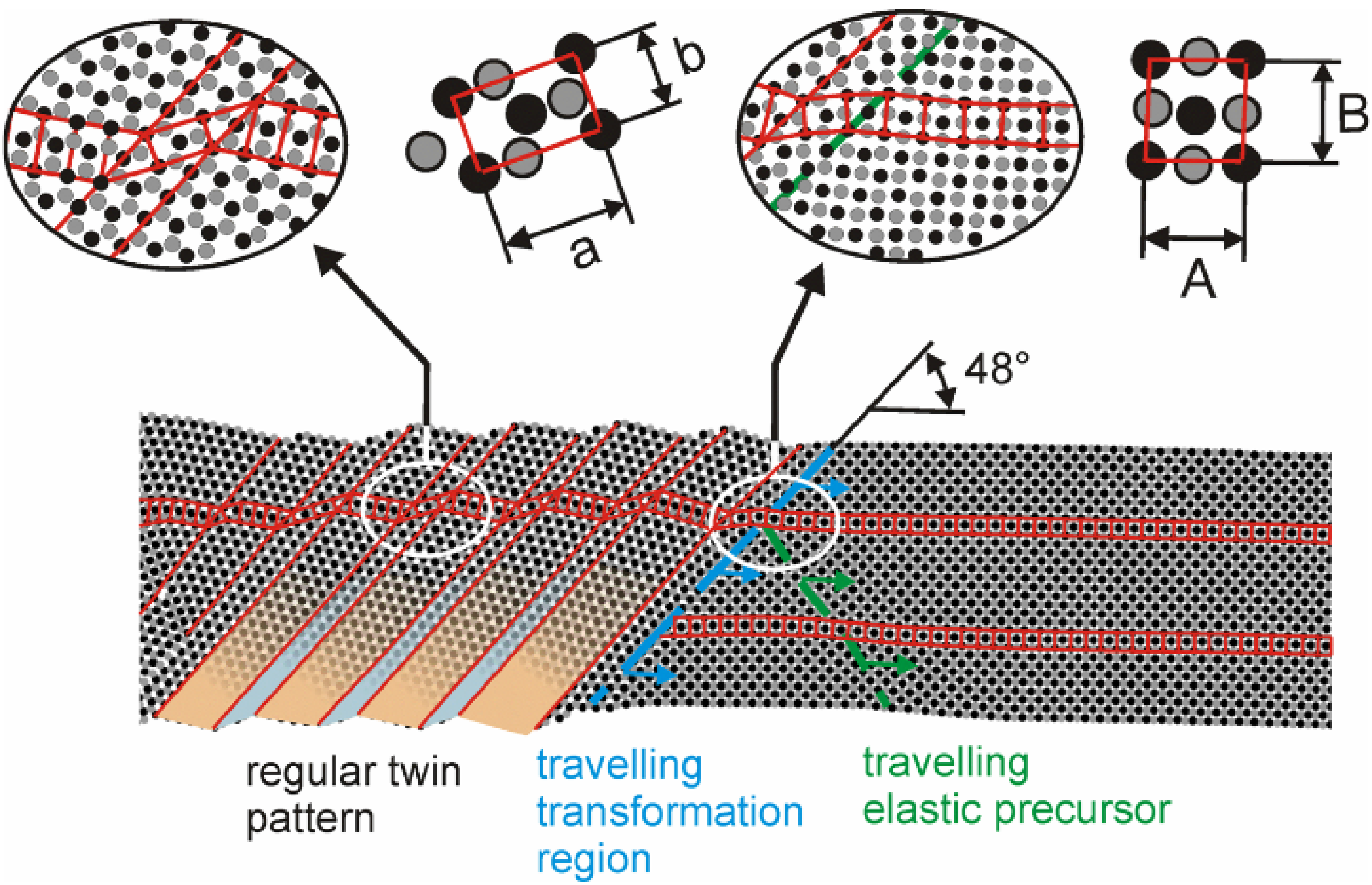
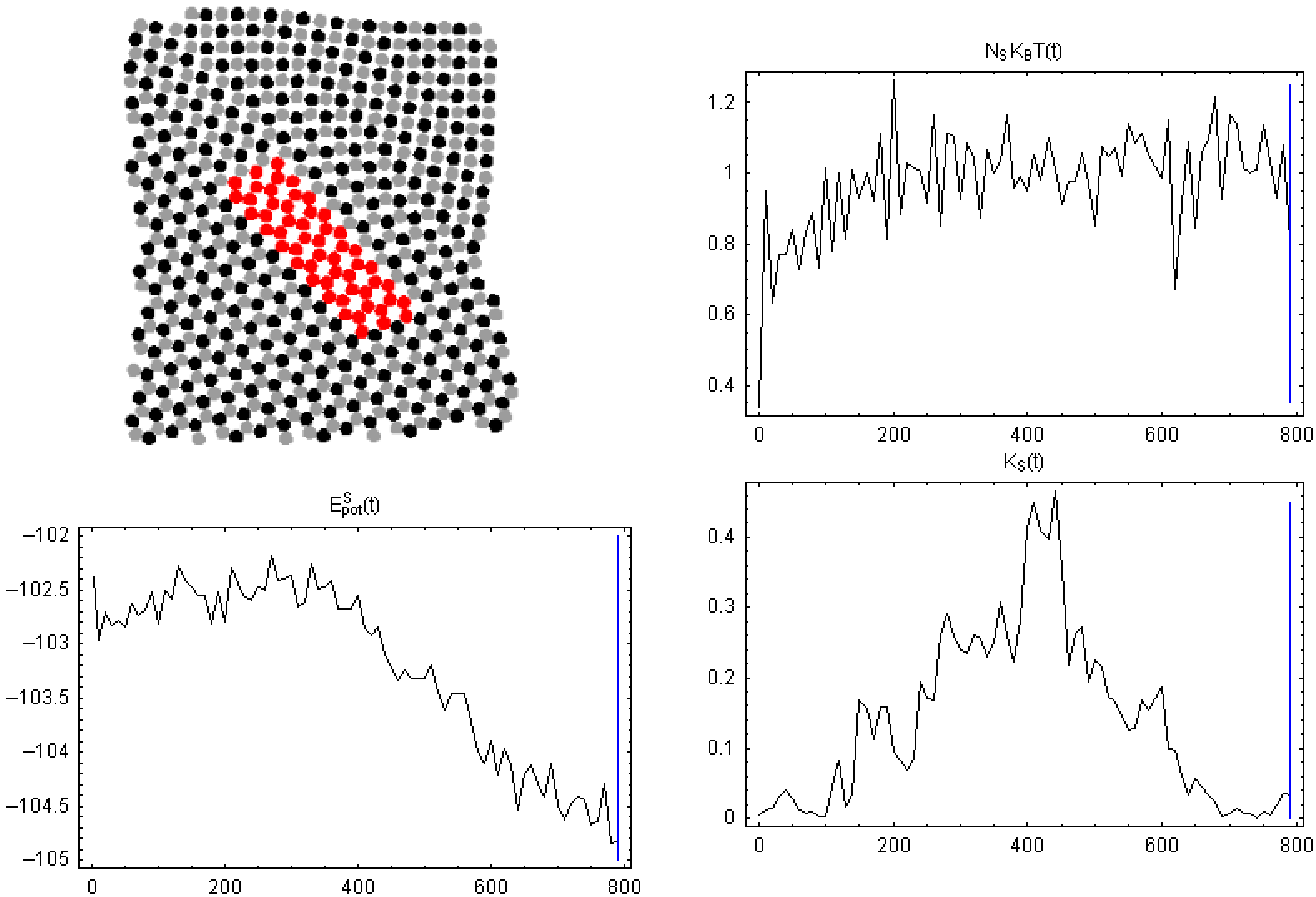
Bar details



