Quasiparticle Atomistic Approach to model a Self-Assembly Kinetics of Complex Structures and Structural Defects.

Helena Zapolsky, M. Lavrskyi, A. Vaugeois, R. Patte
University of Rouen Normandie, GPM, UMR 6634, Saint-Etienne du Rouvray, France
A.G. Khachaturyan
Department of Materials Science and Engineering, Rutgers University, Piscataway, NJ

Workshop II: Stochastic Sampling and Accelerated Time Dynamics on Multidimensional Surfaces, Octobre 16-20,2017, UCLA, IPAM

Stability of the system with respect to infinitesimal fluctuations $\delta c(r) = c(r) - \bar{c}$

Free energy of heterogeneous system in continuous approximation

$$F = \int_V \left[(f(c) + \frac{1}{2}\beta(c)(\nabla c)^2) dV \right]$$

Variation of free energy with respect to small fluctuations

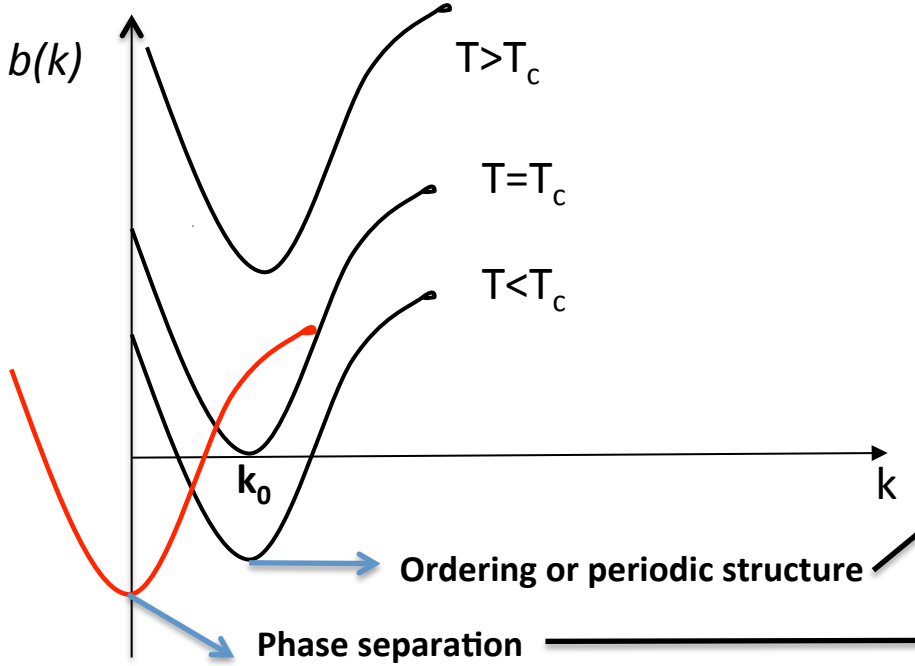
$$\Delta F = \int_V \left[\frac{1}{2}\frac{d^2 f(\bar{c})}{dc^2}\delta c^2(r) + \frac{1}{2}\beta(\bar{c})(\nabla \delta c(r))^2 dV \right]$$

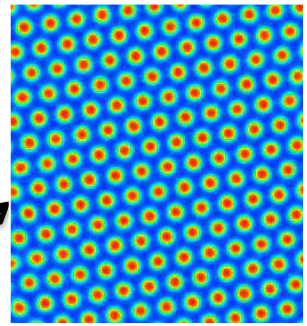
$$\delta c(r) = c(r) - \bar{c} = \frac{1}{N}\sum_k c(k) e^{ikr}$$

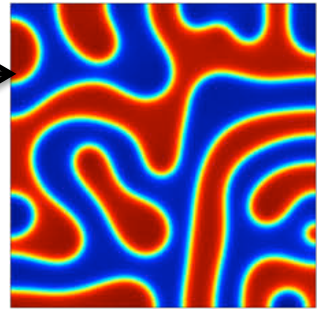
FT

$$\Delta F = \frac{1}{2}\int b(k)\left|c(k)\right|^2 \frac{d^3 k}{(2\pi)^3}$$

$$b(k) = v\left[\frac{d^2 f(\bar{c})}{dc^2} + \beta(\bar{c})k^2 \right]$$







Two types of minima:

$$\left.\frac{\partial b(k)}{\partial k}\right|_{k=k_j} = 0$$

k=0 separation

k≠0 periodic structures

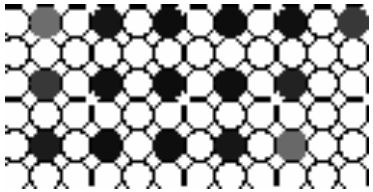
Landau Khalatnikov kinetic equation (1954)

Landau-Khalatnikov relaxation equation

$$\frac{d\psi(\vec{r},t)}{dt} = -\gamma \frac{\partial F}{\partial \psi(\vec{r},t)}$$

Microscopique kinetic equation
Atomic density function theory

$$\frac{dP(\vec{r},t)}{dt} = \sum_{\vec{r}'} L(\vec{r}-\vec{r}') \frac{\partial F}{\partial P(\vec{r}',t)}$$



P(r) is the probability to find atom in position r.

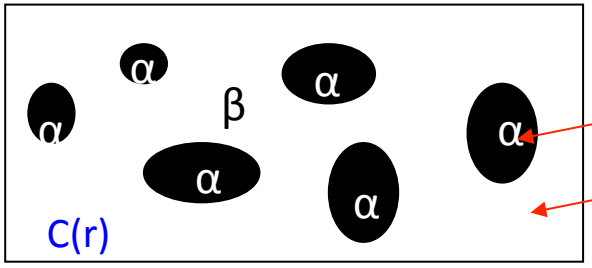
Time dependent Ginzburg-Landau equation

$$\frac{\partial \eta(\vec{r},t)}{\partial t} = -L\left(\frac{\delta F}{\delta \eta(\vec{r},t)}\right) + \zeta_\eta(\vec{r},t)$$

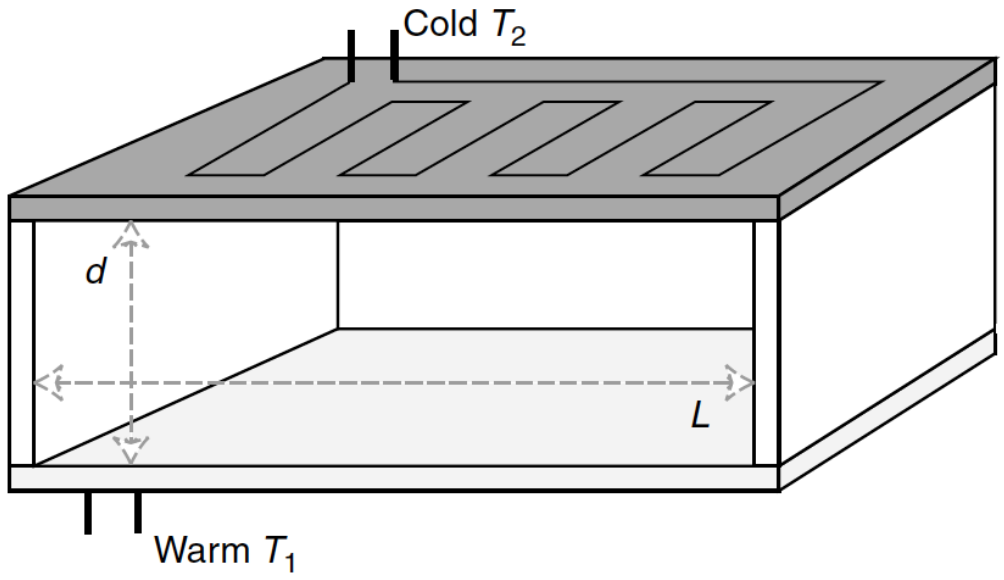
Cahn-Hilliard equation for concentrations

