Atomistic modeling of austenite-ferrite interface migration in pure iron

O. Nakonechna [1*], H. Zapolsly[1], F. Danoix[1], M. Gouné[2], D. Huin[3]

(olha.nakonechna2@univ-Rouen.fr)

[1] Groupe de Physique des Matériaux (GPM)

[2] ICMCB – UPR CNRS 90481,87 Avenue du Docteur Schweitzer, 33608 Pessac, France

[3] ArcelorMittal research SA, voie romaine, 57 280 Maizières Les Metz, France

17th ALEMI Meeting: July 5-6, Metz, France

Introduction

- Quasi-particles approach: Theory and Modeling.
- Application for austenite to ferrite phase transformation.
- Conclusion & perspectives

Introduction

Mechanical properties of steels are determined by their microstructure features.

- volume fraction
- size distribution
- topology and morphology of phases

chemical composition

heat treatment processing

solid-state phase transformations that take place during cooling of steel

Austenite to ferrite phase transformation

Main goal (task):

to understand deeply the mechanism of austenite to ferrite phase transformation (kinetics of ferrite growth) and study the influence of different factors on it.

- ❑ Transformation temperature
- ❑ Chemical composition
- ❑ Moving α/γ transformation interface

Introduction

Atomistic modeling approaches:

❑ Molecular dynamic (MD):

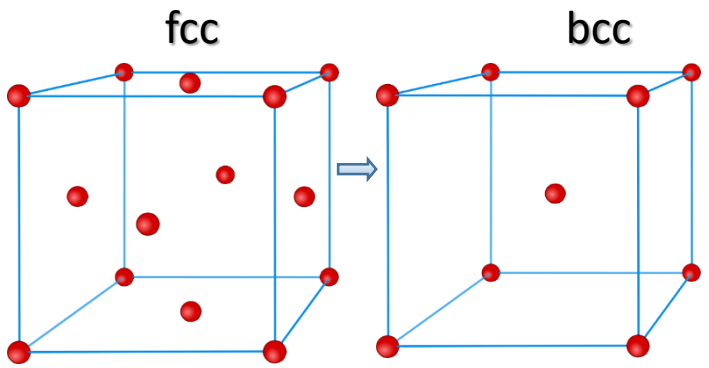
- ∀ atoms : solve motion equation
- Total number of atom is limited
- Time scale second ~10^{-12} second
- Relaxation around equilibrium positions

❑ Monte Carlo (MK):

- Rigid lattice & difficulties to include elastic interactions
- Stochastic method & no geometric relaxation near equilibrium position
- Many configurations should be tested to converge to minimum of free energy.

The austenite to ferrite phase transformation involve two main phenomena:

- ❑ Diffusional process: the redistribution of interstitial and substitutional elements.
- ❑ The change in crystal structure.



Our goal :

- ➢ *Construct atomistic model that be able to reproduce phase transformation at diffusion time scale.*
- ➢ *Provide possibility of moving atoms on a smaller distance than an interatomic distance.*

Outline

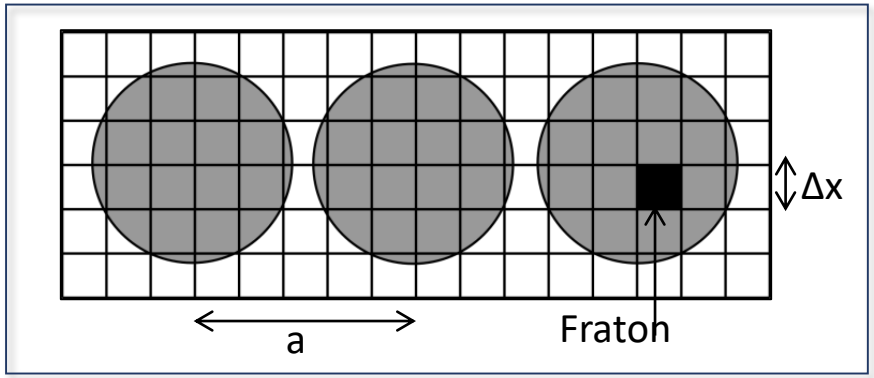
- Introduction
- **Quasi-particles approach: Theory and Modeling**
- Application for austenite to ferrite phase transformation.
- Conclusion & perspectives

Atomic fragment theory (AFT)

A small parameter determining the transition from discrete to continuum version of the ADF model is:

$$\Delta x < a$$

a – lattice parameter; Δx – Ising lattice parameter



Occupation number:

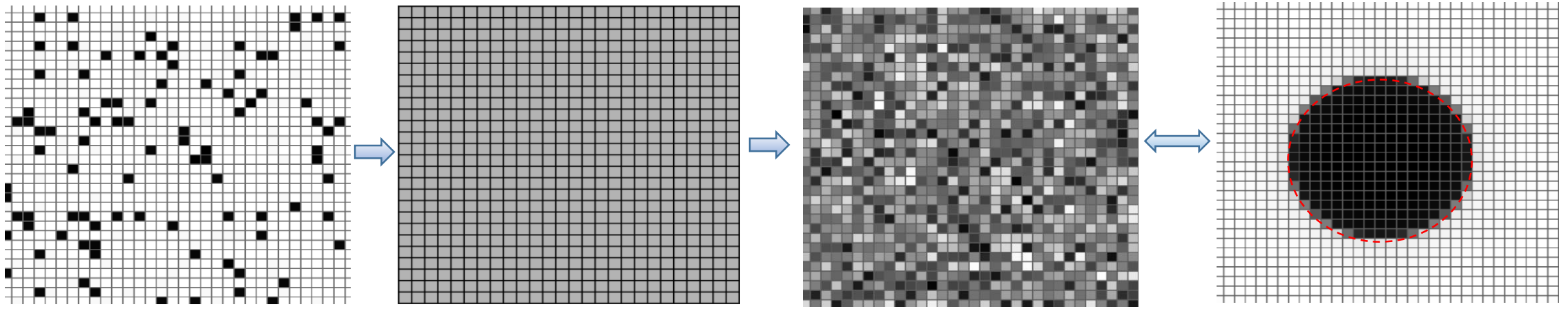
$$c(\mathbf{r}) = \begin{cases} 1 & \text{if site r is within any point of any atom} \\ 0 & \text{if site } \mathbf{r} \text{ is outside of any atom} \end{cases}$$

The occupation probability of finding a **fraton** at the point *r:*

$$\rho(\mathbf{r}) = < c(\mathbf{r}) >_t$$

$$\sum_r \rho_A^{fratons}(\mathbf{r}) = N_A^{fratons}$$

Schematic representation of condensation of randomly distributed pseudo-particles (fratons) in atomic sphere



c(r): ocupation number — ρ(r) homogeneous: liquid — Random fluctuations — ρ(r) heterogeneous

Free energy functional

Free energy functional is:

$$F = \frac{1}{2}\sum_{\alpha}\sum_{\beta}\sum_{\mathbf{r},\mathbf{r}'} w_{\alpha\beta}(\mathbf{r}-\mathbf{r}')\rho_{\alpha}(\mathbf{r})\rho_{\beta}(\mathbf{r}') + k_B T \sum_{\mathbf{r}}\sum_{\alpha}\left[\rho_{\alpha}(\mathbf{r})\ln\rho_{\alpha}(\mathbf{r}) + \left(1-\sum_{\alpha}\rho_{\alpha}(\mathbf{r})\right)\ln\left(1-\sum_{\alpha}\rho_{\alpha}(\mathbf{r})\right)\right]$$

Non-local term

Local term

The pairwise interaction energy of α-β pair of atoms situated at **r** and **r'**: $w_{\alpha\beta}(\boldsymbol{r}-\boldsymbol{r}')$

Model potential

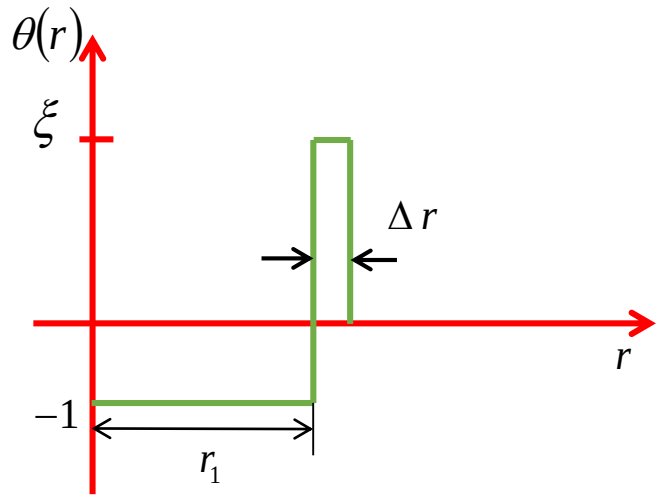
Model potential

$$\tilde{w}_{\alpha\beta}(\mathbf{k}) = \lambda_1 \tilde{w}^{SR}_{\alpha\beta}(\mathbf{k}) + \lambda_2(\mathbf{k})\tilde{w}^{LR}_{\alpha\beta}(\mathbf{k})$$

λ_1 – the strength of the short-range atomic interaction

$\lambda_2(\mathbf{k})$ – the strength of the long-range interaction

Short range potential: $\theta(\mathbf{r})$



r_1 - length parameter determining the atomic radius

Δr - width of the repulsion of fraton-fraton interaction

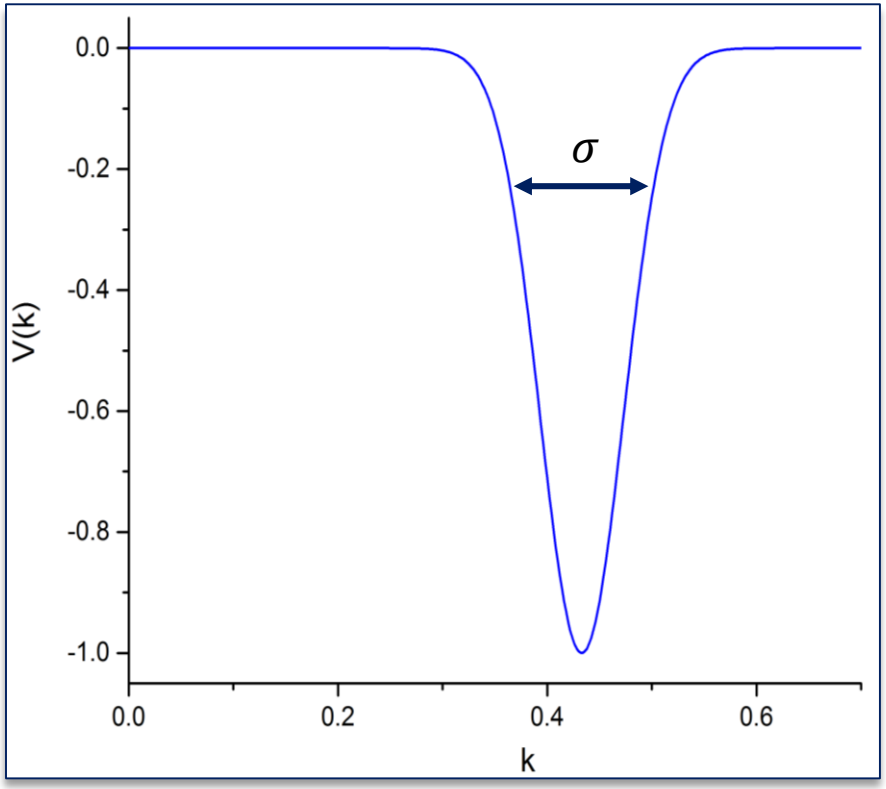
ξ - height of the repulsion part

Long-range potential

Gaussian function: $$f(x) = \exp\left(-\frac{(x-x_0)^2}{2\sigma^2}\right)$$

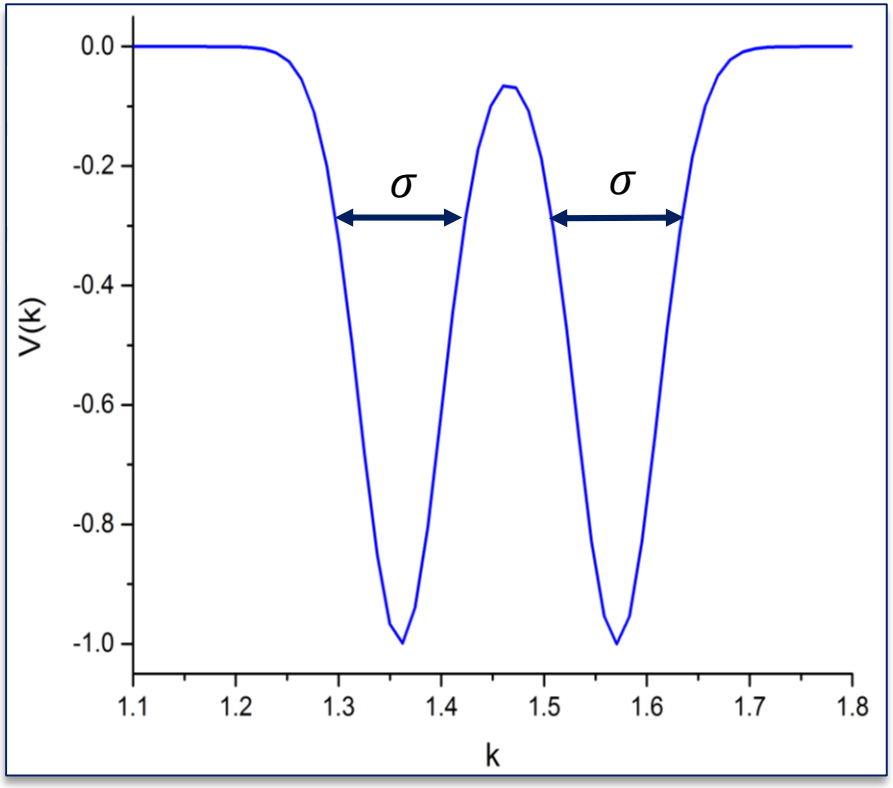
Long-range potential for bcc:

$$\tilde{w}_{LR}^{bcc}(\mathbf{k}) = \lambda_2\left(\exp\left(-\frac{(k-k_{01}^{bcc})^2}{2\sigma^2}\right)\right)$$