Transformation kinetics of a crystallographic layer



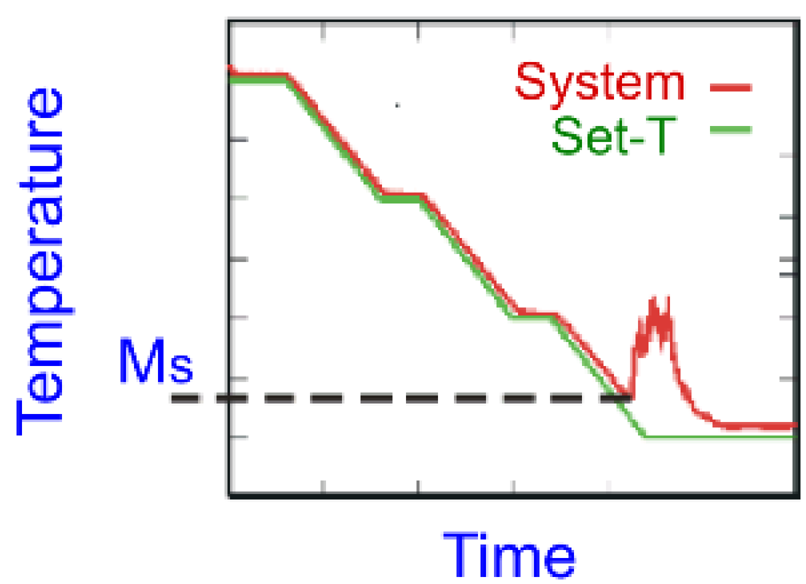
Nukleation and growth of MT in a 2D quad