$$\frac{\partial c(\vec{r},t)}{\partial t} = \vec{\nabla} M \vec{\nabla}\left(\left(\frac{\delta F}{\delta c(\vec{r},t)}\right)\right) + \varsigma_c(\vec{r},t)$$

Phase field variables:
Concentration c(r)
Ordre parametre η(r)



Rayleigh–Bénard convection



Rayleigh–Bénard convection of a fluid layer between two horizontal plates is one of the simplest sustained nonequilibrium systems. When the temperature difference ΔT = T1−T2 is sufficiently large, the warm less-dense air near the floor and the cold more-dense air near the ceiling spontaneously start to move, i.e. convection sets in. The rising and falling regions of air eventually forms cellular structures known as convection rolls. The characteristic roll size is about the depth d of the air.

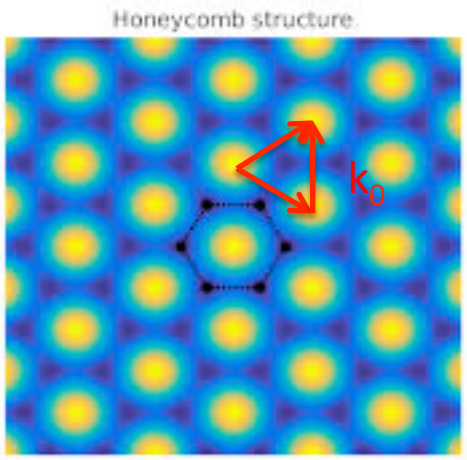
Swift-Hohenberg model of convection

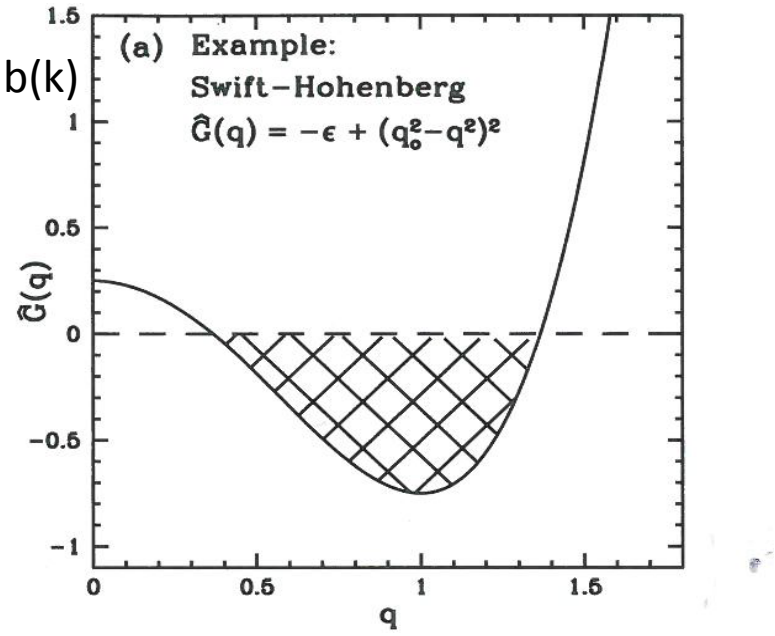
The addition Ψ^3 in the free energy functional break ± symmetry (Brazovskii energy, 1976)

$$\rho(r) = \rho + \sum_k Q(k) e^{-ikr}$$

$$F = \int d\mathbf{r} \left[\frac{1}{2} \psi(-\varepsilon + (k_0^2 + \nabla^2)^2)\psi + \alpha \frac{\psi^3}{3} + \frac{\psi^4}{4} \right]$$

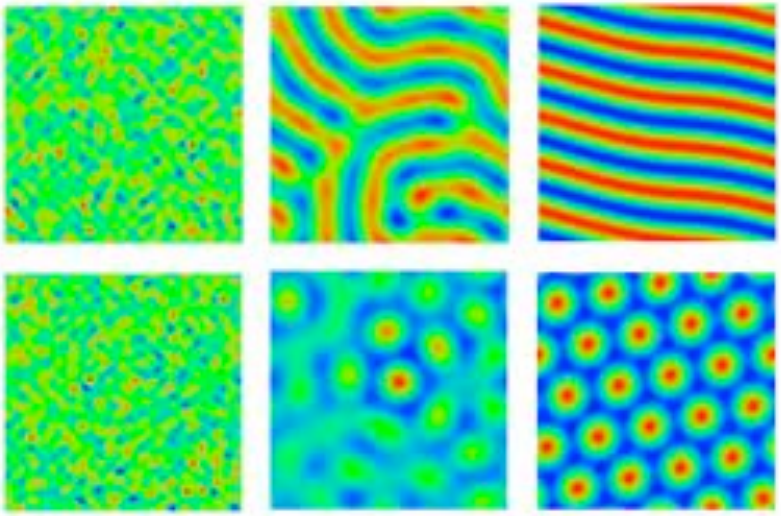
$$\Delta F = \frac{1}{2} \sum_k b(k) |Q(k)|^2$$





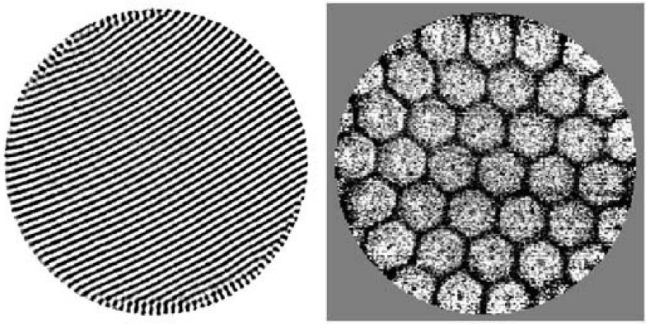
for ε=3/4 and k_0=1

$$\frac{\partial \psi}{\partial t} = -L\frac{\delta F}{\delta \psi} = L(\varepsilon - (q_0^2 + \nabla^2)^2 \psi - \alpha\psi^2 - \psi^3)$$



stripes

honeycomb structure.