Long-range potential for fcc:

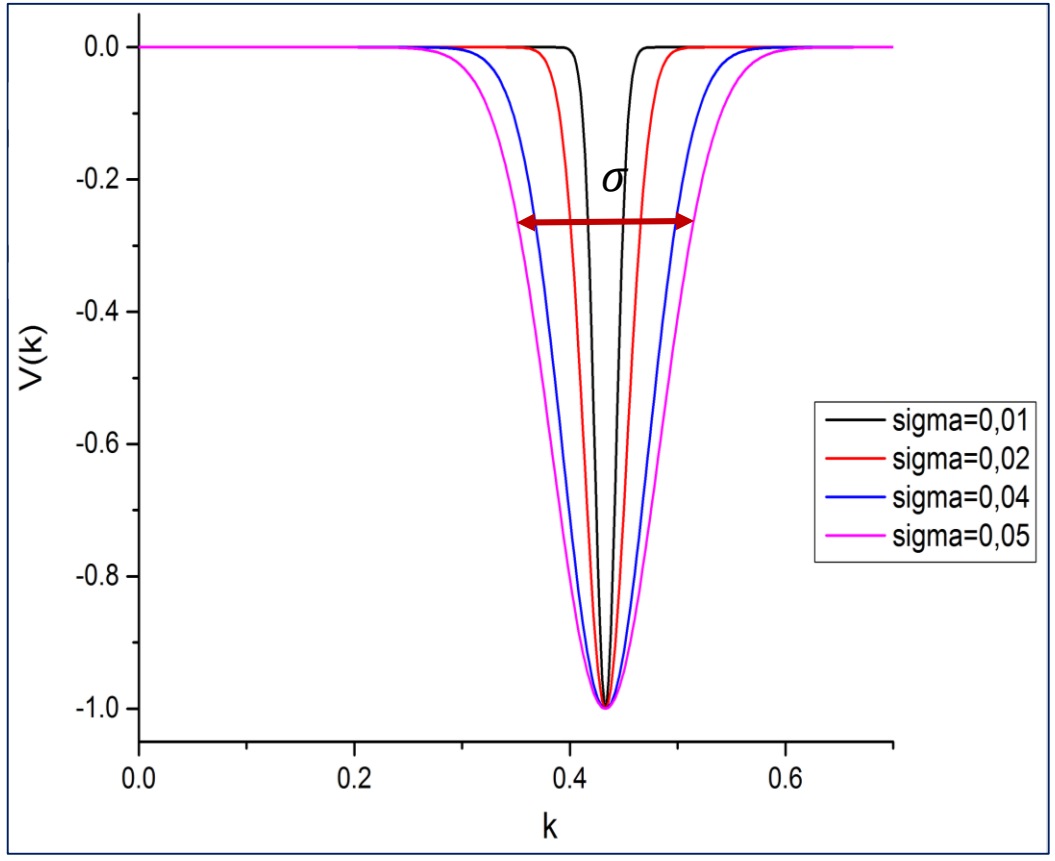
$$\tilde{w}_{LR}^{fcc}(\mathbf{k}) = \lambda_2\left(\exp\left(-\frac{(k-k_{01}^{fcc})^2}{2\sigma^2}\right) + \exp\left(-\frac{(k-k_{02}^{fcc})^2}{2\sigma^2}\right)\right)$$



Long-range potential

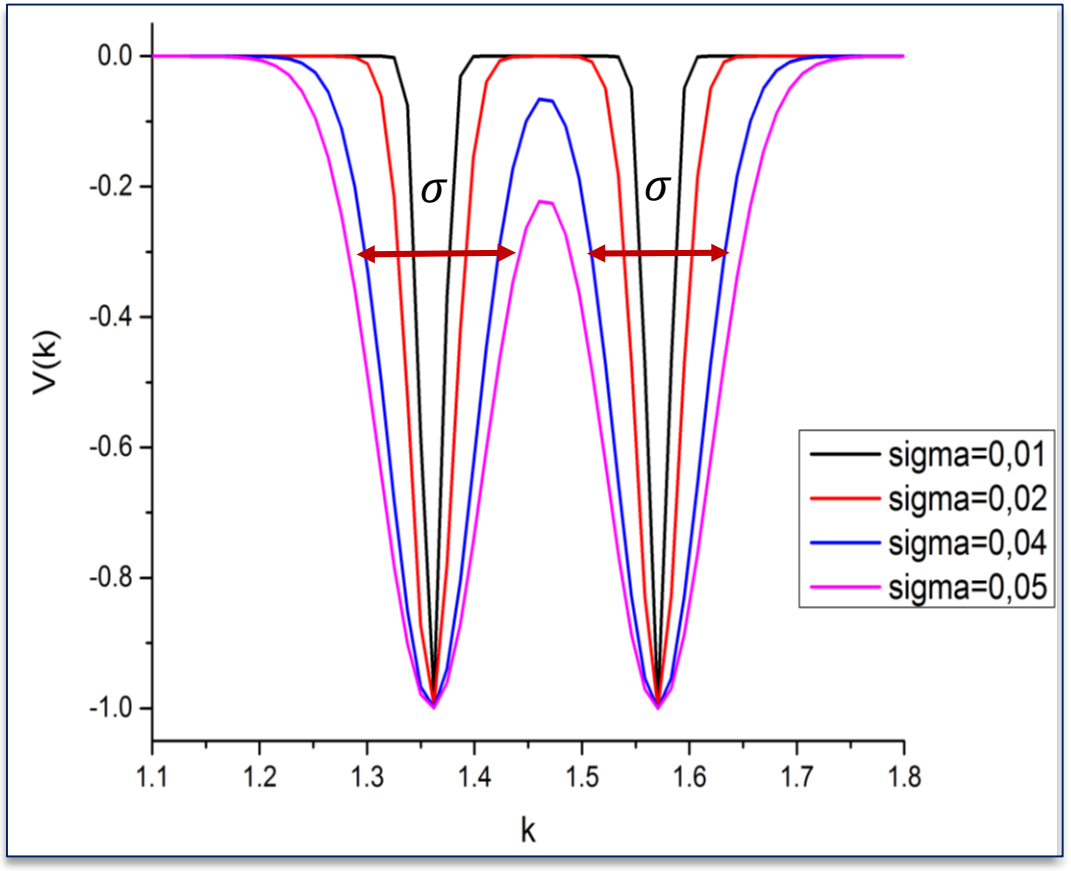
Long-range potential for bcc:

$$\tilde{w}_{LR}^{bcc}(\mathbf{k}) = \lambda_2 \left(\exp\left(-\frac{\left(k - k_{01}^{bcc}\right)^2}{2\sigma^2} \right) \right)$$



Long-range potential for fcc:

$$\tilde{w}_{LR}^{fcc}(\mathbf{k}) = \lambda_2 \left(\exp\left(-\frac{\left(k - k_{01}^{fcc}\right)^2}{2\sigma^2} \right) + \exp\left(-\frac{\left(k - k_{02}^{fcc}\right)^2}{2\sigma^2} \right) \right)$$



Kinetic equation

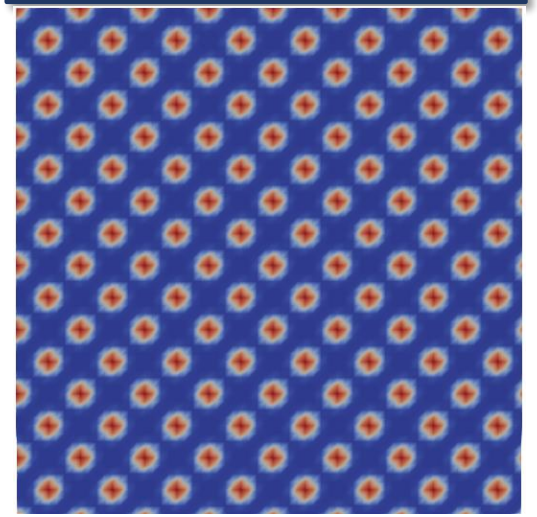
Kinetic equation assumes a linear proportionality of the evolution rate, $\frac{\partial \rho_\alpha(\mathbf{r},t)}{\partial t}$, to the transformation driving force, $\frac{\delta F}{\delta \rho_\beta(\mathbf{r}',t)}$:

$$\frac{d\ \rho_\alpha(\mathbf{r},t)}{dt} = \sum_{\mathbf{r}'}\sum_{\beta} L_{\alpha\beta}(\mathbf{r},\mathbf{r}')\frac{\delta F}{\delta \rho_\beta(\mathbf{r}',t)}$$

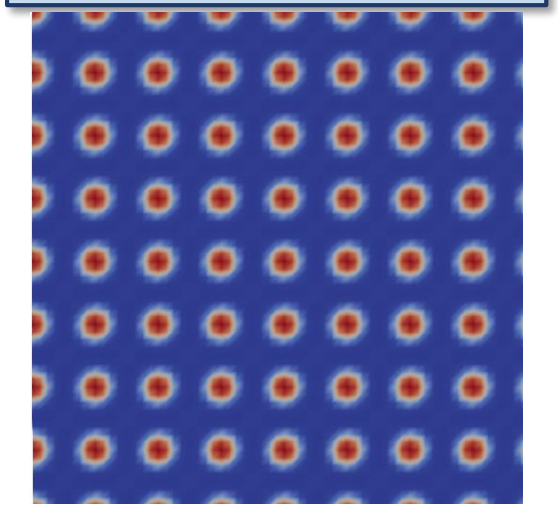
$L_{\alpha\beta}(\mathbf{r}-\mathbf{r}')$ – the matrix of kinetic coefficients proportional to the probability of an elementary diffusional jump from site the r to r' during the time unit.

Simulation details

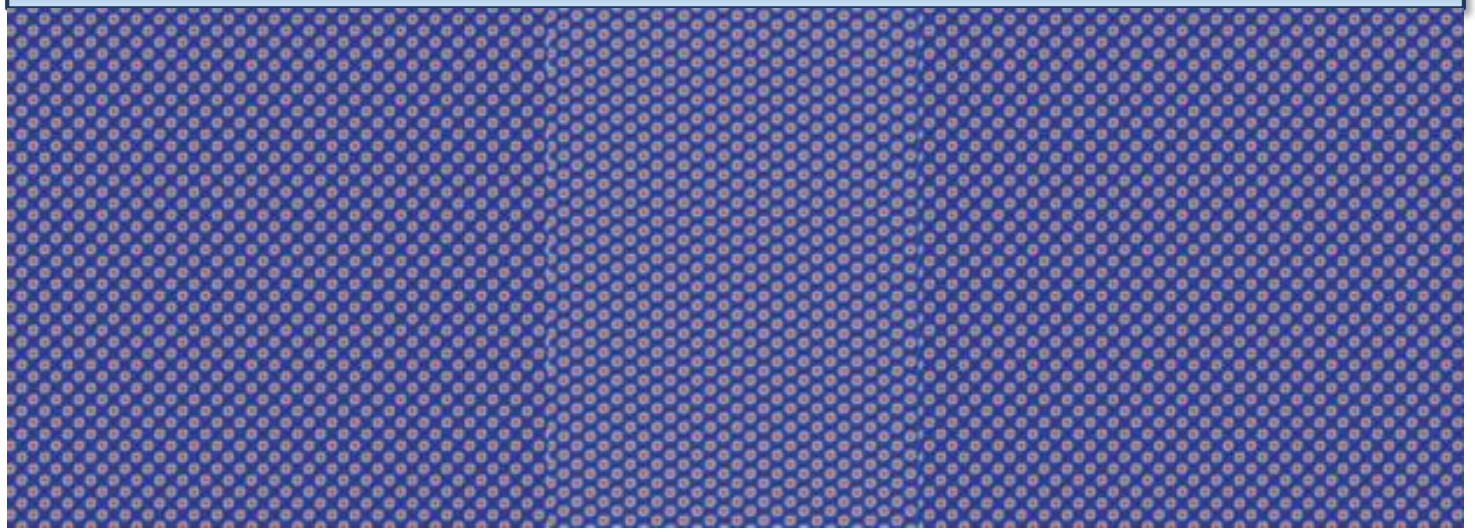
1. Build equilibrium state of fcc.