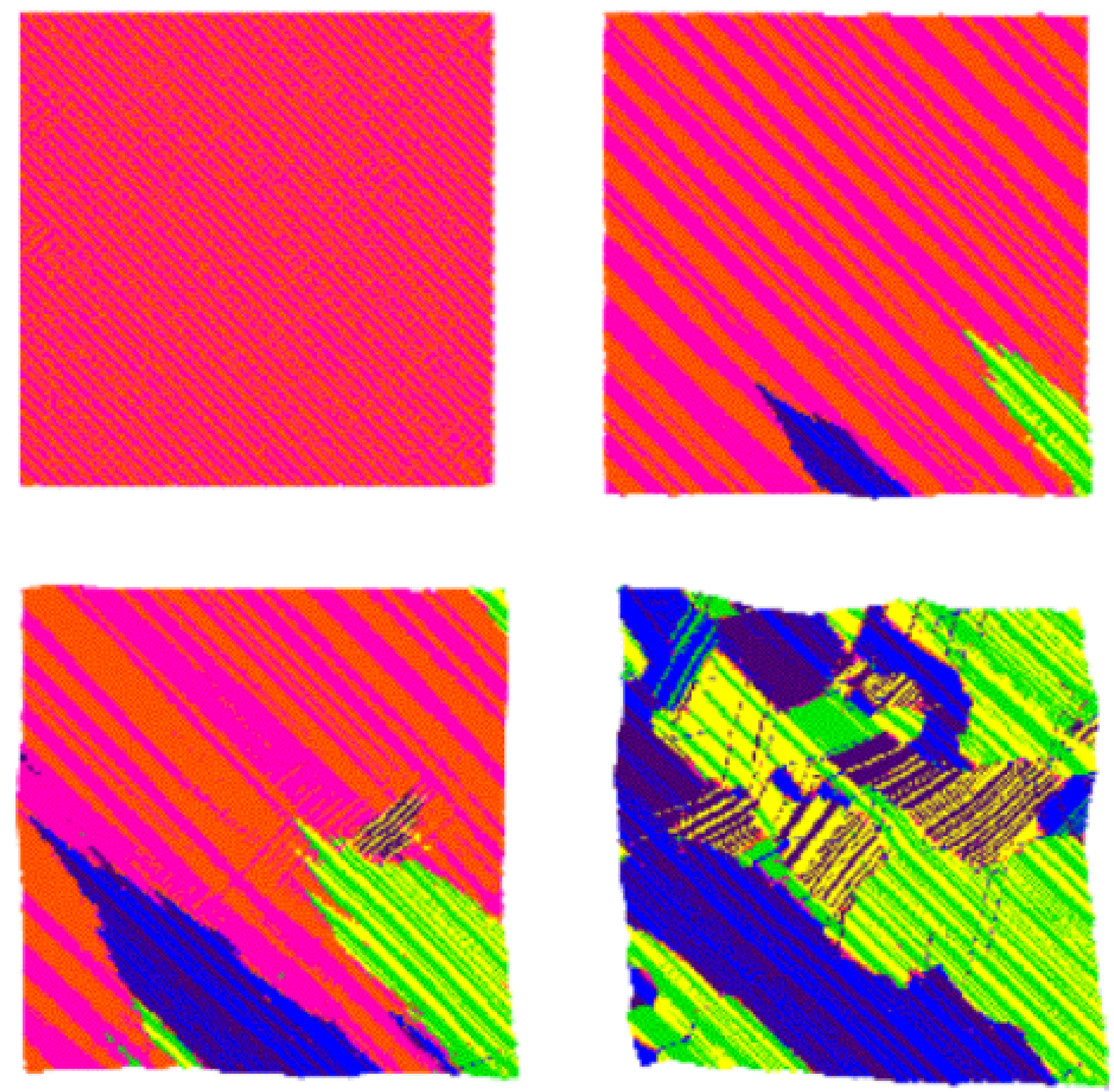
262,144 atom quad

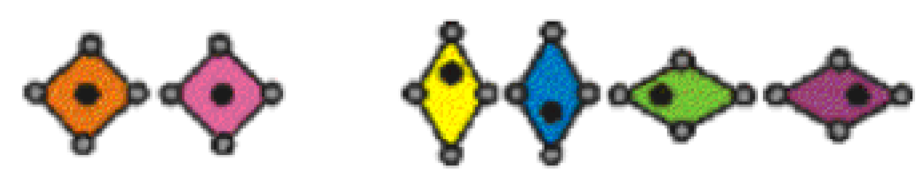
Thermostat

Free Surface

Parallel Computation







...Video...