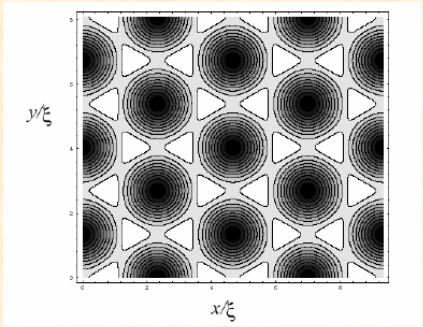
Rayleigh–Bénard convection

SOVIET PHYSICS JETP VOLUME 5, NUMBER 6 DECEMBER 15, 1957

On the Magnetic Properties of Superconductors of the Second Group

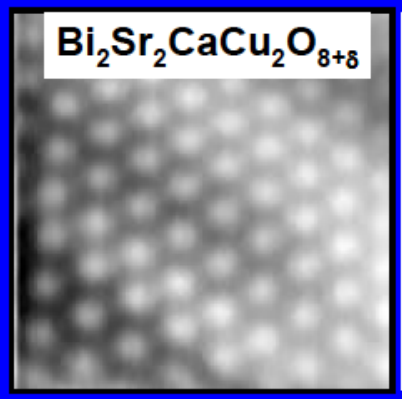
A. A. ABRIKOSOV
Institute of Physical Problems, Academy of Sciences, U.S.S.R.
(Submitted to JETP editor November 15, 1956)
J. Exptl. Theoret. Phys. (U.S.S.R.) 32, 1442-1452 (June, 1957)

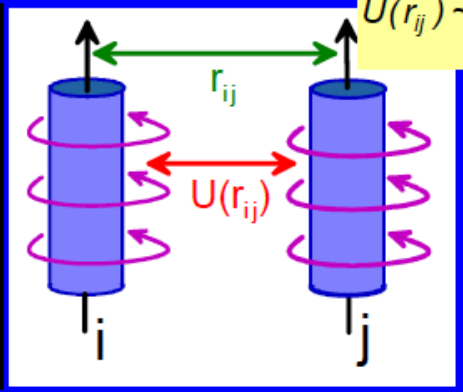
A study is made of the magnetic properties of bulk superconductors for which the parameter κ of the Ginzburg-Landau theory is greater than $1/\sqrt{2}$ (superconductors of the second group). The results explain some of the experimental data on the behavior of superconductive alloys in a magnetic field.



Carte du paramètre d'ordre selon le calcul d 'Abrikosov

$|\psi|^2$ proportional to the density of superconducting electrons



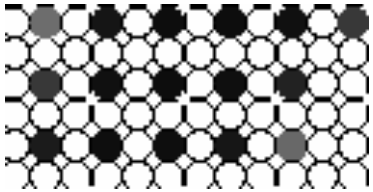


Vortices are mutually repulsive - leads to formation of an ordered triangular lattice.

Interaction between the **vortex**:
repulsion -> two wires with currents in opposite directions
attraction->the superconductor prefering to be in a state with no defects.

Atomic density function theory on constrained lattice

$$F = F_{chem} + E_{elast}$$



$$F_{chem} = \frac{1}{2}\sum_{r,r'} V(r-r')p(r)p(r') + k_B T \sum_{\vec{r}} \left\{ p(r) Ln(p(r) + \left[1 - p(r)\right] Ln\left[1 - (p(r)\right]\right\}$$

$$E_{elast} = \frac{1}{2}\sum_{pq} \int \frac{d^3k}{(2\pi)^3} B_{pq}(\mathbf{n})\theta_p(\mathbf{k})\theta_q^*(\mathbf{k})$$

Microscopic kinetic Onsager equation

$$\frac{dP(r,t)}{dt} = \frac{1}{k_B T}\sum_{\alpha,\beta}\sum_{r'} L_{\alpha\beta}(r-r')c_\alpha c_\beta \frac{\partial F}{\partial P(r',t)}$$

Conserved dynamic if: $\sum_r L(r-r') = 0$

Dynamics of Simultaneous Ordering and Phase Separation and Effect of Long-Range Coulomb Interactions

L.Q. Chen, A.G. Khachaturyan, PRL 1993

The finite range interaction (attraction)

$$V(\mathbf{k})_{\text{fi}} = 2W_1[\cos 2\pi h + \cos 2\pi l] + 4W_2 \cos 2\pi h \cos 2\pi l + 2W_3[\cos 4\pi h + \cos 4\pi l], \quad (3)$$

The long-range interaction (repulsion)

$$W(\mathbf{r})_{\text{Coul}} = \frac{A}{r}\exp\left(-\frac{r}{r_D}\right), \xrightarrow{\text{FT}} V_{coul}(k) = \frac{4\pi A}{\upsilon_0(k^2 + k_D^2)}$$

$$\frac{dP(r,t)}{dt} = \frac{1}{k_B T}\sum_{\alpha,\beta}\sum_{r'} L_{\alpha\beta}(r - r')c_\alpha c_\beta \frac{\partial F}{\partial P(r',t)}$$

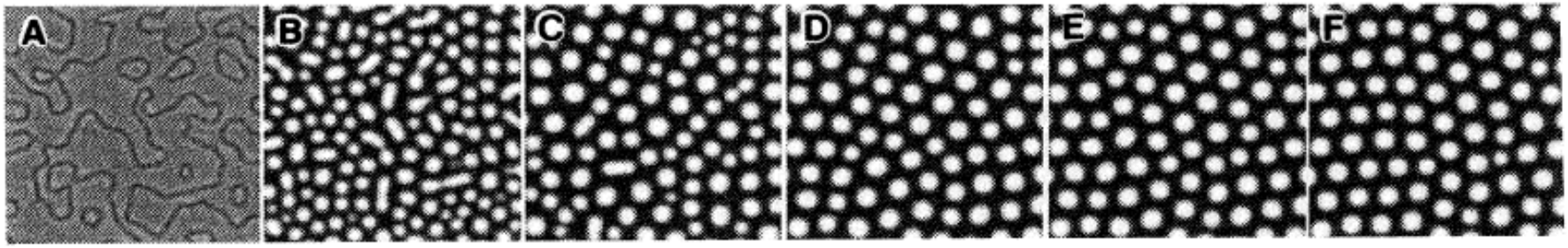


FIG. 2. Temporal morphological evolution started from a completely disordered state with $A = 0.25$ eV and composition $c = 0.175$. The gray level represents the different magnitudes of the absolute value of $c\eta$, where c is the local composition and η is the local long-range order parameter of the ordered phase; c and η are related to the occupation probability by $n(\mathbf{r}) = c(\mathbf{r}) + c(\mathbf{r})\eta(\mathbf{r})$. In this representation, bright regions are ordered domains and dark regions are disordered phase domains. (a) $t^* = 2.5$; (b) $t^* = 10$; (c) $t^* = 100$; (d) $t^* = 500$; (e) $t^* = 1000$; (f) $t^* = 2000$.

In system with only finite-range interactions, the resultant two-phase mixture will continuously coarsen reducing its interfacial energy. The Coulomb interaction stops the coarsening after the ordered particles reach certain size. Eventuelly, all ordered particles reach the same size and form a spectacular regular pattern of a triangular lattice.