2. Build equilibrium state of bcc.



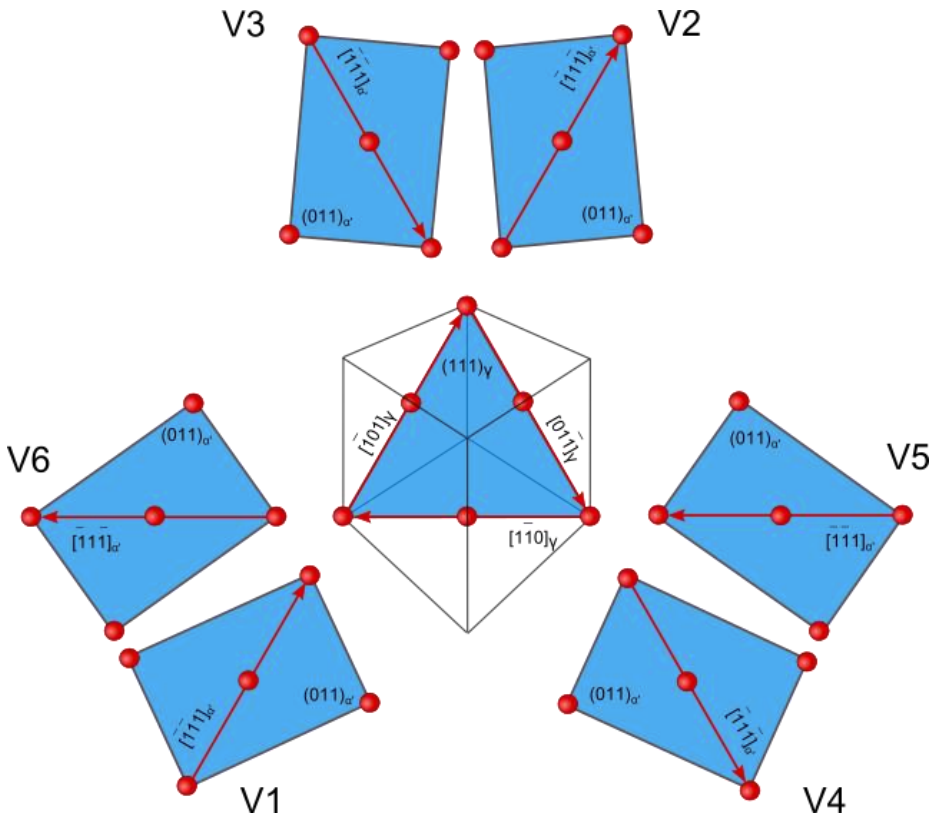
3. Put some volume of bcc in fcc.



Crystallography of austenite/ferrite interphase

Typically, for ferrite in steels orientation relationship (OR) is close to Kurdjumov-Sachs (KS) and Nishiyama-Wassermann (NW).

Six crystallographic KS variants (V1-V6)



Four the close-packed $\{111\}_\gamma$ planes

24 KS-ORs

Sets the close packed $(011)_\alpha$ plane of the bcc ferrite parallel to the $(111)_\gamma$ plane of the fcc austenite.

Kurdjumov-Sachs (KS):

$$\{111\}_\gamma \text{ II } \{110\}_\alpha$$
$$\langle\bar{1}01\rangle_\gamma \text{ II} \langle\bar{1}\bar{1}1\rangle_\alpha$$

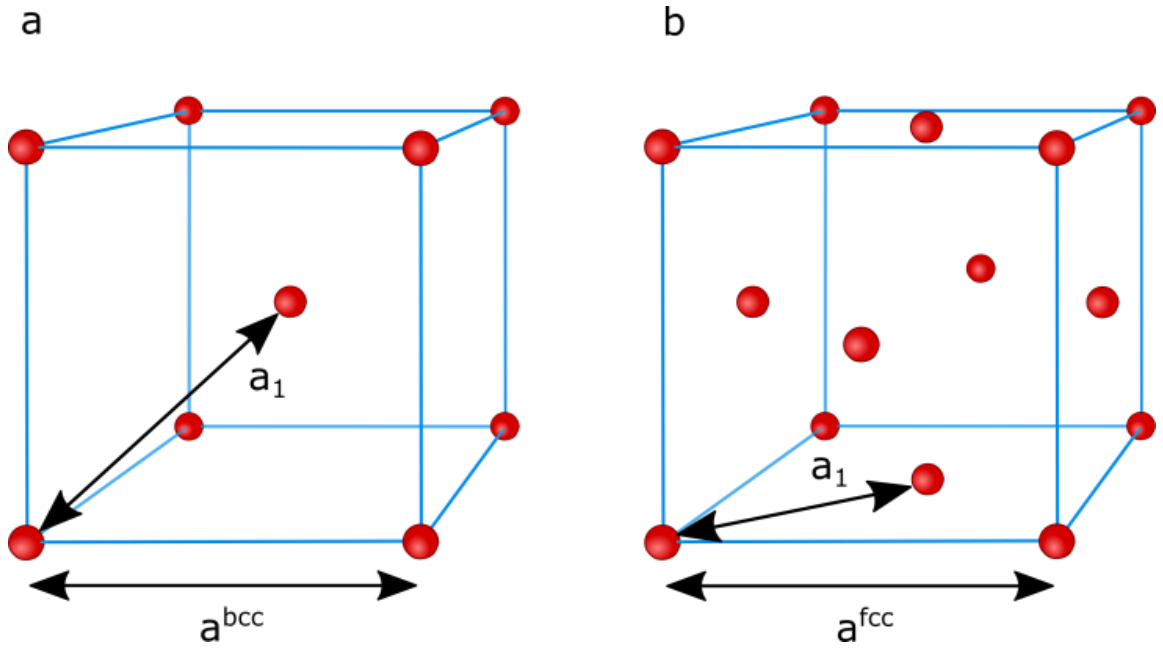
Nishiyama-Wassermann (NW):

$$\{111\}_\gamma \text{ II } \{110\}_\alpha$$
$$\langle\bar{1}01\rangle_\gamma \text{ II} \langle\bar{1}\bar{1}1\rangle_\alpha$$

Bain OR: $\{010\}_\gamma \text{ II } \{001\}_\alpha$
$\langle 110\rangle_\gamma \text{ II} \langle 100\rangle_\alpha$

Pitsch OR: $\{010\}_\gamma \text{ II } \{101\}_\alpha$
$\langle 101\rangle_\gamma \text{ II} \langle\bar{1}11\rangle_\alpha$

Simulation details



$$a_{fcc} = 8 \Rightarrow R = \frac{\sqrt{2}}{4} a_{fcc} \approx 2.8$$

$$\Rightarrow R = \frac{\sqrt{3}}{4} a_{bcc} \Rightarrow a_{bcc} \approx 6.5$$

$$\frac{a_0^{fcc}}{a_0^{bcc}} = \sqrt{\frac{3}{2}} \approx 1.231$$

$$\frac{a_{\exp er}^{fcc}}{a_{\exp er}^{bcc}} = \frac{0.3562}{0.2860} \approx 1.245$$

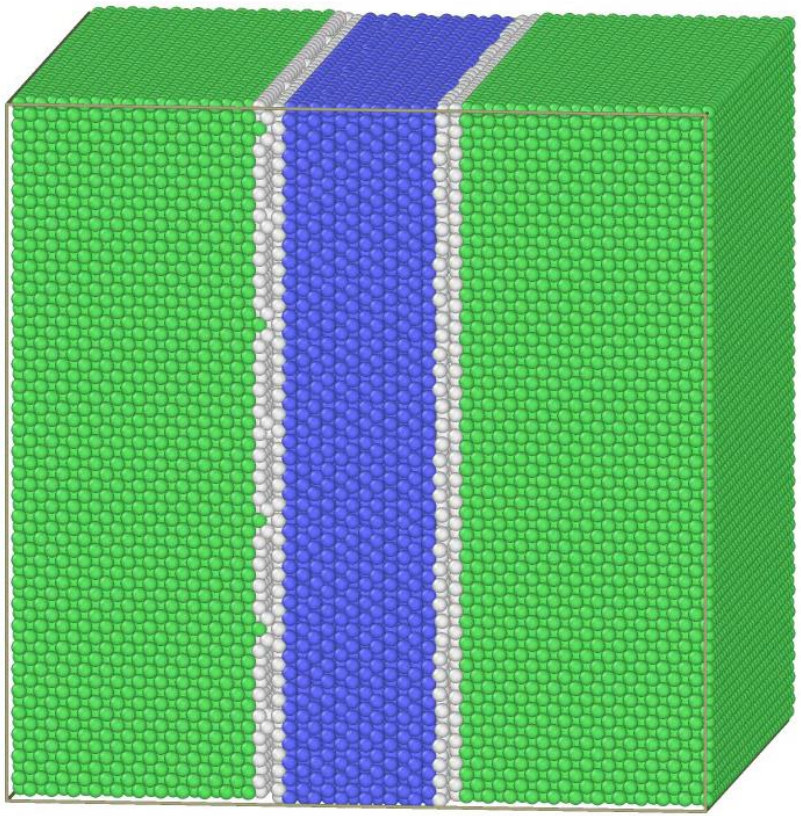
Long-range potential to model the fcc-to-bcc transition:

$$\tilde{w}_{LR}(\mathbf{k}) = \exp\left(-\frac{(k-k_{01})^2}{2\sigma^2}\right) + 0.1\exp\left(-\frac{(k-k_{02})^2}{2\sigma^2}\right)$$

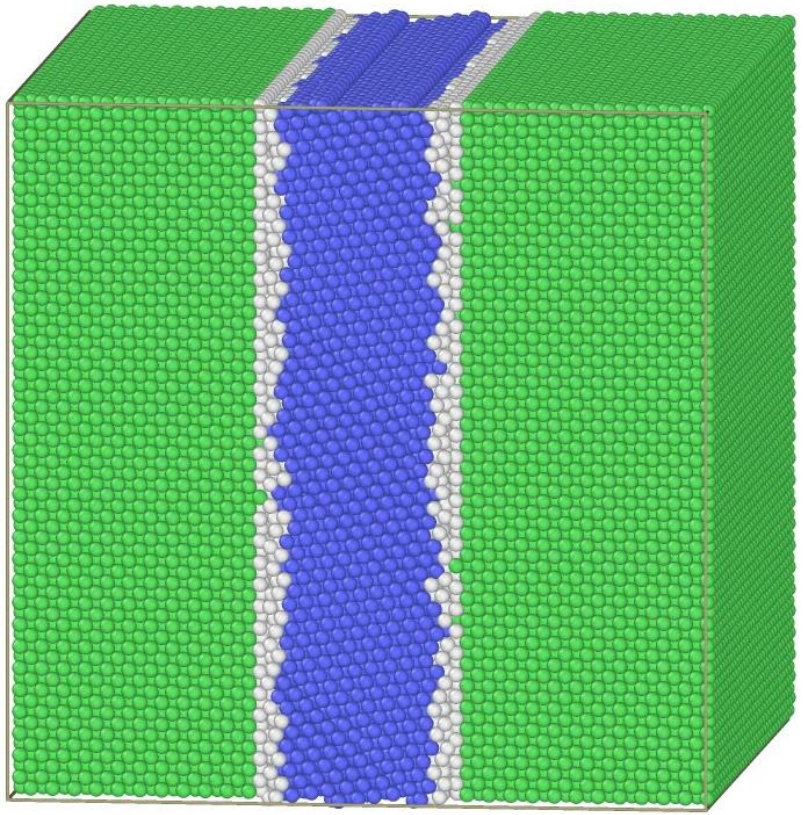
OVITO software: ● BCC; ● FCC; ● "other"; ● HCC;

L=256, $a_{fcc} = 8$, $a_{bcc} \approx 6.5$

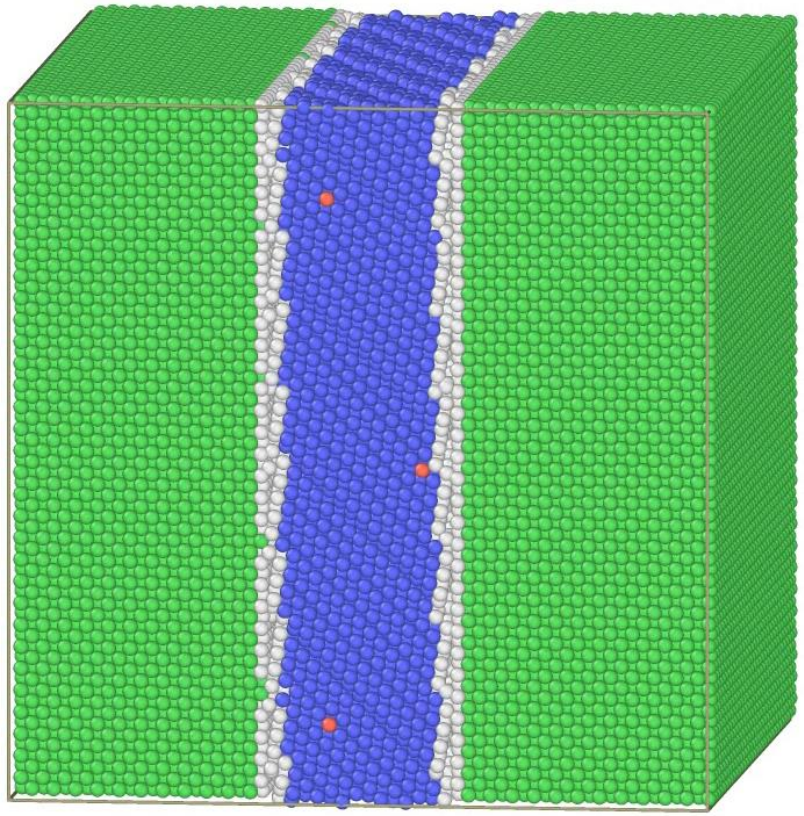
Bain OR: $\{010\}_\gamma \text{ II } \{001\}_\alpha$
$\langle 110\rangle_\gamma \text{ II} \langle 100\rangle_\alpha$