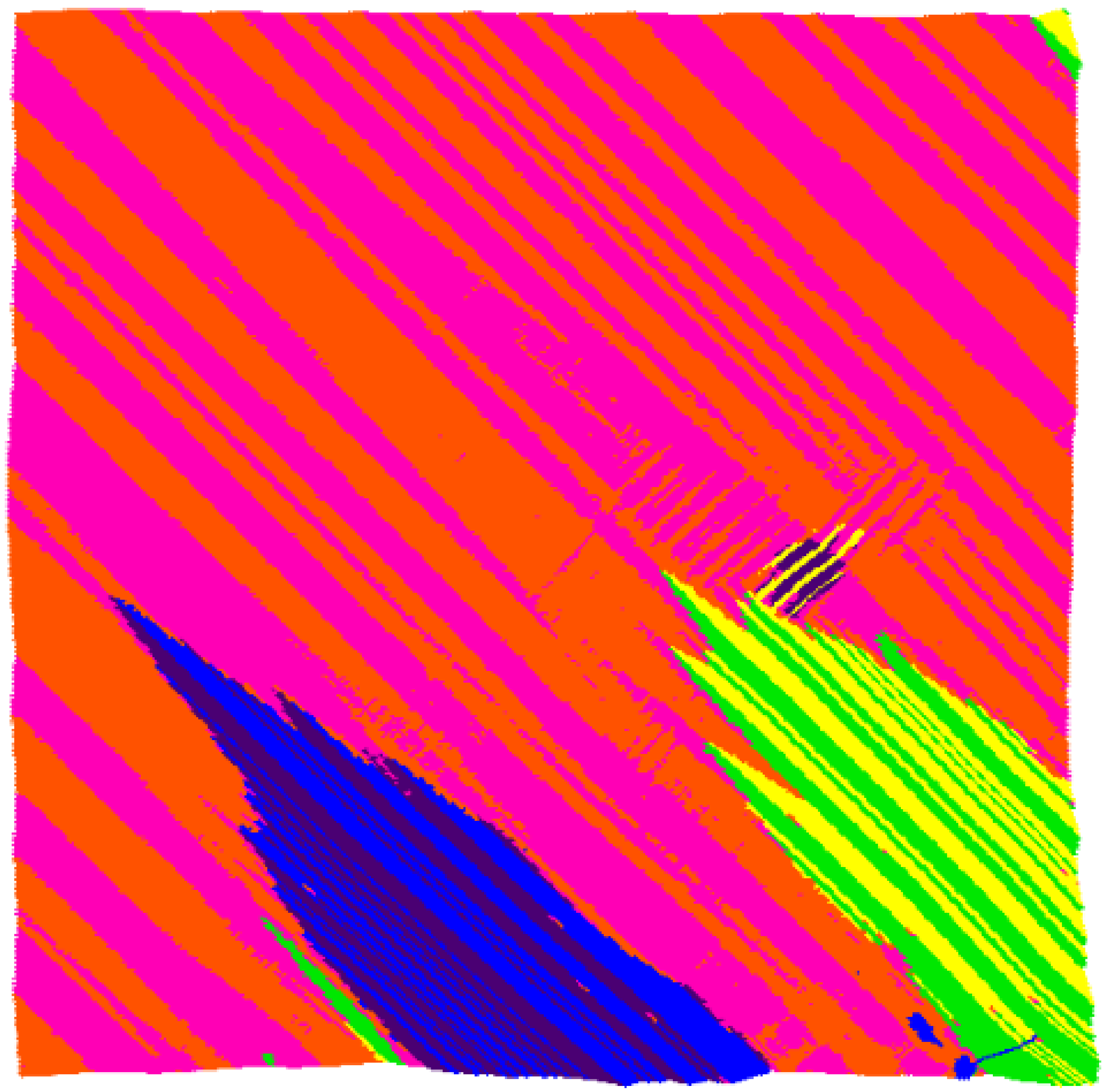


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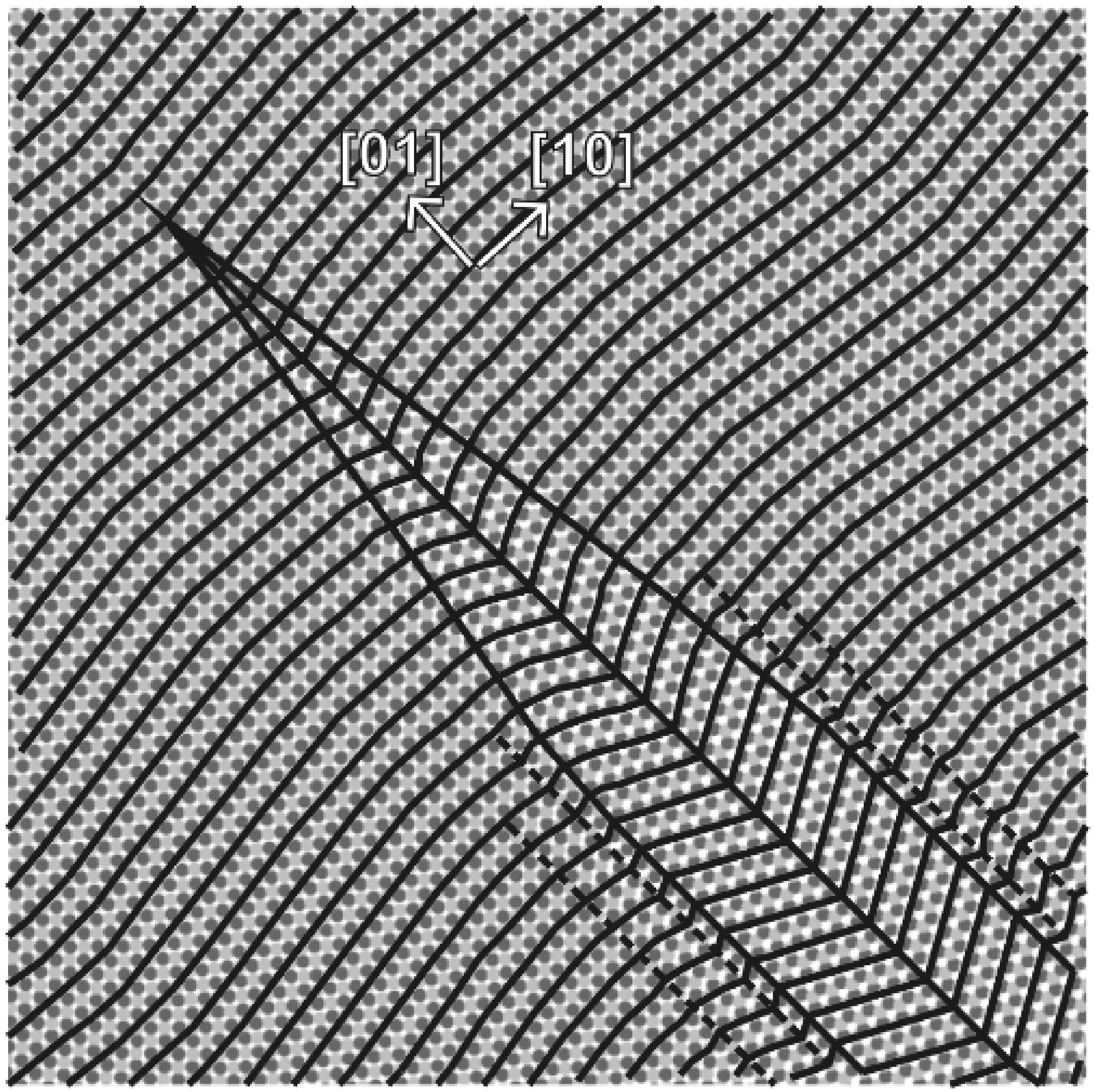
Plate growth I