Phase Field Crystal method (K. Elder, 2002) -> zones with high concentration-> atoms

Free energy change with respect to homogeneous state is :

$$\Delta F = \frac{1}{2}\iint_V \sum_{\alpha\beta}\left[V_{\alpha\beta}(\mathbf{r}-\mathbf{r}') + \frac{\partial^2 f(\{c_\alpha\})}{\partial c_\alpha \partial c_\beta}\right]\Delta c_\alpha(\mathbf{r})\Delta c_\beta(\mathbf{r}')d^3r d^3r'$$

$D_{\alpha\beta}(k,T,\{c_\alpha\})$ Response function

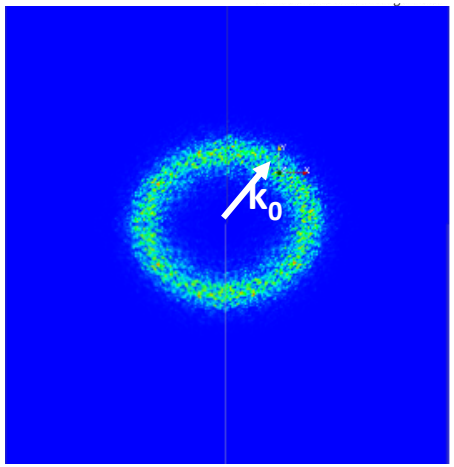
Response function can be estimated from the elastic diffuse scattering

$$I(k) \propto k_B T D^{-1}_{\alpha\beta}(\mathbf{k})$$

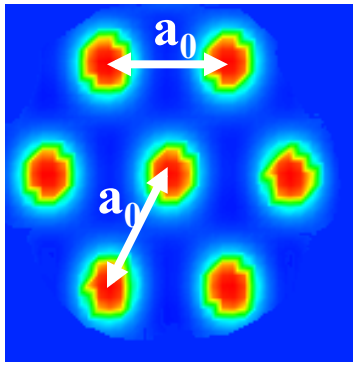
Y. Jin et al. JAP 100, 013519 2006

Why one minima potential gives only “honeycomb” structure in 2D and bcc in 3D simulations ?

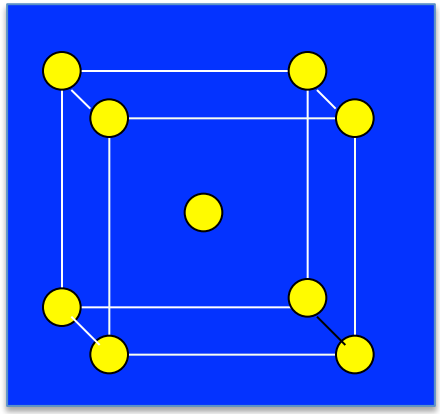
Diffraction pattern of liquid



$$I = c\left(\vec{k}\right)\ c\left(\vec{k}\right)^*$$



2D structure with one characteristic distance and maximum number of first neighbors.



In 3D bcc lattice (fcc reciprocal lattice) the number of first neighbors is maximum

Free energy minima

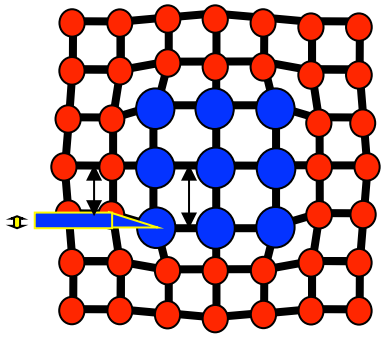
The most stable high temperature modification of the crystalline phase is the one whose reciprocal lattice has maximum possible number of the nearest neighbor sites.

D(k) works as a filter of spatial frequencies.

Anisotropic long range interaction (elastic interaction)

Misfit → **elastic energy**

$$F = F_{chem} + E_{elast}$$



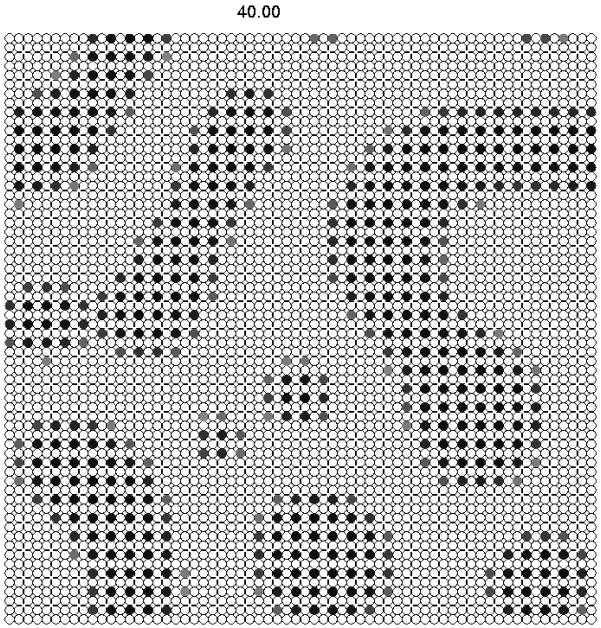
$$E_{elast} = \frac{1}{2}\sum_{p,q}\int \frac{d^3k}{(2\pi)^3}[\lambda_{ijkl}\varepsilon^0_{ij}(p)\varepsilon^0_{kl}(q) - (n\hat{\sigma}^0(p)\hat{\Omega}(n)\hat{\sigma}^0(q)n]\theta_p(k)\theta^*_q(k)$$

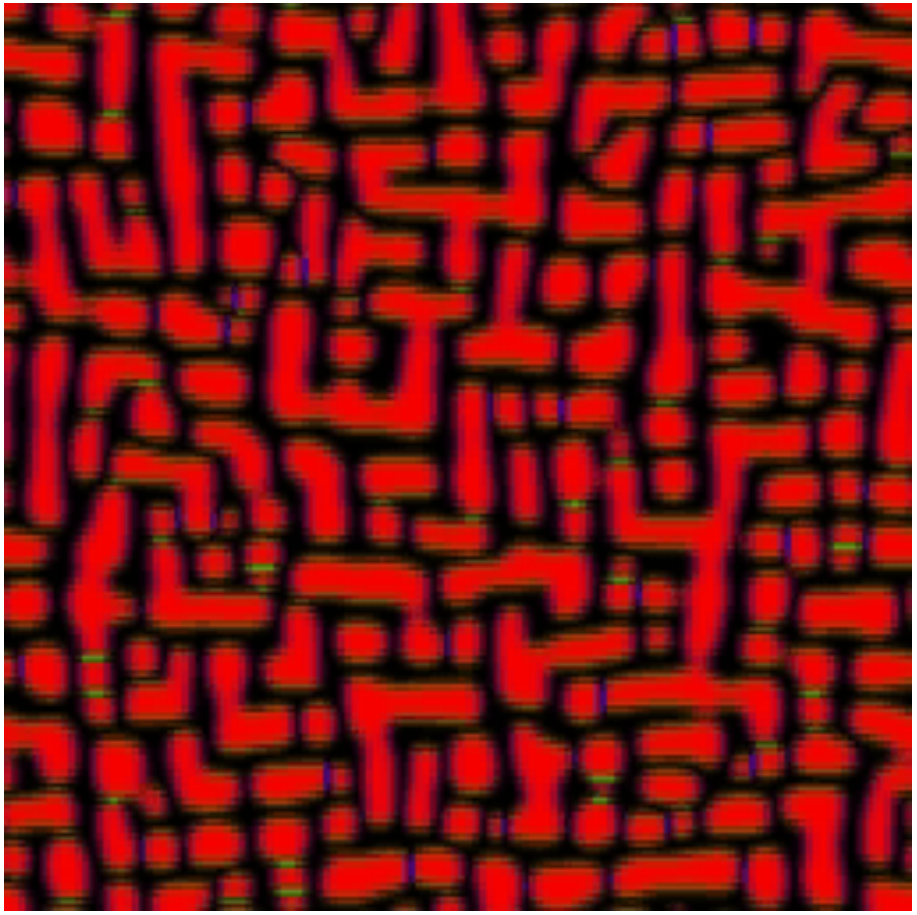
$$\Omega^{-1}_{ij}(\mathbf{n}) = \lambda_{ijkl}n_k n_l \qquad \mathbf{n} = \frac{\mathbf{k}}{k}$$