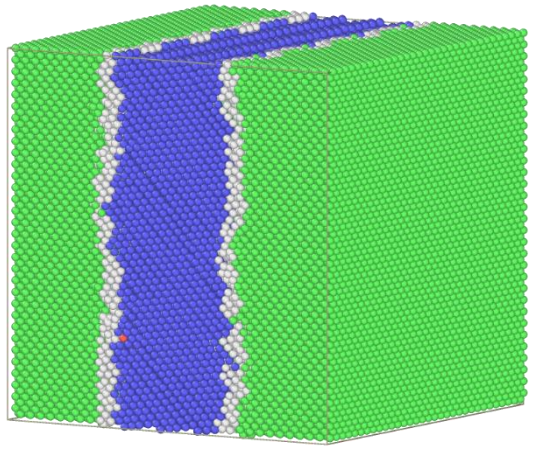
Pitsch OR: $\{010\}_\gamma \text{ II } \{101\}_\alpha$
$\langle 101\rangle_\gamma \text{ II} \langle \bar{1}11\rangle_\alpha$



Kurdjumov-Sachs (KS):
$\{111\}_\gamma \text{ II } \{110\}_\alpha$
$\langle \bar{1}01\rangle_\gamma \text{ II} \langle \bar{1}\bar{1}1\rangle_\alpha$

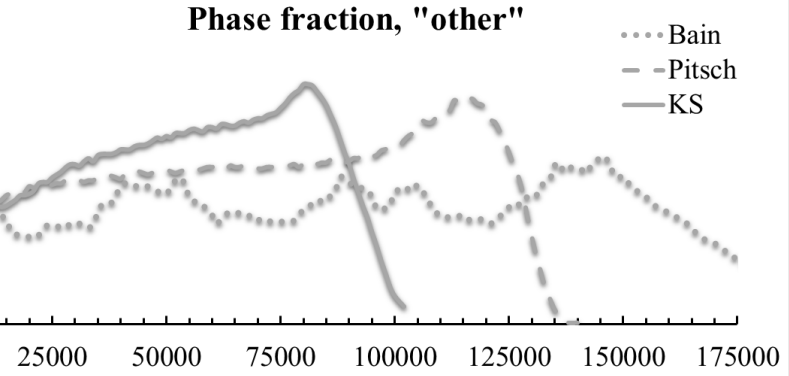


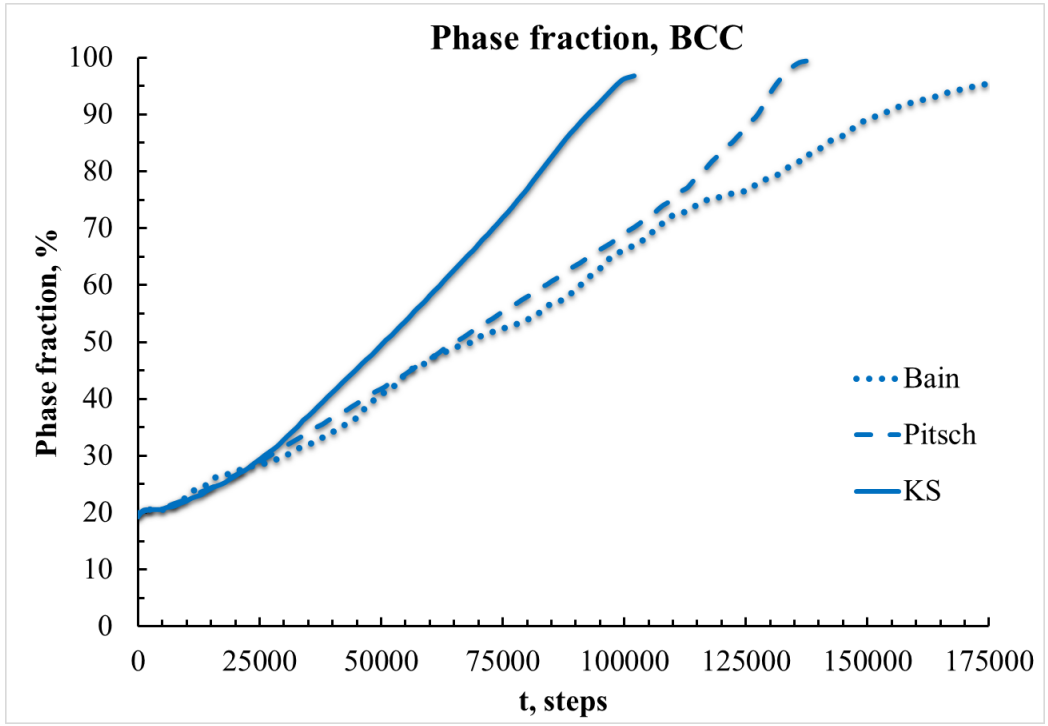
First results: kinetics of interface

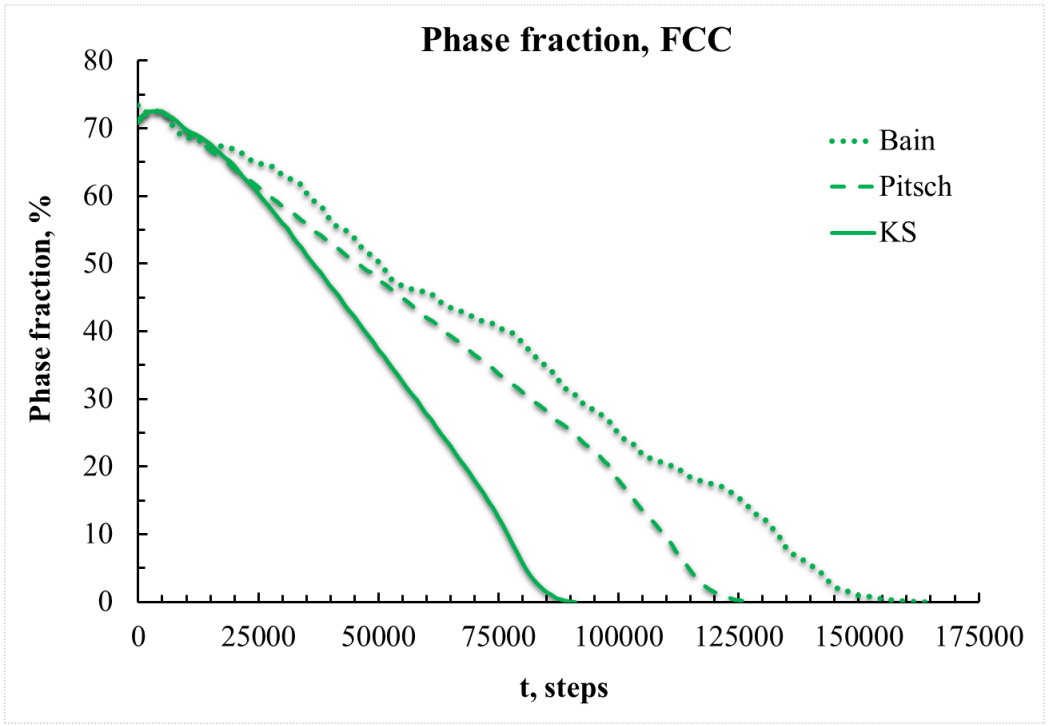


OVITO software:

- BCC;
- FCC;
- "other";





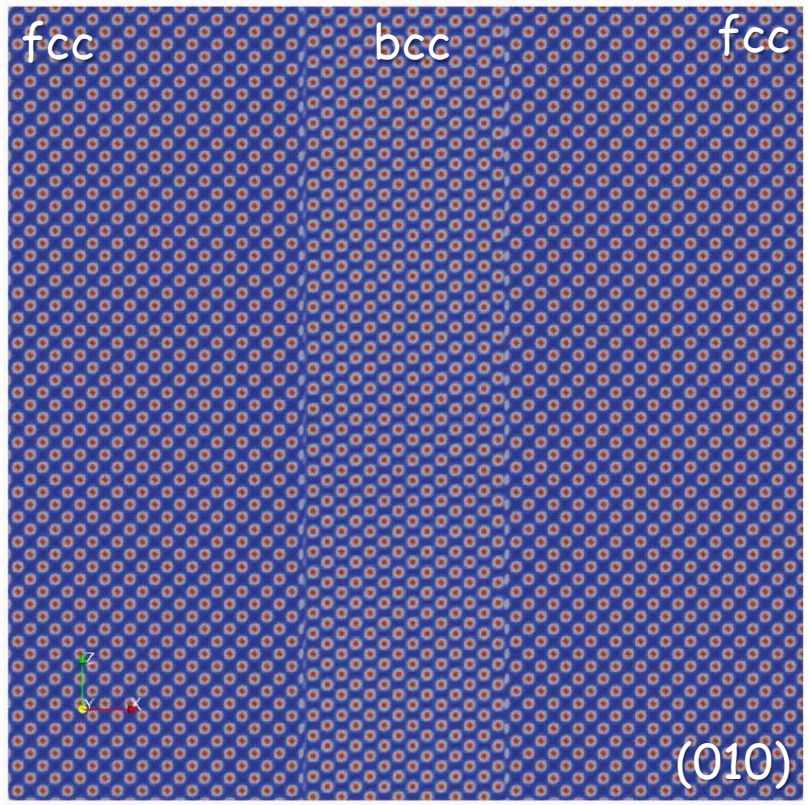


First results: structure of interface

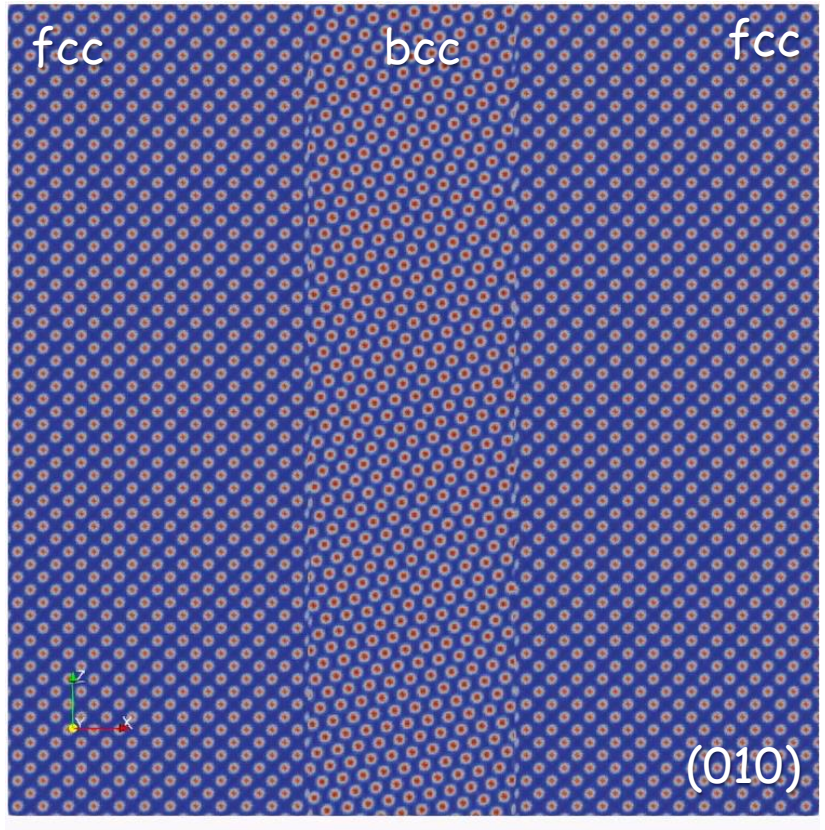
ParaView software:

L=256, $a_{fcc} = 8$, $a_{bcc} \approx 6.5$

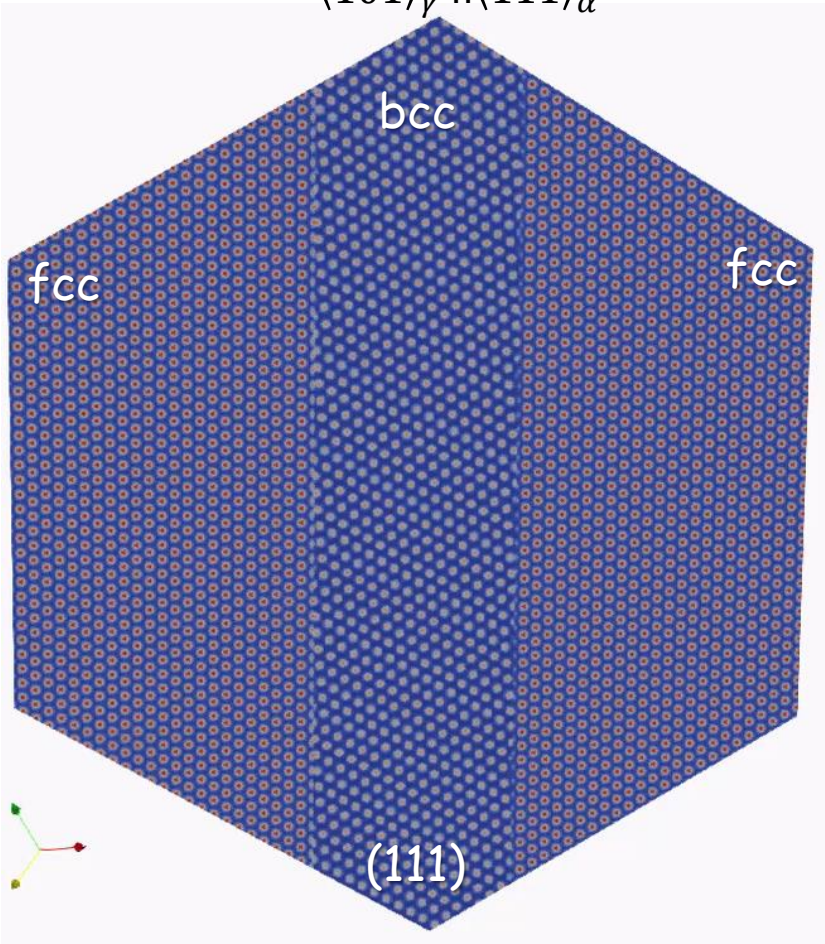
Bain OR: $\{010\}_\gamma \text{ II } \{001\}_\alpha$
$\langle 110\rangle_\gamma \text{ II} \langle 100\rangle_\alpha$



Pitsch OR: $\{010\}_\gamma \text{ II } \{101\}_\alpha$
$\langle 101\rangle_\gamma \text{ II} \langle \bar{1}11\rangle_\alpha$



Kurdjumov-Sachs (KS):
$\{111\}_\gamma \text{ II } \{110\}_\alpha$
$\langle \bar{1}01\rangle_\gamma \text{ II} \langle \bar{1}\bar{1}1\rangle_\alpha$



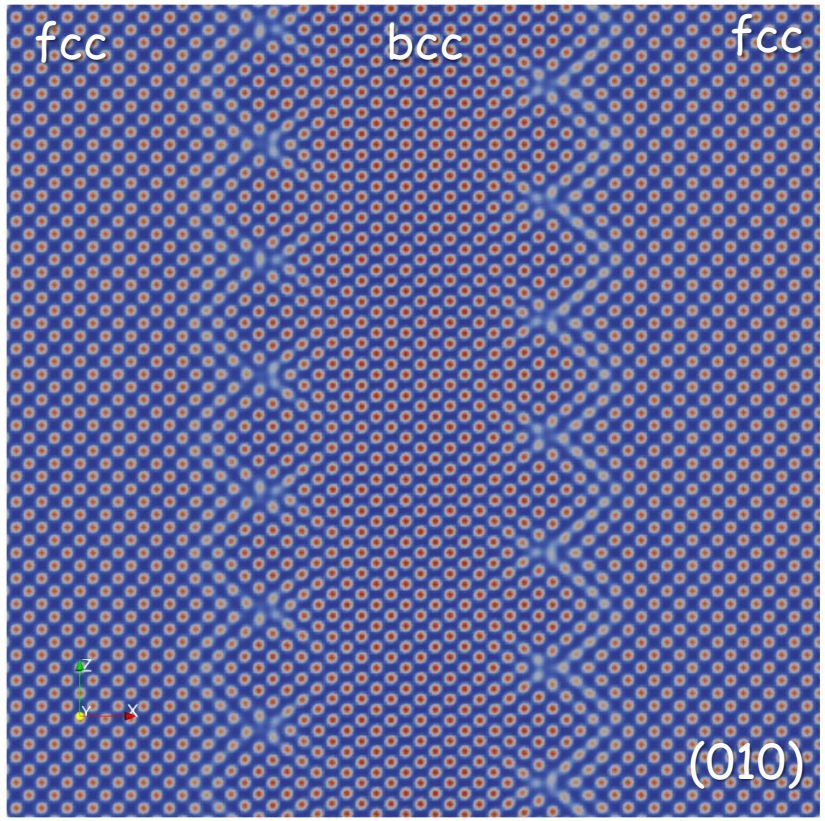
First results: structure of interface

ParaView software:

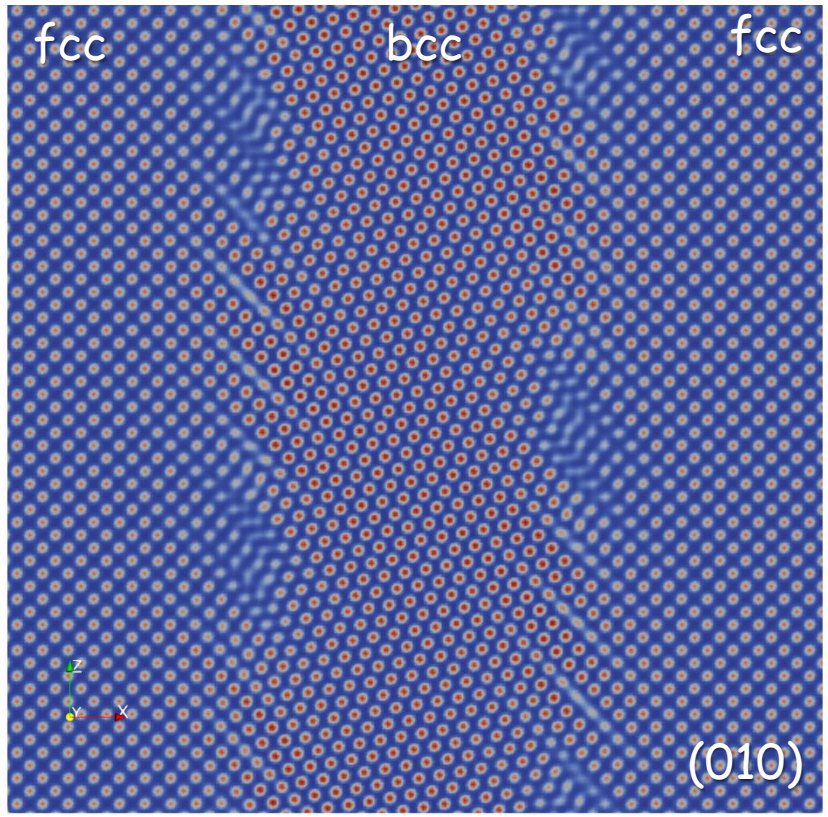
L=256, $a_{fcc} = 8$, $a_{bcc} \approx 6.5$

30000 steps

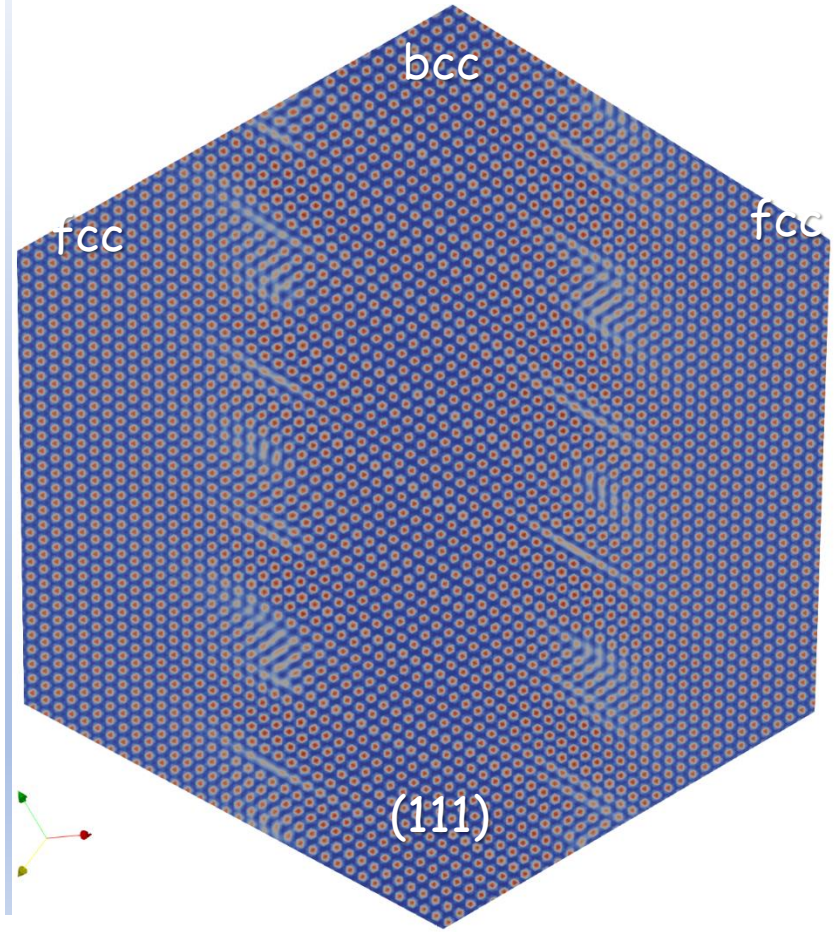
Bain OR: $\{010\}_\gamma \text{ II } \{001\}_\alpha$
$\langle 110\rangle_\gamma \text{ II} \langle 100\rangle_\alpha$



Pitsch OR: $\{010\}_\gamma \text{ II } \{101\}_\alpha$
$\langle 101\rangle_\gamma \text{ II} \langle \bar{1}11\rangle_\alpha$



Kurdjumov-Sachs (KS):
$\{111\}_\gamma \text{ II } \{110\}_\alpha$
$\langle \bar{1}01\rangle_\gamma \text{ II} \langle \bar{1}\bar{1}1\rangle_\alpha$

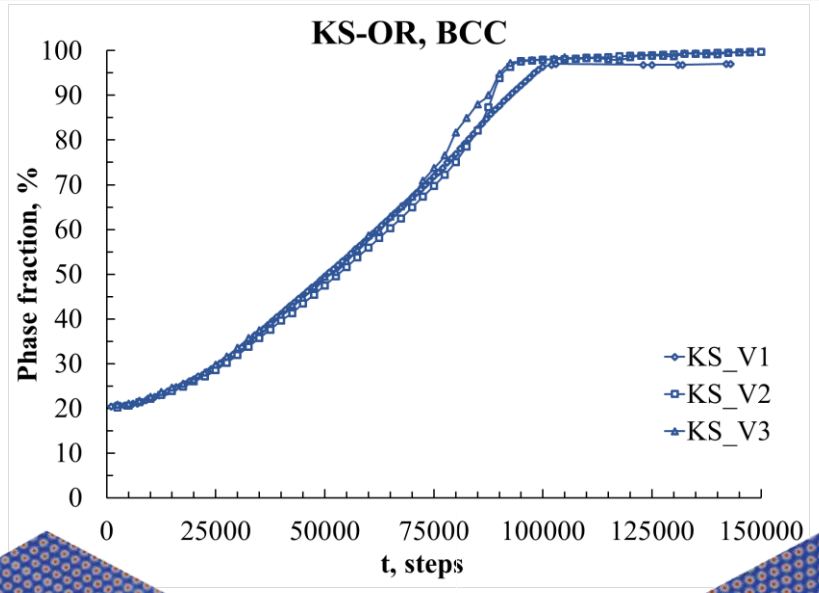


First results: structure of interface

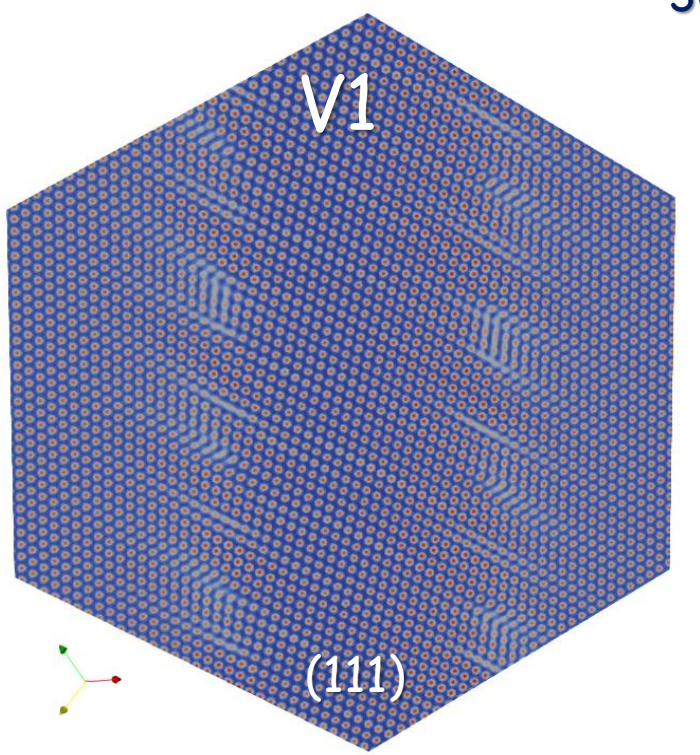
KS_V1: $\{111\}_\gamma \text{ II } \{110\}_\alpha$
$\langle\bar{1}01\rangle_\gamma \text{ II} \langle\bar{1}\bar{1}1\rangle_\gamma$