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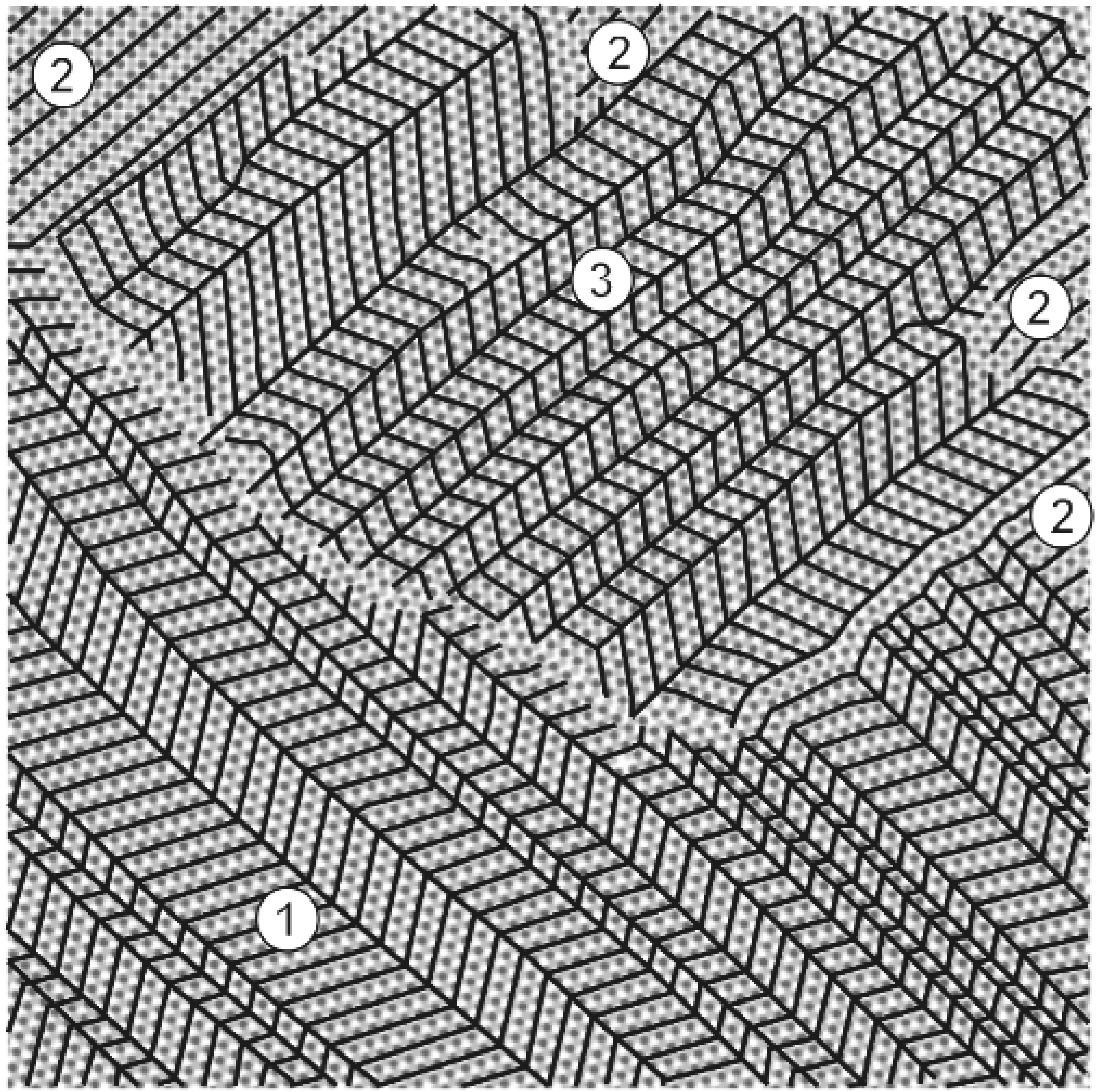
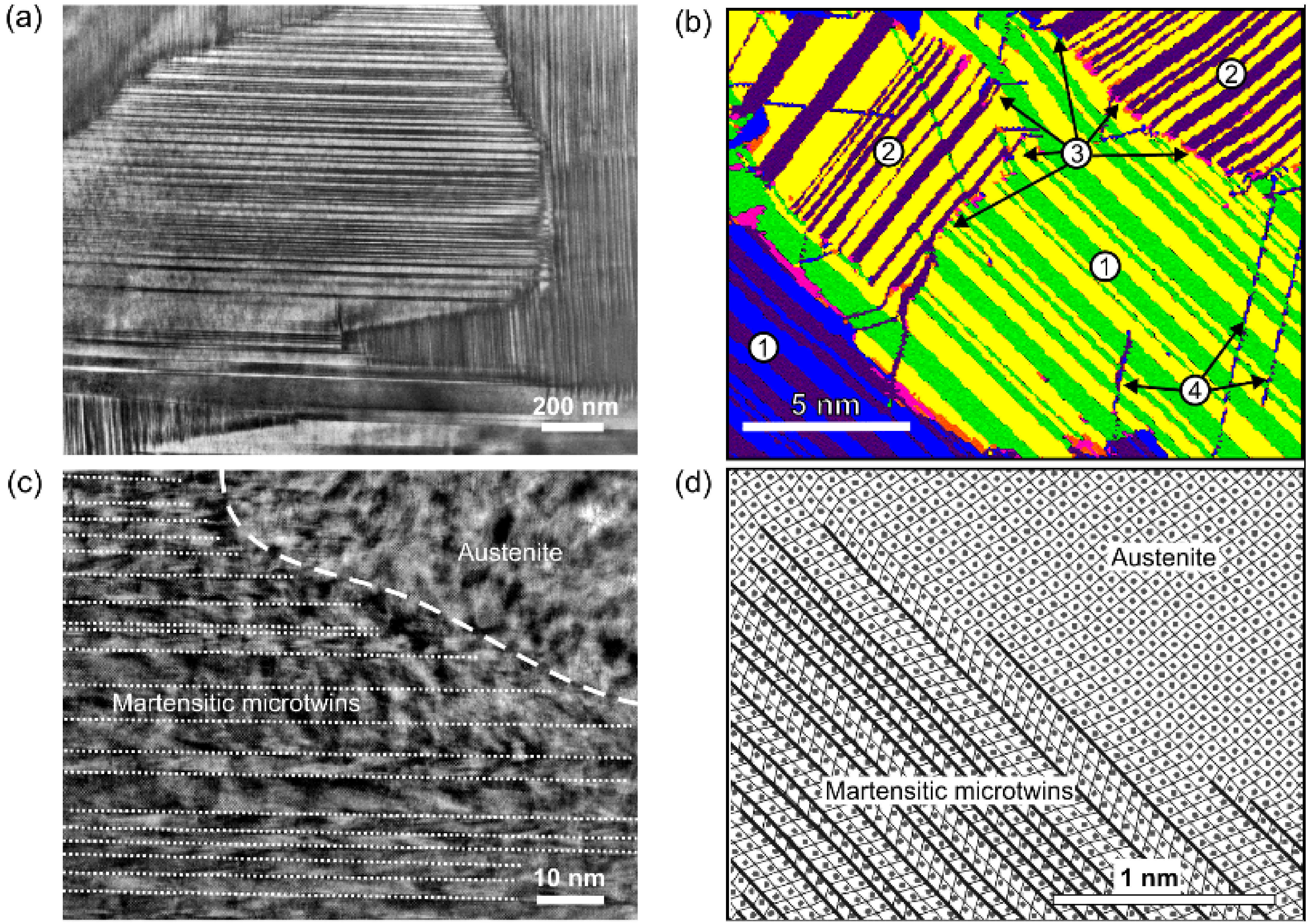
Domain formation III