$$\varepsilon_0 = \frac{a_{L12} - a_{fcc}}{a_{fcc}(c_{L12} - c_{fcc})}$$

$$E_{elast} = \frac{1}{2}\sum_{pq}\int \frac{d^3k}{(2\pi)^3}B_{pq}(\mathbf{n})\theta_p(\mathbf{k})\theta^*_q(\mathbf{k})$$

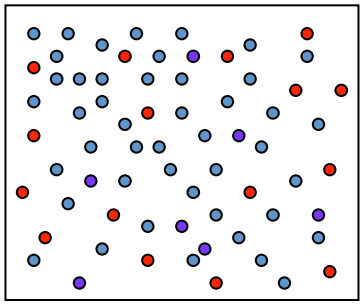
Microstructure evolution in Ni-13%Al à T=800°C with elastic interactions





$L1_2$ phase is presented in red and fcc matrix in black

Atomic density function model (ADF)



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

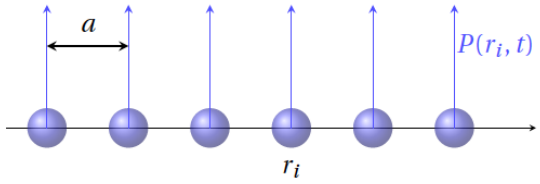
$$\frac{a}{R_{W\alpha\beta}} << 1$$

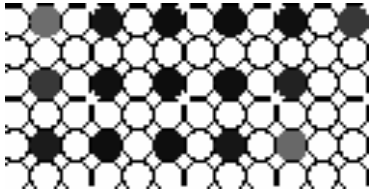
a- Ising lattice parameter

$R_{W\alpha\beta}$- characteristic distance of interatomic interaction

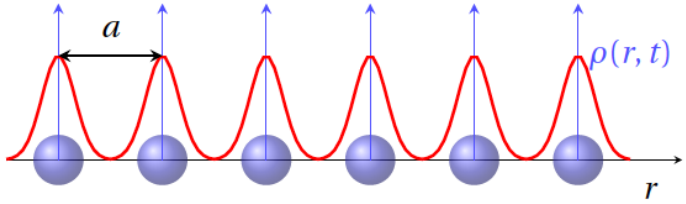
ADF on constrained lattice → **ADF on unconstrained lattice**

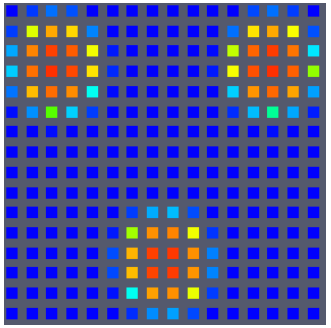
P(r) - probability to find atom at position r





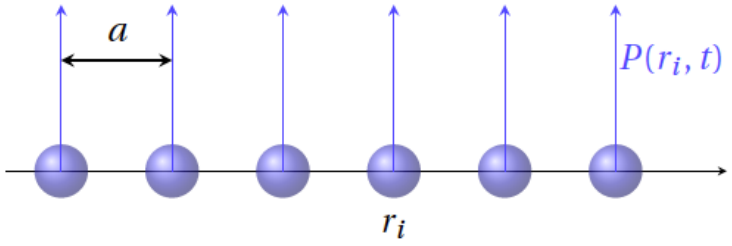
Atomic density function ρ(r)





From discrete to continuum ADF model

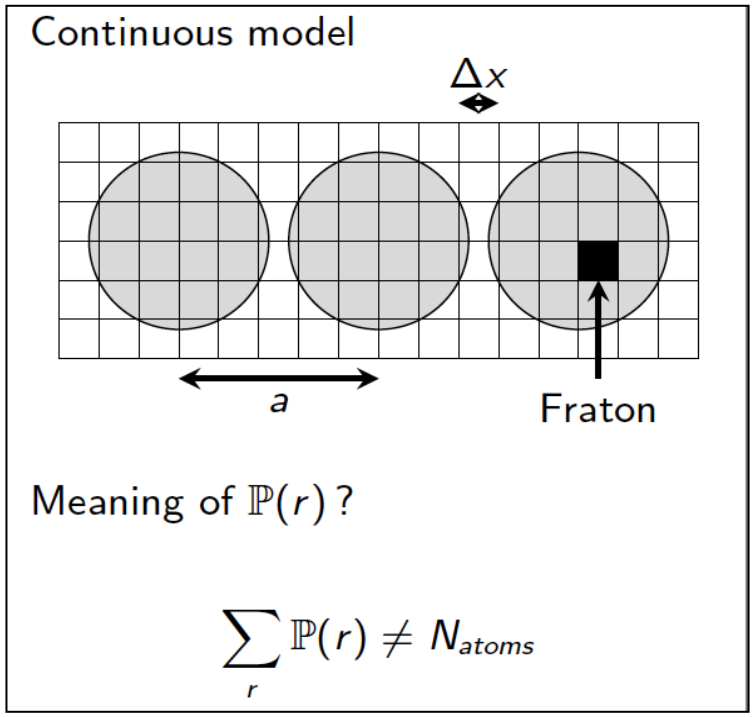
Rigide Ising lattice



(a) Probability $P(r_i, t)$ to find atom on site r_i

- $\mathbb{P}(r)$: probability to find atom at position r
- 1 atome $\Leftrightarrow$ 1 site

$$\sum_r \mathbb{P}(r) = N_{atoms}$$



(M. Lavrskiy et al.,npj computational materials 2016)

Configurational degrees of freedom:

The use of a set of occupation numbers , $c(r)$, equal 1 or 0 for each points, r, of the continuum space rather than a choice of coordinates of centers all of atoms