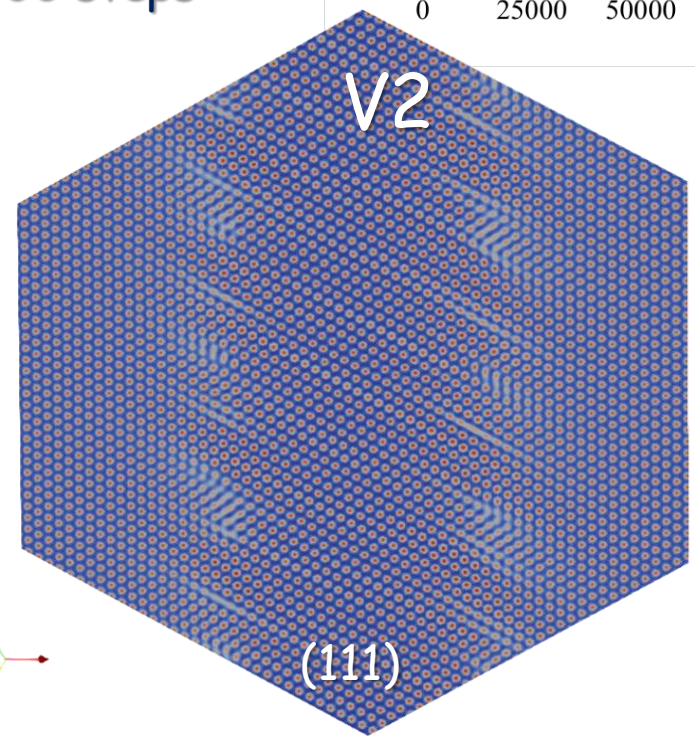
KS_V2: $\{111\}_\gamma \text{ II } \{110\}_\alpha$
$\langle\bar{1}01\rangle_\gamma \text{ II} \langle\bar{1}1\bar{1}\rangle_\gamma$

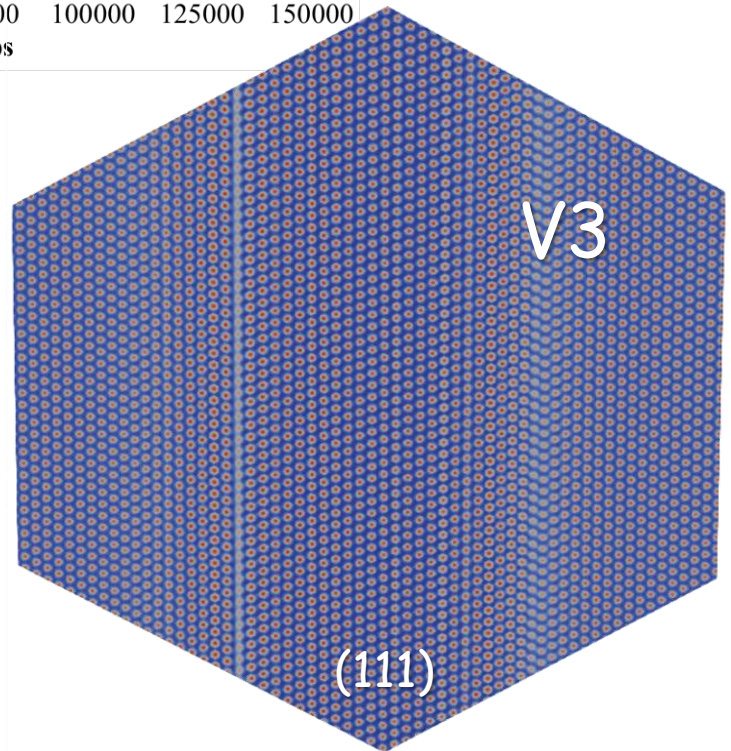
KS_V3: $\{111\}_\gamma \text{ II } \{110\}_\alpha$
$\langle 01\bar{1}\rangle_\gamma \text{ II} \langle\bar{1}\bar{1}1\rangle_\gamma$



30000 steps

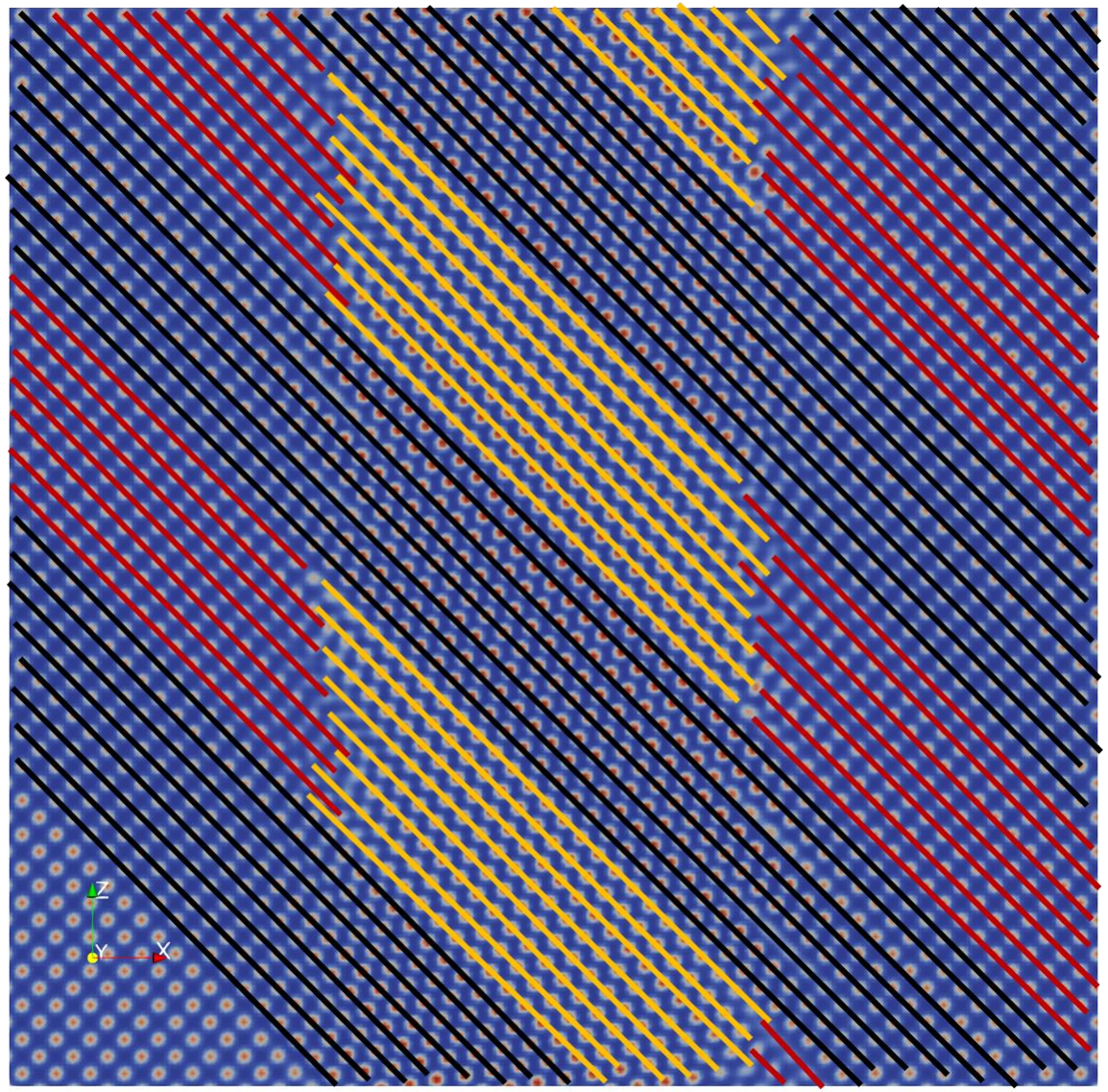




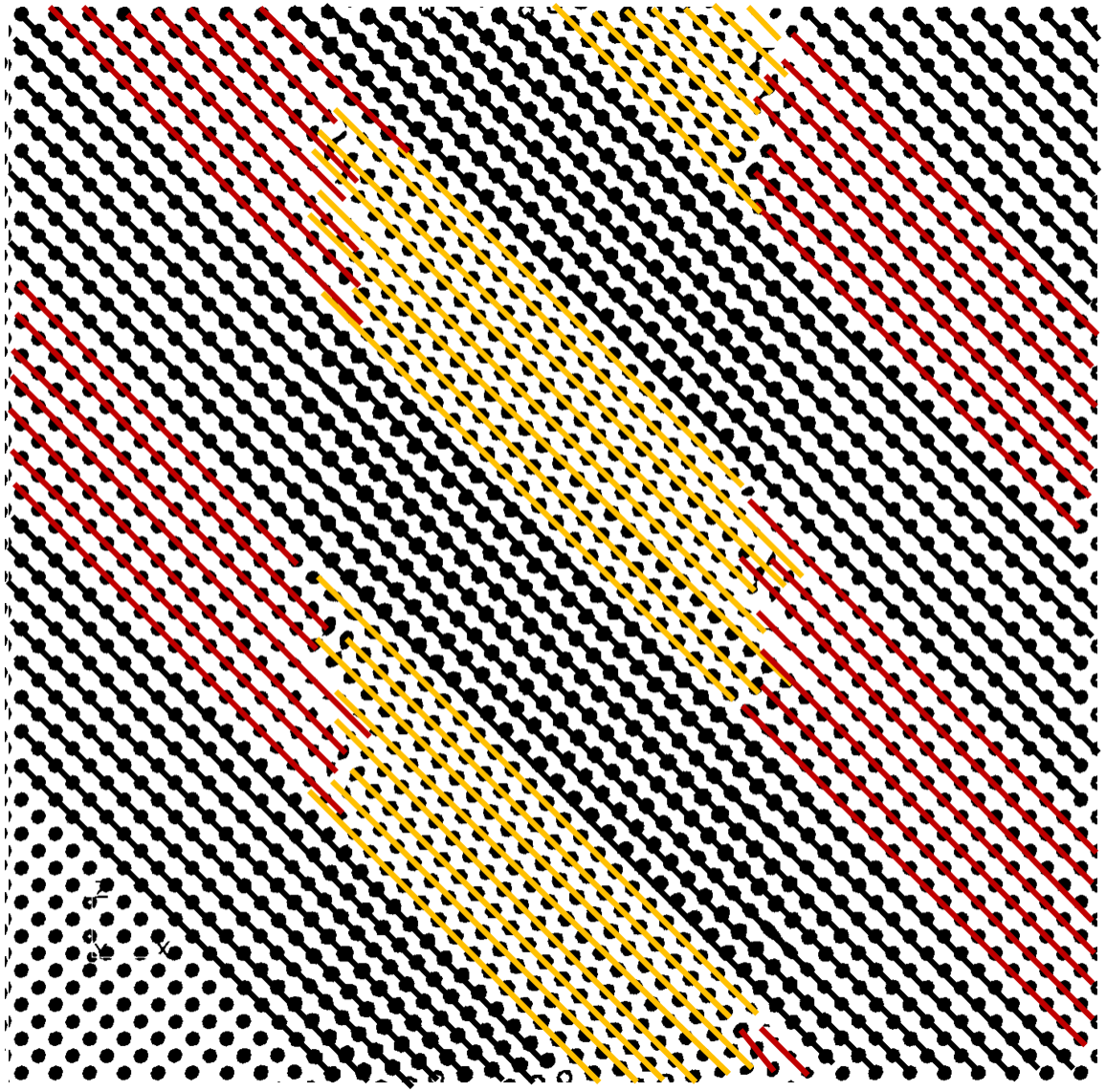


First results: dislocation

Pitsch OR: $\{010\}_\gamma$ II $\{101\}_\alpha$, $\langle 101\rangle_\gamma$ II$\langle \bar{1}11\rangle_\alpha$