Significance



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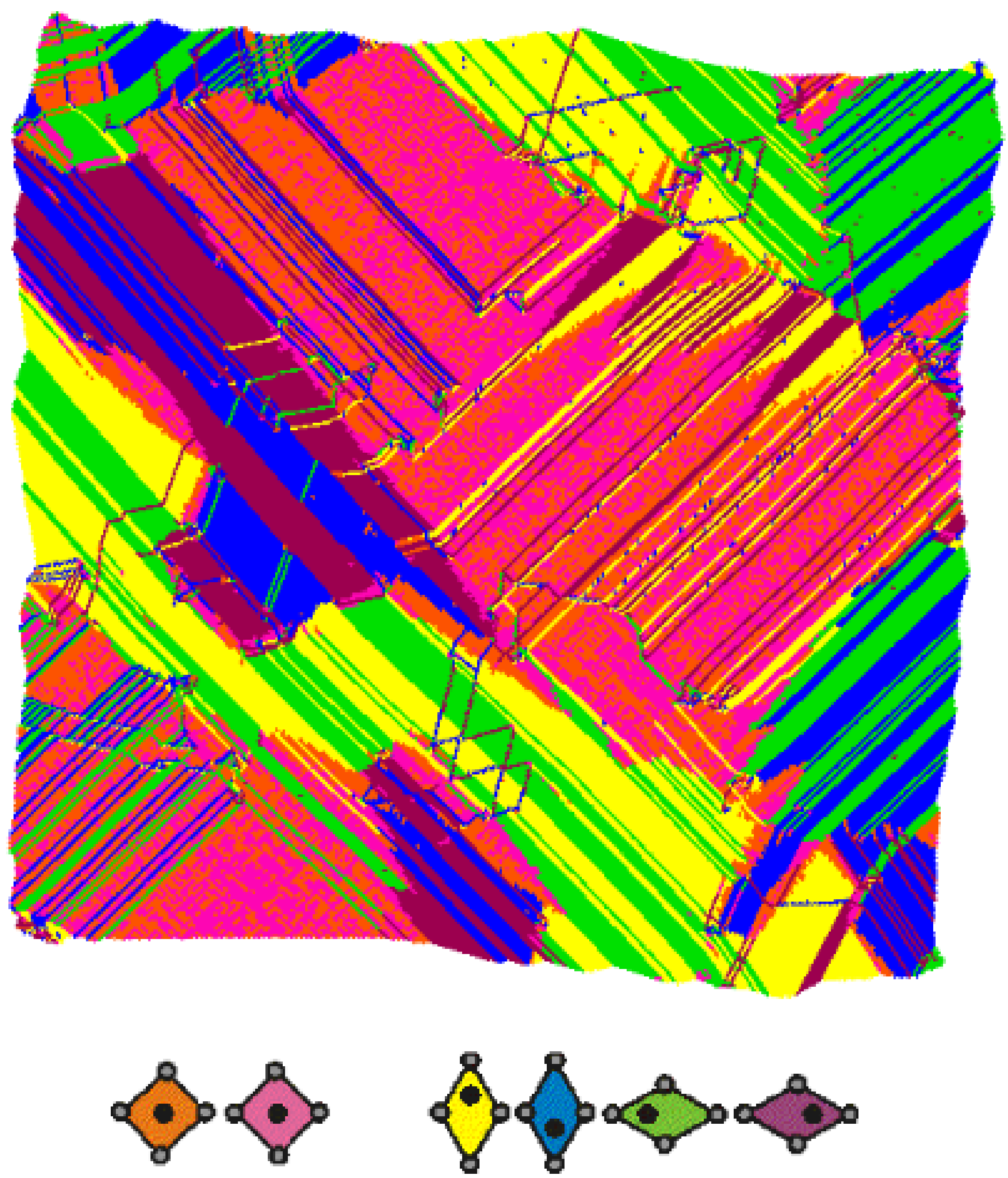
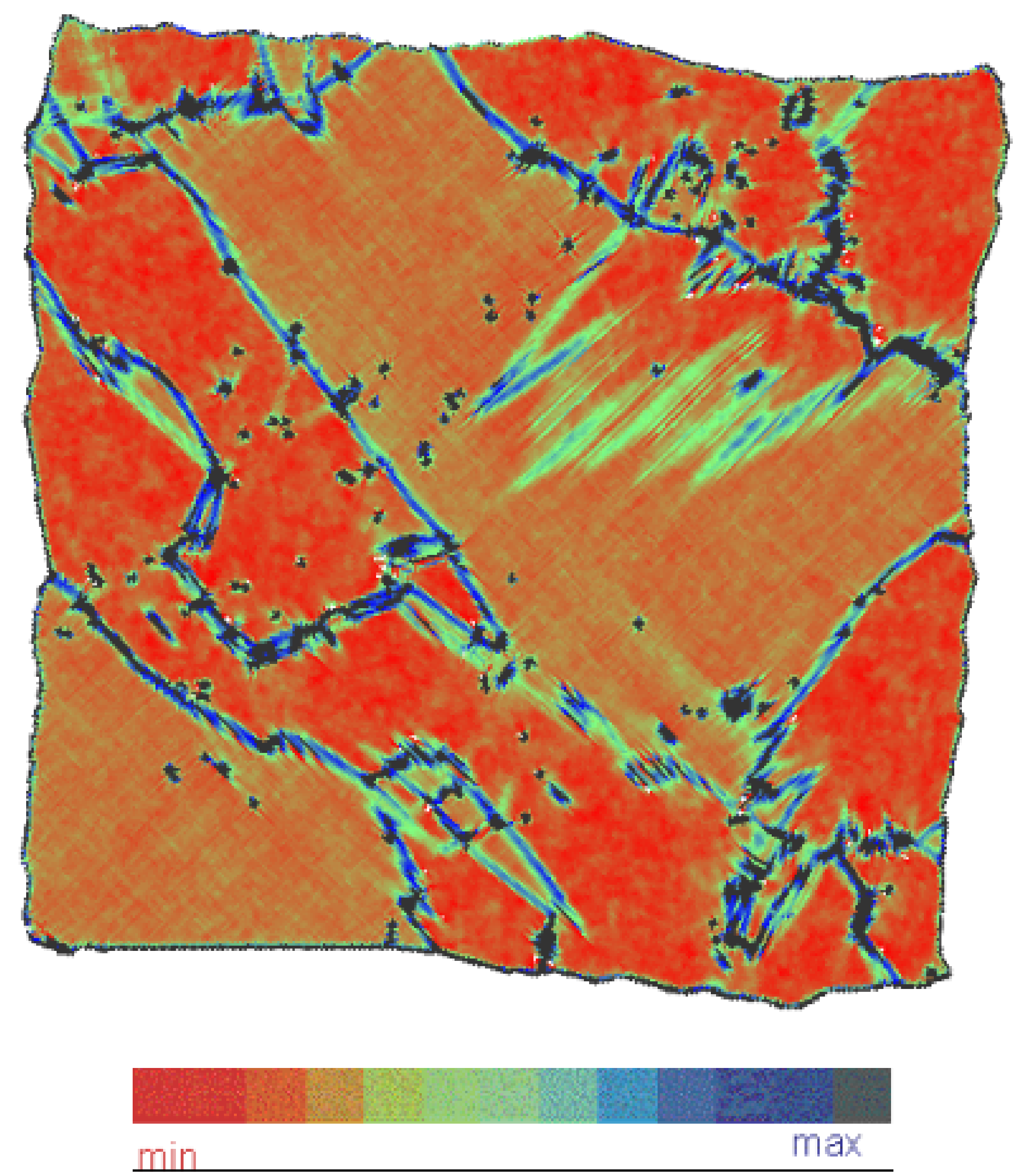
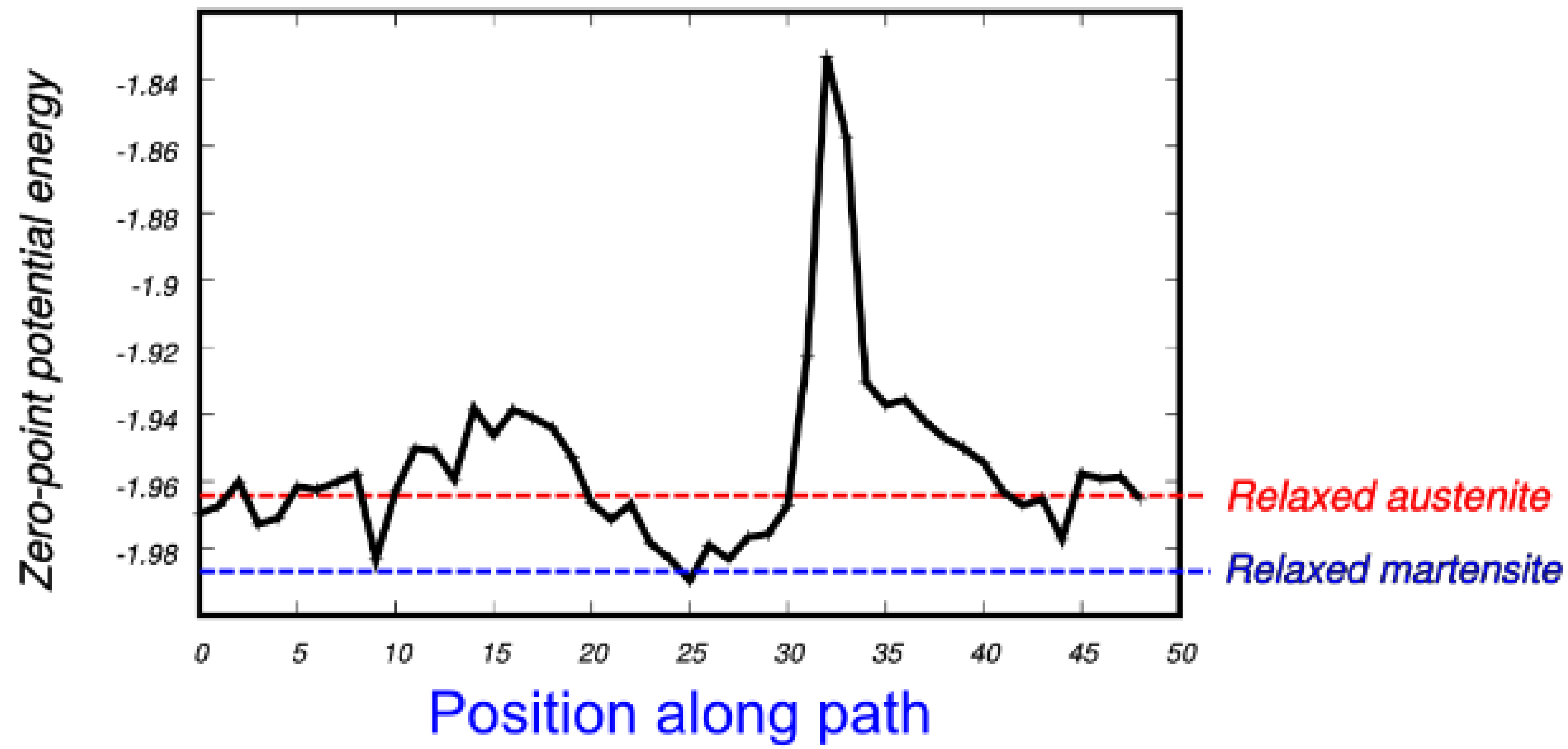
Microstructure evolution and hysteresis