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

$$\sum_r \mathrm{P}(\mathbf{r}) = N_{fraton}$$

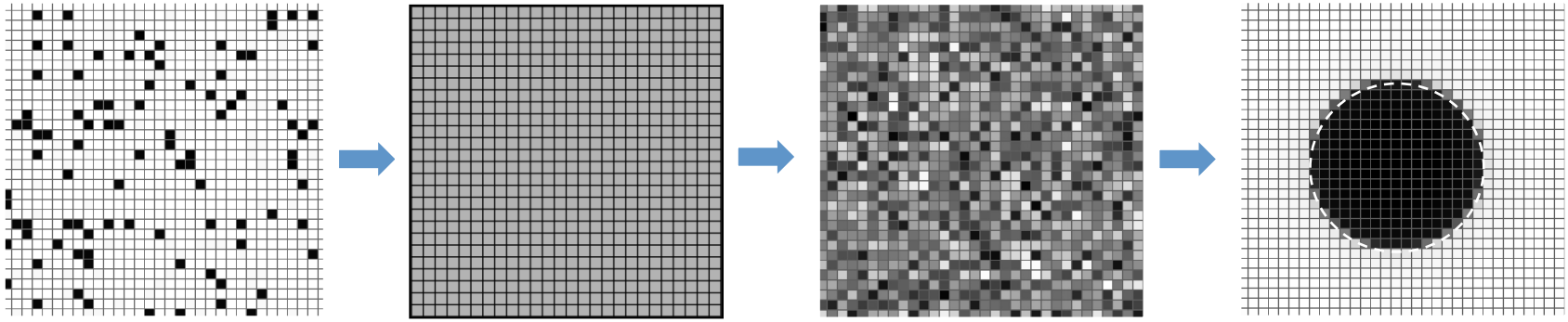
Introduction of occupation numbers, c(r), mimics a transition to the "secondary quantization", by an introduction of creation and annihilation of pseudo-particle. For brevity we name them fratons.

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) | **Homogeneous density of fratons ρ(r)** | **Random fluctuations** | **atoms**

Model Hamiltonian:

$$H = \frac{1}{2}\sum_{r,r'}\sum_{\alpha=1}^{\alpha=m}\sum_{\beta=1}^{\beta=m} w_{\alpha\beta}(\boldsymbol{r}-\boldsymbol{r}')\,\rho_{\alpha}(\boldsymbol{r})\rho_{\beta}(\boldsymbol{r}')$$

the occupation probability of finding a fraton of the kind α (α = 1, 2, ..., m) at the point, *r*

$$\rho_{\alpha}(\boldsymbol{r}) = < c_{\alpha}(\boldsymbol{r}) >$$

interaction potential of two fratons of the kind α and β at sites *r* and *r'* , respectively

$$w_{\alpha\beta}(\boldsymbol{r}-\boldsymbol{r}')$$

Fermi-Dirac statistic

$$\rho_{\alpha}(\mathbf{r}) = \left[\exp\left(\frac{-\mu_{\alpha}+\Phi_{\alpha}(\mathbf{r})}{k_B T}\right)+1\right]^{-1}$$

$$\Phi_{\alpha}(\mathbf{r}) = \sum_{\beta}\sum_{\mathbf{r}'} w_{\alpha\beta}(\mathbf{r}-\mathbf{r}')\rho_{\beta}(\mathbf{r}')$$

The Fourier Transform representation of the model Hamiltonian:

$$H = \frac{1}{2N} \sum_{\boldsymbol{k}} \sum_{\alpha=1}^{\alpha=m} \sum_{\beta=1}^{\beta=m} \tilde{w}_{\alpha\beta}(\boldsymbol{k})\, \tilde{\rho}_{\alpha}(\boldsymbol{k}) \tilde{\rho}_{\beta}(\boldsymbol{k})^{*}$$

Model Potential $\tilde{w}_{\alpha\beta}(\mathrm{k}) = \lambda_1 \underbrace{\tilde{\theta}_{\alpha}(\mathrm{k})}_{\text{Short range}} \delta_{\alpha\beta} + \lambda_2 \underbrace{(\mathrm{k})\ \Psi_{\alpha}^{cltr}(\mathrm{k})\ \Psi_{\beta}^{cltr}(\mathrm{k})^{*}}_{\text{Long range}}$

The structural cluster function $\Psi_{\alpha}^{clstr}(\mathrm{k}) = \sum_{j_\alpha} \omega_j(\alpha, \mathrm{k}) e^{-i\,\mathrm{k}\mathrm{r}_{j\alpha}}$

Structural cluster

A structural cluster for atoms of the kind, α, is a minimum size group of several geometric points numbered by index j_α. Their number and mutual location is chosen to reproduce the topological features of the desirable final configuration of the α-atoms.

In fact, the structural cluster function has a built-in info about length, directions, and rigidity of the bonds.

Limit transition to the Landau theory

$$F = \int \frac{1}{2} \sum_{\alpha\beta} V_{\alpha\beta}(k) \Phi_{\alpha}(k) \Phi^{*}_{\beta}(k) \frac{d^3k}{(2\pi)^3} + \int_V f(\{\rho_{\alpha}(r)\}) d^3r \qquad (1)$$

Where $V_{\alpha\beta}(\mathbf{k})$ is the Fourier transforms of the effective potentials $W_{\alpha\beta}(\mathbf{r})$:

$$\mathrm{V}(\boldsymbol{k}) = \int_{\mathrm{V}} \mathrm{W}(\boldsymbol{r}) \exp(-\mathrm{i}\boldsymbol{k}\boldsymbol{r}) \mathrm{d}^3\mathrm{r}$$

Using Taylor expansion of $V_{\alpha\beta}(\mathbf{k})$ in k

$$V_{\alpha\beta}(k) = A_0^{\alpha\beta} + \frac{1}{2!} A_2^{\alpha\beta} k^2 + \frac{1}{4!} A_4^{\alpha\beta} k^4 + \ldots + \frac{1}{n!} A_n^{\alpha\beta}$$

Eq.(1) is a generalized **Landau gradient expression**:

$$F = \int_V \sum_{\alpha\beta} \left(\frac{1}{2!} A_o^{\alpha\beta} \rho_{\alpha}(\mathbf{r}) \rho_{\beta}(\mathbf{r}) + \frac{1}{2!} A_2^{\alpha\beta} \nabla\rho_{\alpha}(\mathbf{r}) \nabla\rho_{\beta}(\mathbf{r}) + \frac{1}{4!} A_4^{\alpha\beta} \nabla^2\rho_{\alpha}(\mathbf{r}) \nabla^2\rho_{\beta}(\mathbf{r}) + \ldots \right) d^3r$$
$$+ \int_V f(\{\rho(\mathbf{r})_{\alpha}\}) d^3r$$

The **Phase Field Crystal model** has used two first terms of the gradient expansion of the Landau theory.