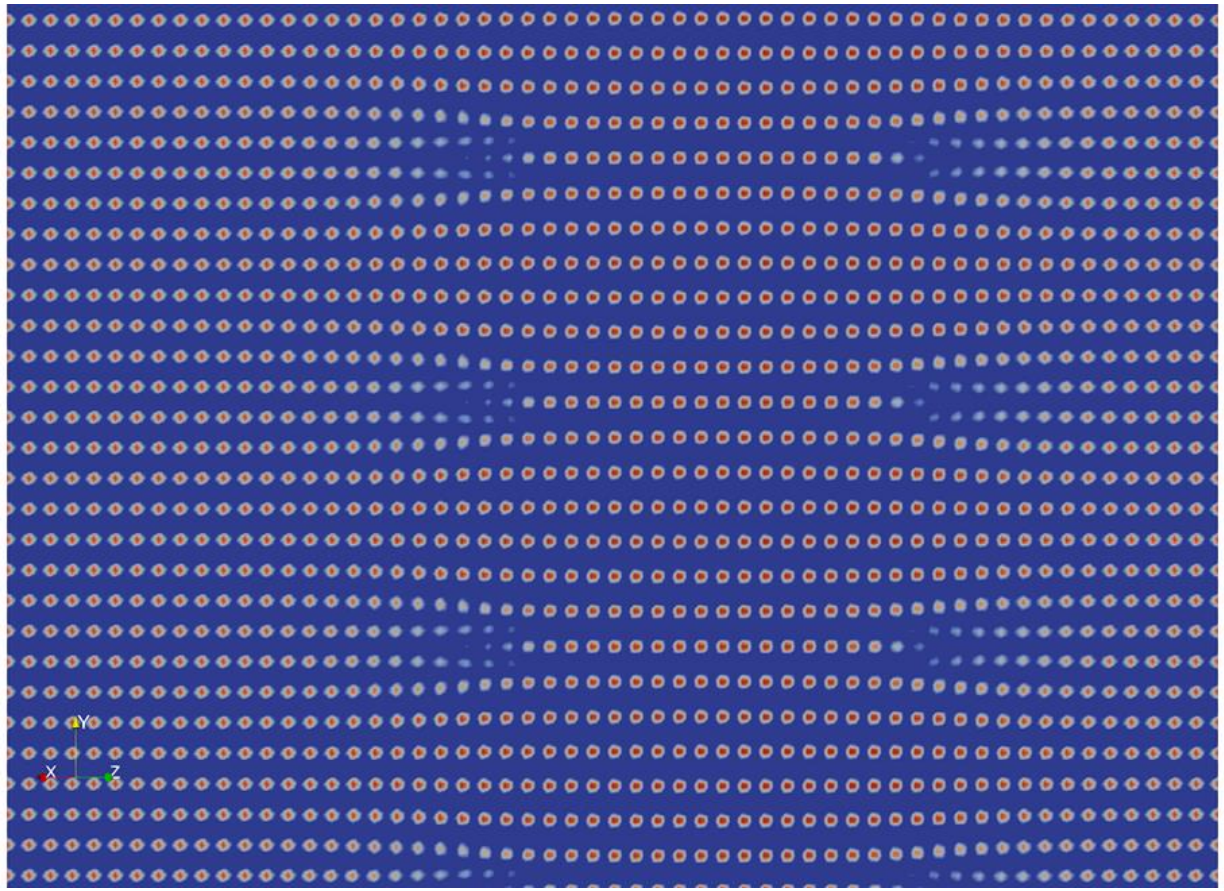


30000 steps : $\{010\}_\gamma$

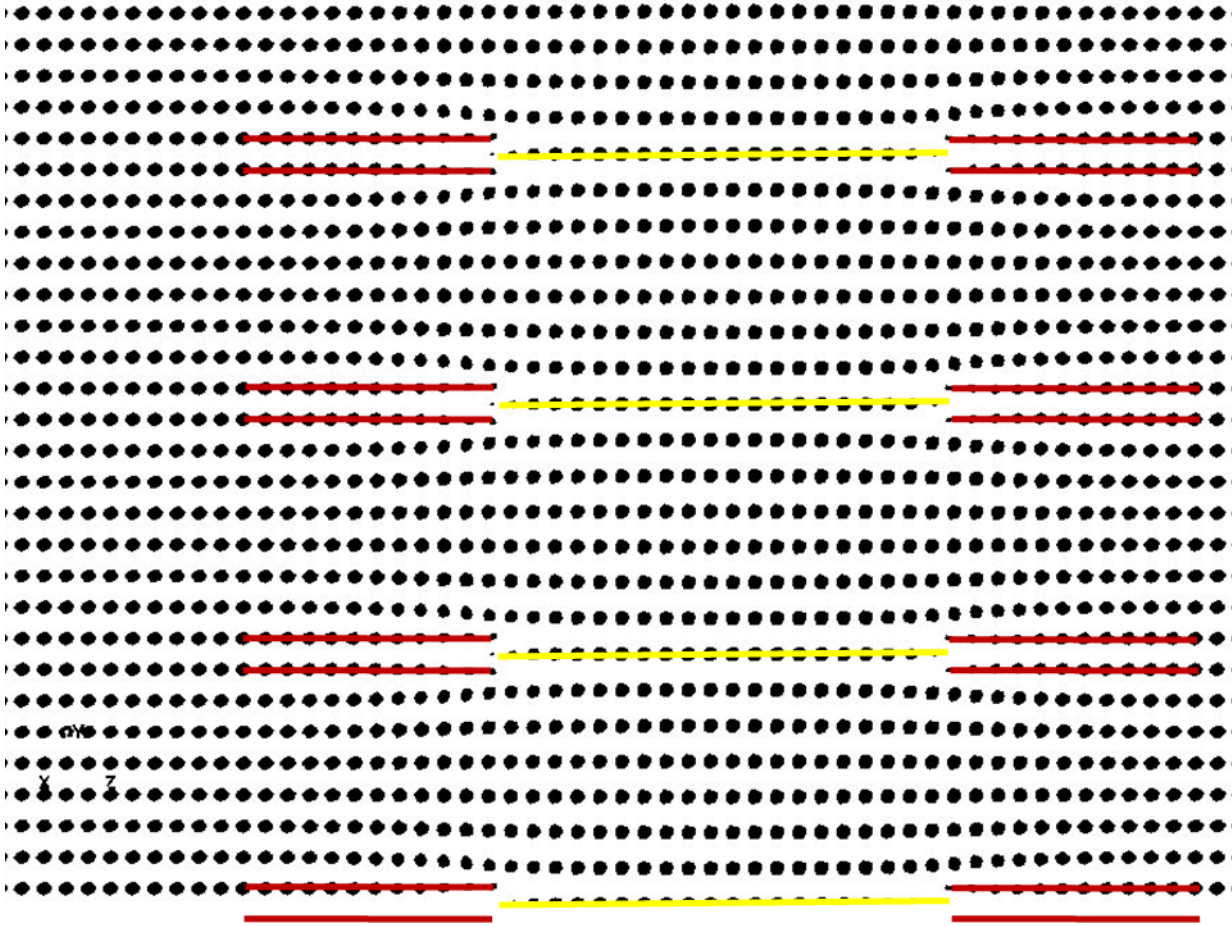


First results: dislocation

Pitsch OR: $\{010\}_\gamma \text{ II } \{101\}_\alpha$, $\langle 101\rangle_\gamma \text{ II} \langle \bar{1}11\rangle_\alpha$



30000 steps : $\{101\}_a$

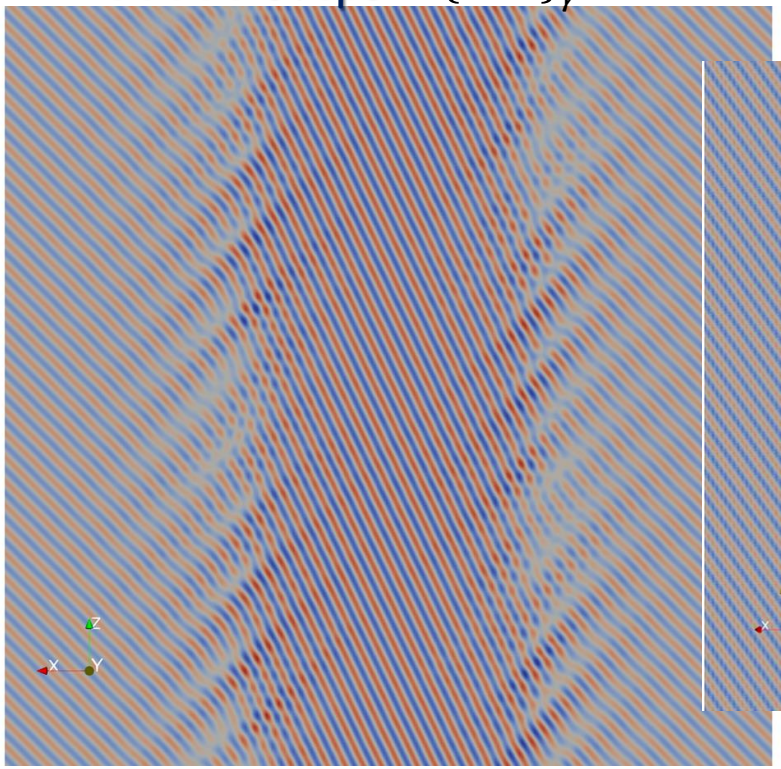


First results: dislocation

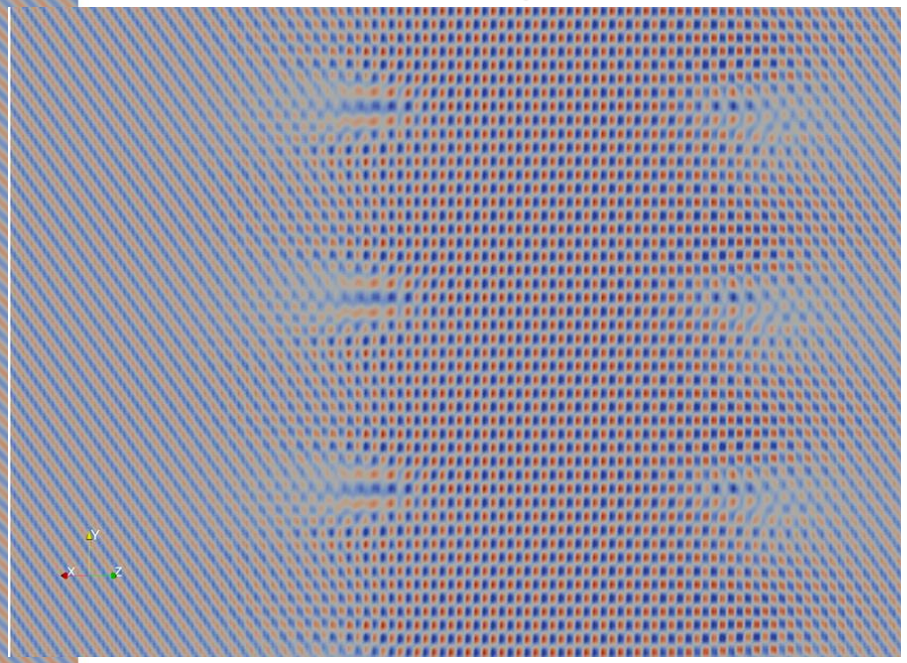
First attempt to do "High resolution image"

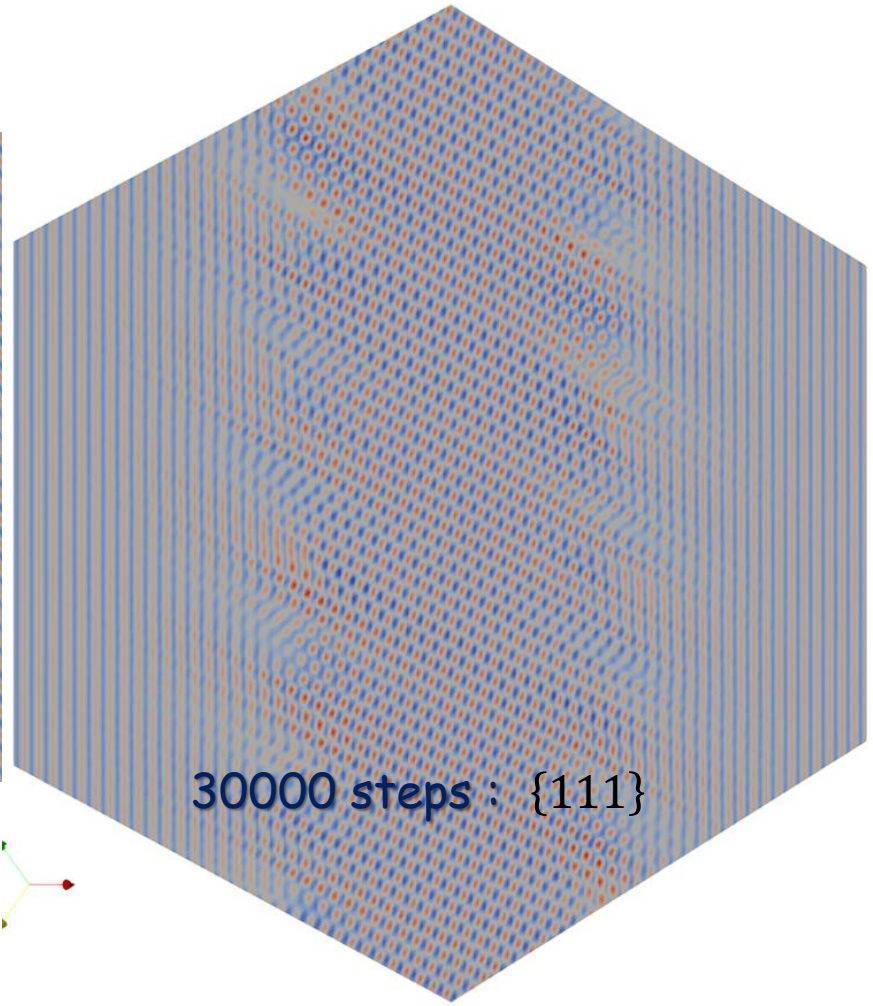
Pitsch OR: $\{010\}_\gamma \text{ II } \{101\}_\alpha$, $\langle 101\rangle_\gamma \text{ II} \langle \bar{1}11\rangle_\alpha$