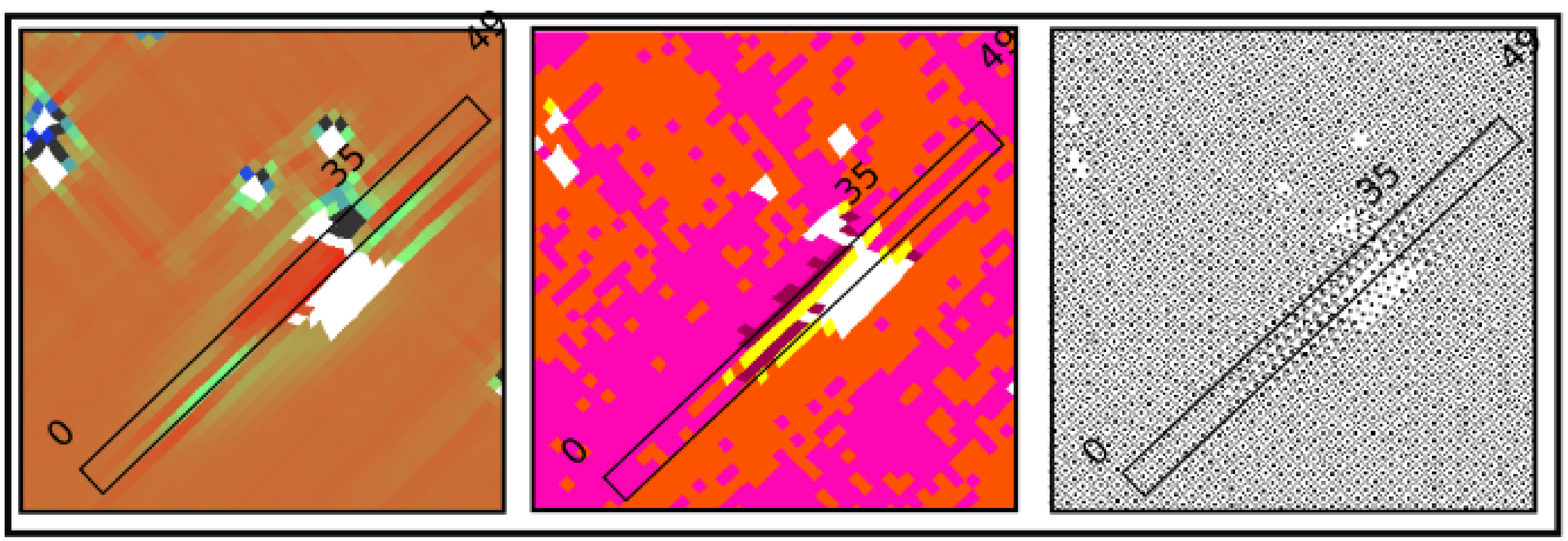
Video: Reverse transformation of a 160,000 atom quad