Kinetic equation (n-components alloy)

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

Free energy functional is:

$$F_{chem} = \frac{1}{2}\sum_{\alpha,\beta}\ \sum_{r,r'} V_{\alpha\beta}(r-r')p_\alpha(r)p_\beta(r') + k_B T \sum_{\alpha}\ \sum_{\vec{r}} \left\{ p_\alpha(r) Ln\left[p_\alpha(r)\right] + \left[1-p_\alpha(r)\ \right] Ln\left[1-(p_\alpha(r)\right]\right\}$$

Reduced variables:

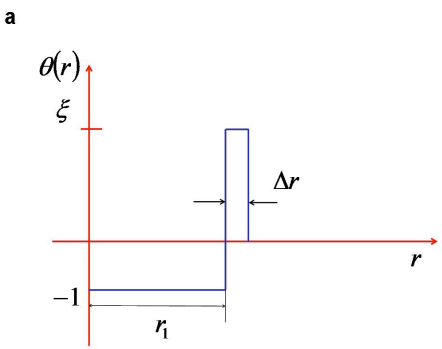
time is measured in units of typical atomic migration time, τ_o

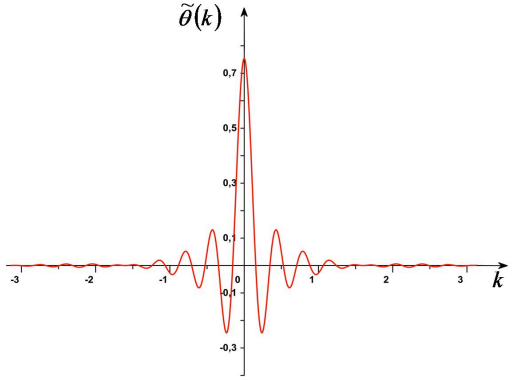
energy is measured in units of $k_B T_o$, where T_o is the solidification temperature

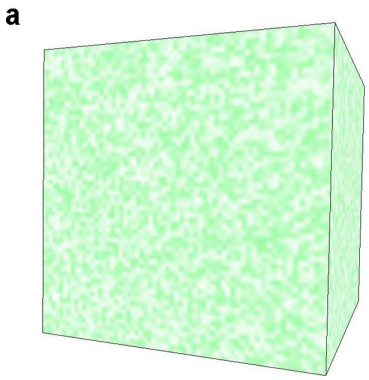
the grid lattice increment, l, (the spacing of the underlying Ising lattice), is defined as a fraction of the atomic radius

The numerical solution -> the semi-implicit Fourier spectral method

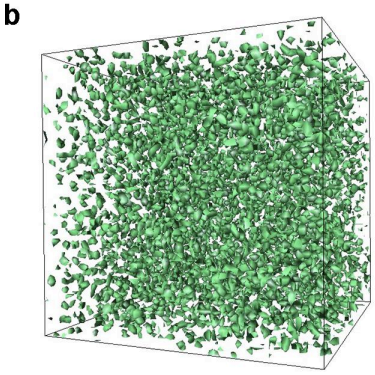
Self-assembly of fratons with only short range interaction



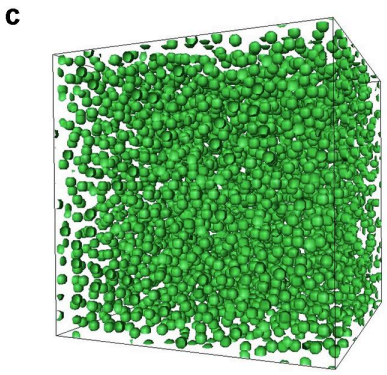




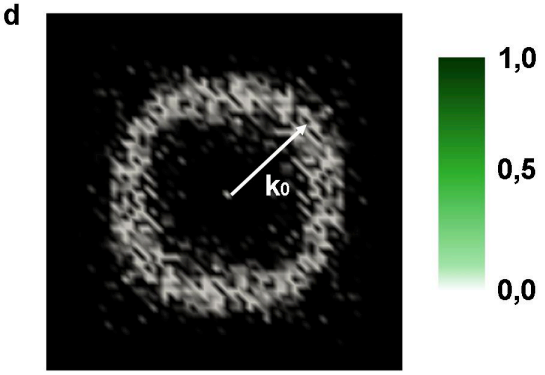
t*=0



t*=50000

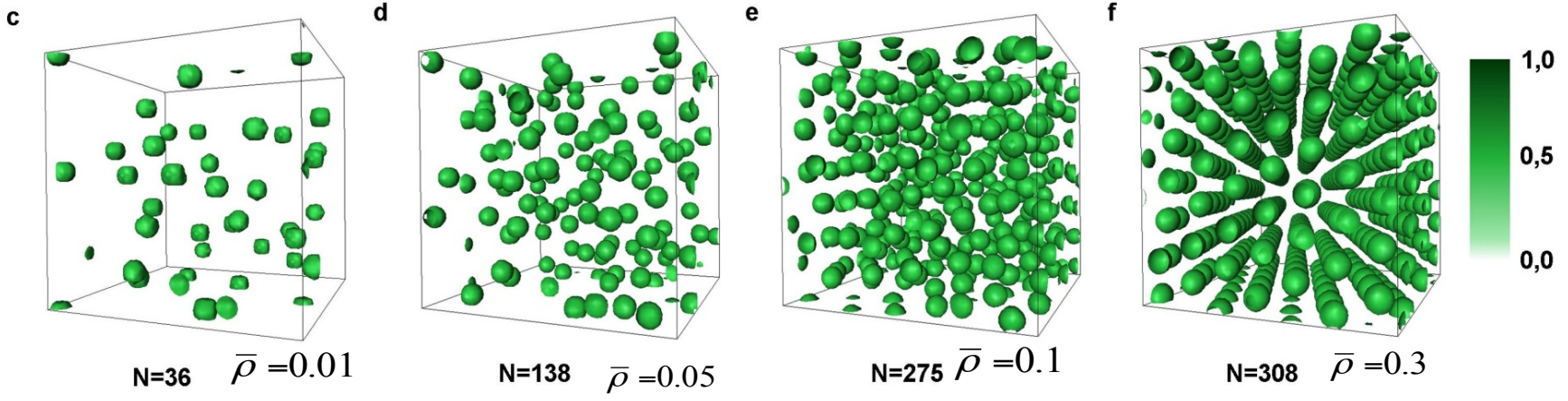


t*=400000



$\hat{\bar{\rho}} = 0.1,\ \hat{l} = 0.5,\ \Delta\hat{r} = 0.17$, and $\hat{T} = 0.63$ $\quad \hat{\lambda}_1 = 45.23,\ \xi = 4$

Equilibrium configuration of fratons with different reduced densities formed by short range potential (r=5Δx)