30000 steps : $\{010\}_\gamma$



30000 steps : $\{101\}_a$





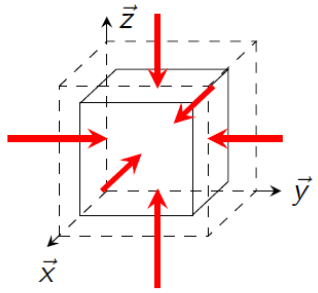
Elastic constants

Potential determine elastic constants C_{ijkl} :

$$C_{ijkl} = \frac{\partial}{\partial \varepsilon_{kl}} \frac{\partial F}{\partial \varepsilon_{ij}}$$

$\underline{\underline{\varepsilon}}$: strain tensor

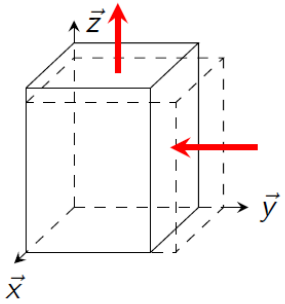
Cubic



Bulk modulus :

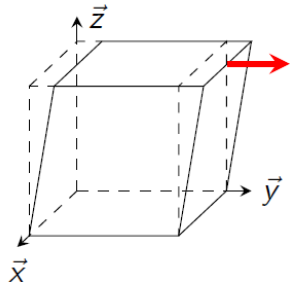
$$B = \frac{C_{11} + 2C_{12}}{3}$$

Orthorombic



C_{44}

Monoclinic



$$C' = \frac{C_{11} - C_{12}}{2}$$

Experimental elastic constants for iron

$$\frac{C_{11}^{bcc}}{C_{11}^{fcc}} \approx 1.60,$$

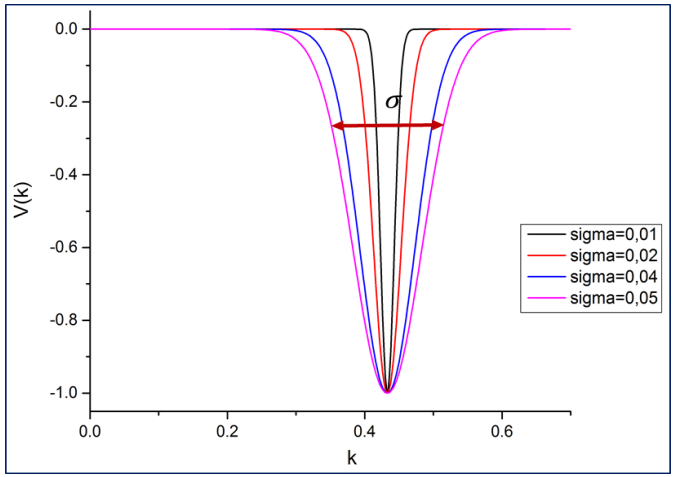
$$\frac{C_{12}^{bcc}}{C_{12}^{fcc}} \approx 1.15,$$

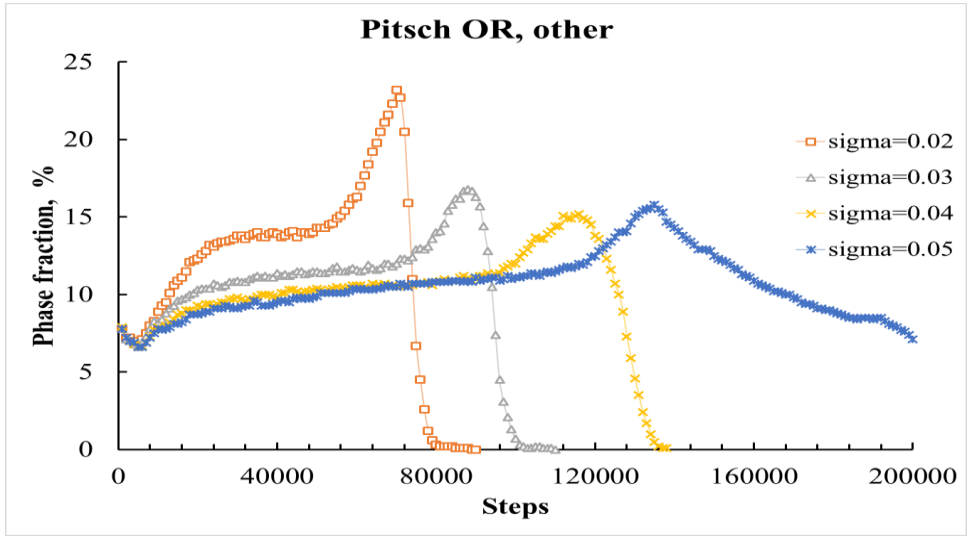
$$\frac{C_{44}^{bcc}}{C_{44}^{fcc}} \approx 1.51$$

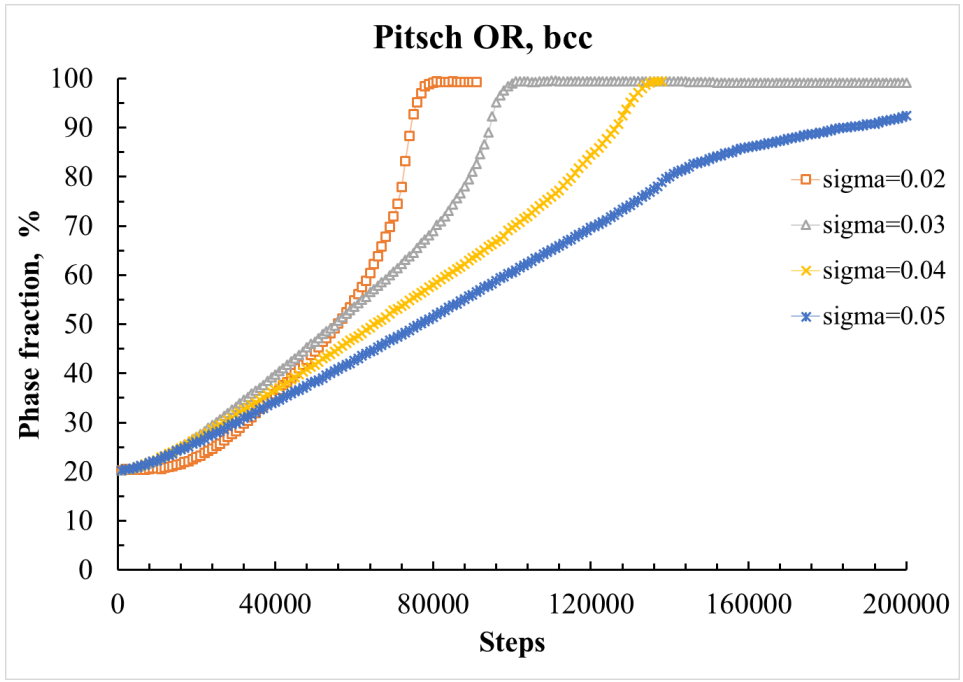
Elactic constans, ρ=0.17

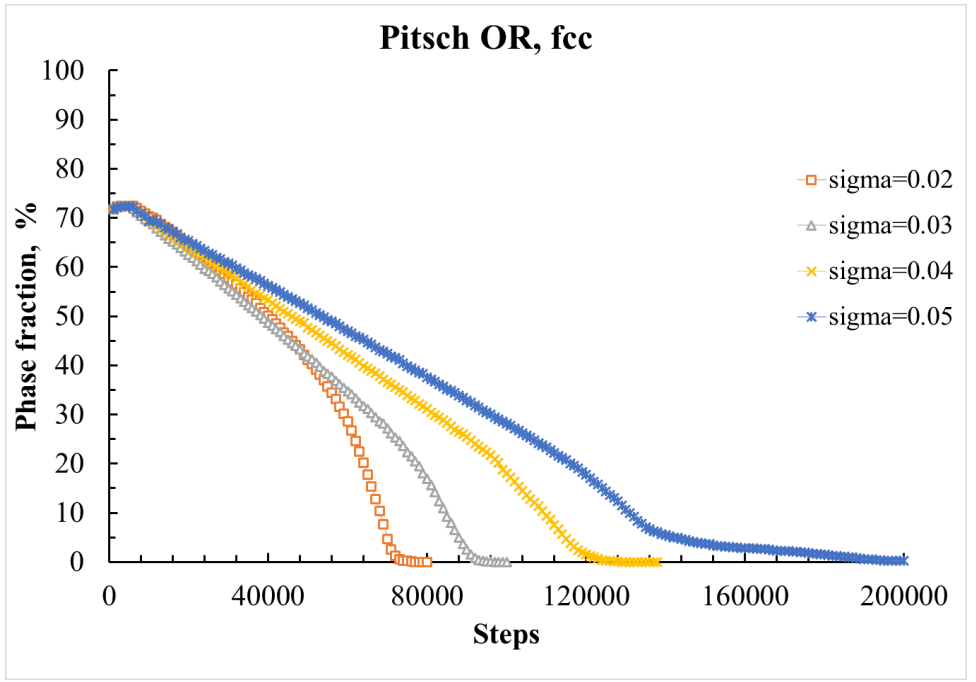
	σ=0.01			σ=0.02			σ=0.03			σ=0.04			σ=0.05		
	bcc	fcc	**bbc/fcc**	bcc	fcc	**bbc/fcc**	bcc	fcc	**bbc/fcc**	bcc	fcc	**bbc/fcc**	bcc	fcc	**bbc/fcc**
C11	6.0328	8.3616	**0.7215**	1.5474	2.5221	**0.6135**	0.6624	1.1634	**0.5694**	0.5092	0.535	**0.9517**	0.2877	0.1857	**1.549**
C12	2.6117	2.4231	**1.0778**	0.6745	0.9889	**0.682**	0.2652	0.4837	**0.5484**	0.277	0.2286	**1.2118**	0.1328	0.0581	**2.2856**
C44	2.2795	2.2451	**1.0153**	0.5805	0.5722	**1.0146**	0.2646	0.2552	**1.0369**	0.1539	0.1637	**0.9404**	0.1026	0.096	**1.0688**

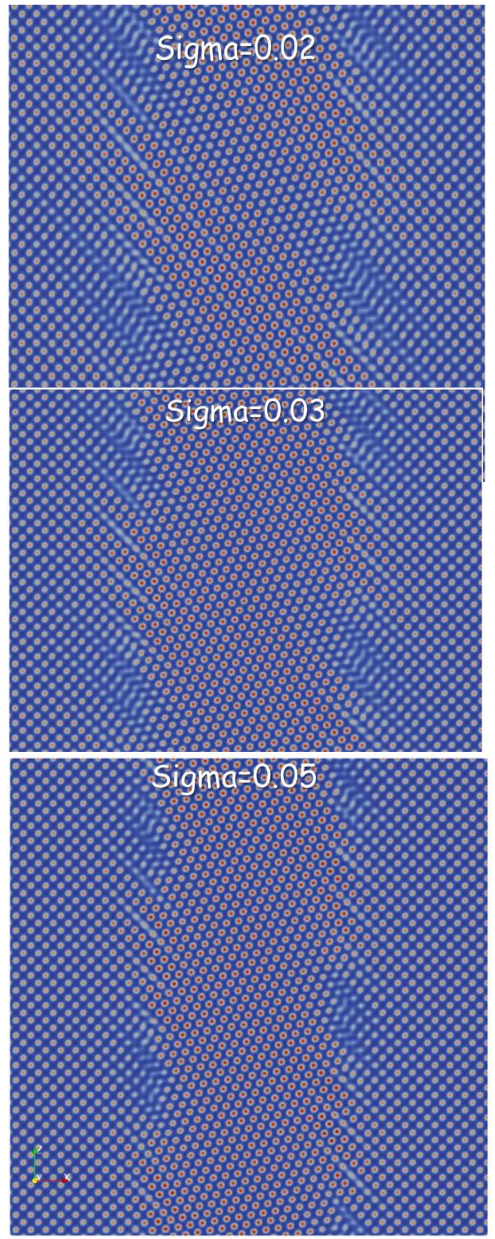
Elastic constants











Conclusions and perspectives

Conclusions :

OR influence on :

- the structure of moving transformation interface;
- kinetics of the propagation interphase interface.

Periodic set of dislocation observed on the interface.

Perspectives:

- Characterization of the interface structure by the dislocation analysis;
- more precise investigation of K-S and N-W ORs;
- move from one to binary component system.

MERCI DE VOTRE ATTENTION !