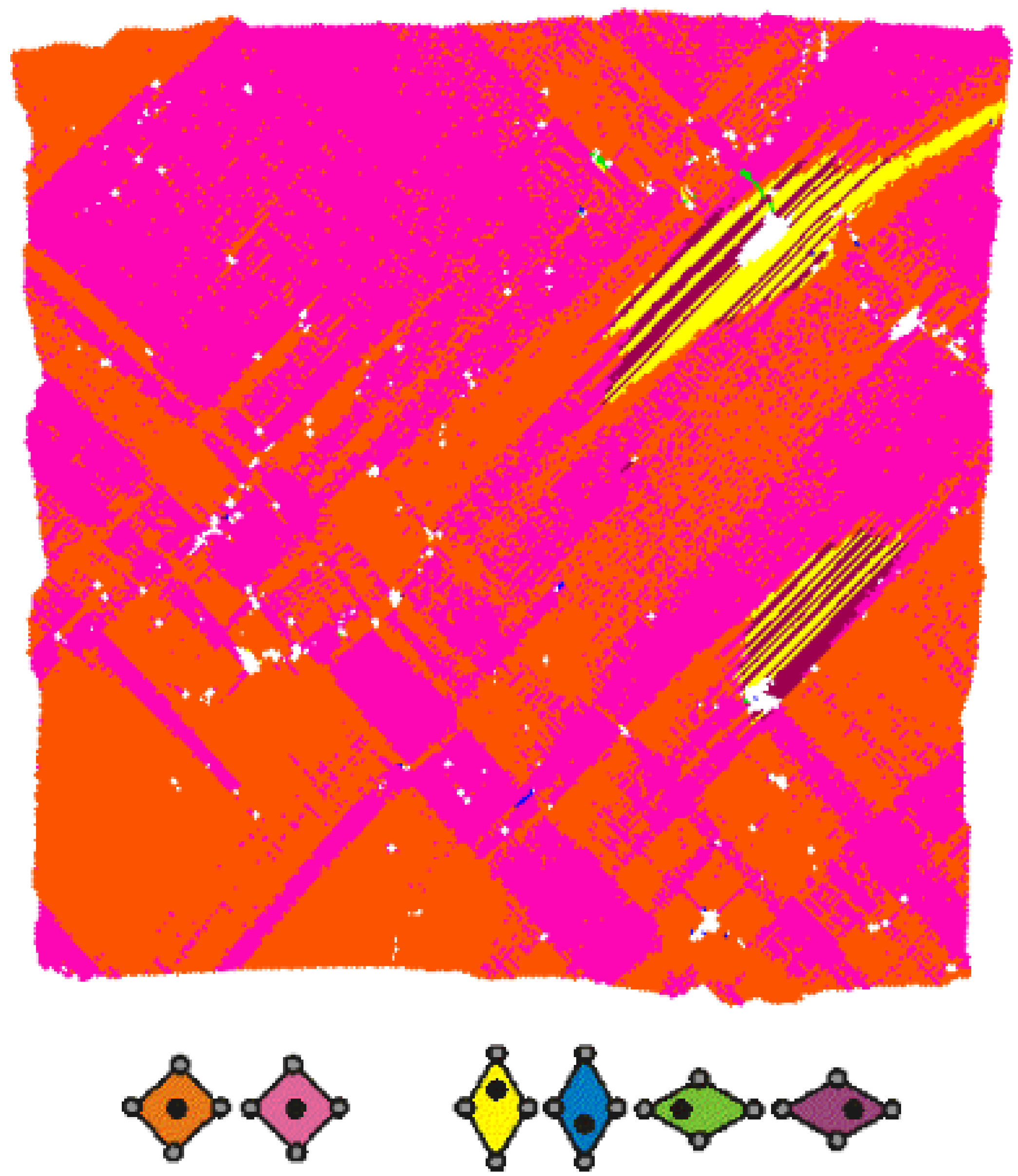


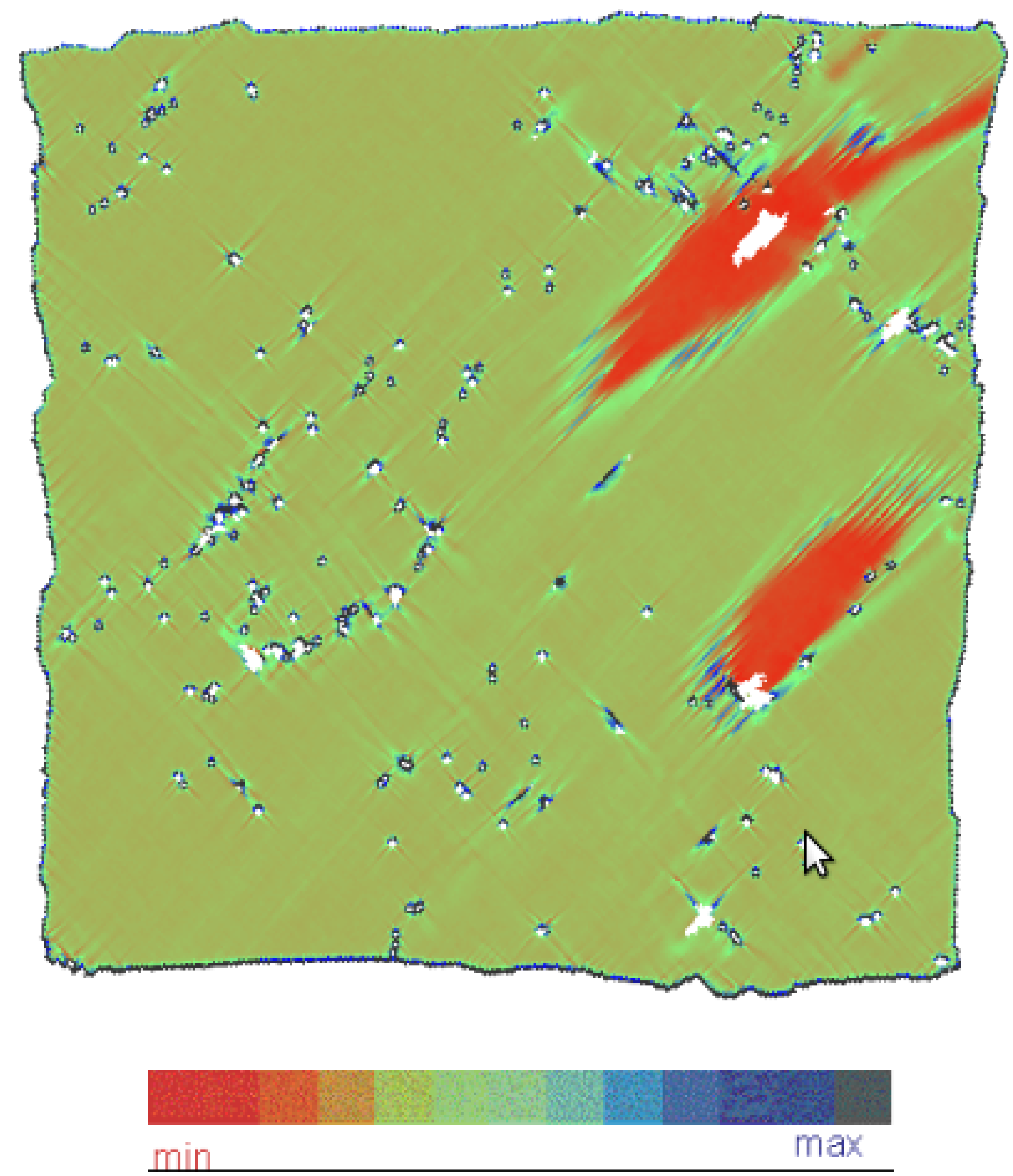
Potential energy across defect





Video: Second transformation cycle





Five cyclic transformations and reverse transformations

Cycle I | *Cycle II* | *Cycle III* | *Cycle IV* | *Cycle V*