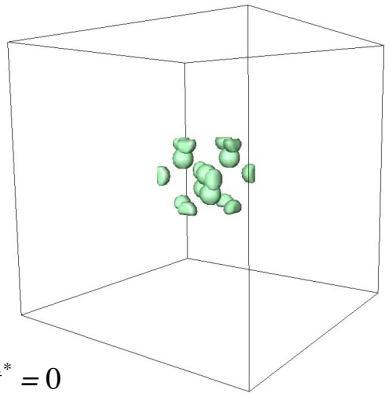


Self-assembly of fratons into diamond structure

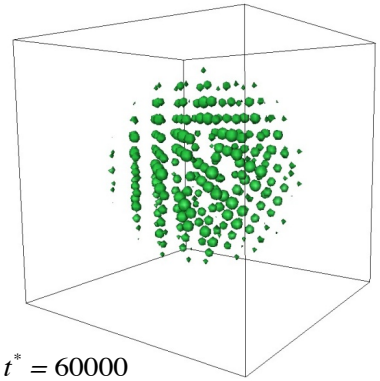
$$\tilde{w}_{LR}(\mathbf{k}) = \lambda_2(\mathbf{k})\tilde{\Omega}_D(\mathbf{k})$$

$$\tilde{\Omega}_D(\mathbf{k}) = \Psi^{cltr}(\mathbf{k})\left(\Psi^{cltr}(\mathbf{k})\right)^* = \left(2+2\cos\left(\frac{a}{4}\left(k_x+k_y+k_z\right)\right)\right)\times$$
$$\times\left(4+4\left(\cos\left(\frac{k_x a}{2}\right)\cos\left(\frac{k_y a}{2}\right)+\cos\left(\frac{k_y a}{2}\right)\cos\left(\frac{k_z a}{2}\right)+\cos\left(\frac{k_x a}{2}\right)\cos\left(\frac{k_z a}{2}\right)\right)\right)$$

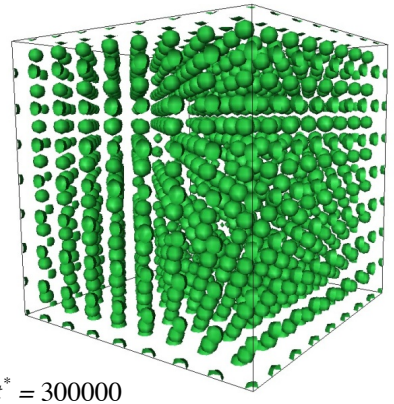
$$\lambda_2(\mathbf{k}) = \begin{cases} \lambda_2 & \text{if} \quad 0 \le \left(k_x+k_y+k_z\right) \le \dfrac{8\pi}{a}+\delta \\ 0 & \text{otherwise} \end{cases}$$



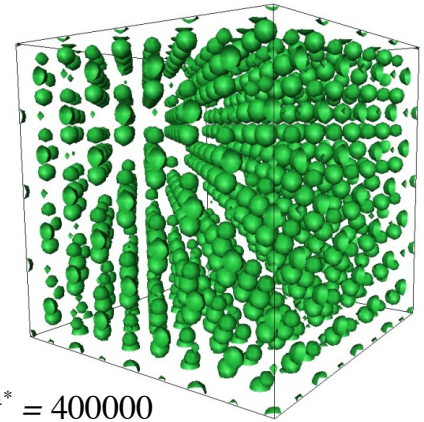
$t^* = 0$



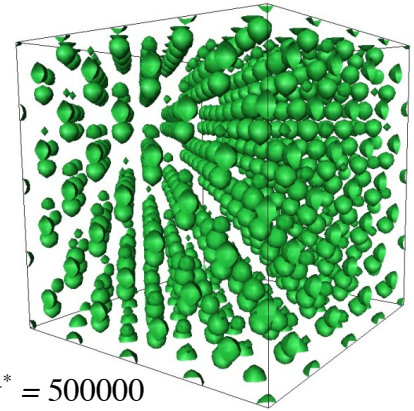
$t^* = 60000$



$t^* = 300000$

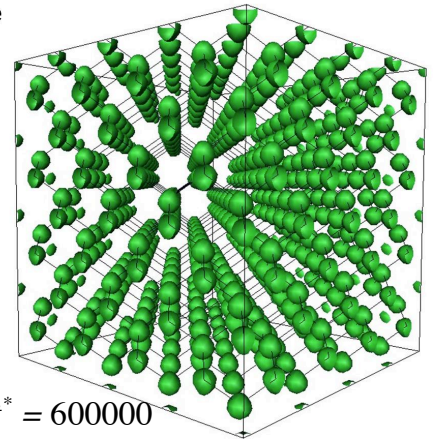


$t^* = 400000$



$t^* = 500000$

e



$t^* = 600000$

Zinc-blende structure

$$V_{AA}(k) = W_{1A}\frac{V_{l.r.}(k)}{maxV_{l.r.}(k) - minV_{l.r.}(k)} + W_{2A}\frac{V_{s.r.}(k, r_A)}{maxV_{s.r.}(k, r_A) - minV_{s.r.}(k, r_A)}$$

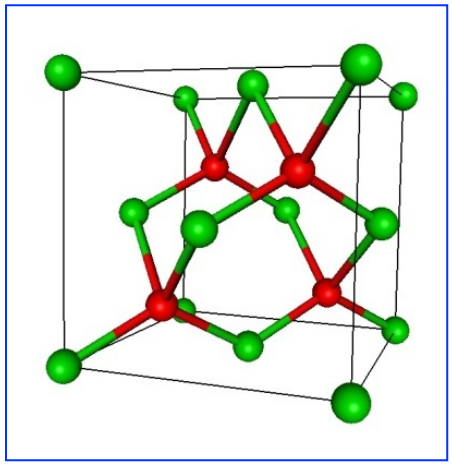
$$V_{BB}(k) = W_{1B}\frac{V_{l.r.}(k)}{maxV_{l.r.}(k) - minV_{l.r.}(k)} + W_{2B}\frac{V_{s.r.}(k, r_B)}{maxV_{s.r.}(k, r_B) - minV_{s.r.}(k, r_B)}$$

$$V_{l.r.}(k) = \left(4 + 4\left(\cos\left(\frac{k_x a}{2}\right)\cos\left(\frac{k_y a}{2}\right) + \cos\left(\frac{k_x a}{2}\right)\cos\left(\frac{k_z a}{2}\right) + \cos\left(\frac{k_y a}{2}\right)\cos\left(\frac{k_z a}{2}\right)\right)\right)$$

$$V_{s.r.}(k) = \frac{4\pi}{k^3}\left(-(\sin(kr) - kr\cos(kr)) + 2(\sin(1.17kr) - 1.17kr\cos(1.17kr) - \sin(kr) + kr\cos(kr))\right)$$

$$V_{AB}(k) = W_{1AB}\frac{V_{AB\,l.r.}(k)}{maxV_{AB\,l.r.}(k) - minV_{AB\,l.r.}(k)}$$

$$w_{LR}^{AB}(k) = 2\cos\left(\frac{a}{4}(k_x + k_y + k_z)\right)\left(4 + 4\left(\cos\left(\frac{k_x a}{2}\right)\cos\left(\frac{k_y a}{2}\right) + \cos\left(\frac{k_x a}{2}\right)\cos\left(\frac{k_z a}{2}\right) + \cos\left(\frac{k_y a}{2}\right)\cos\left(\frac{k_z a}{2}\right)\right)\right)$$



$a = 16dx$

$dx = \pi$

$\frac{k_B T}{k_B T_0} = 0.2354$

$k_B T = 5 \cdot 10^{-3}$

$k_B T_0 = 21.24 \cdot 10^{-3}$

$r_A = 4dx$

$W_{1A} = -0.04$

$W_{2A} = 0.08$

$\bar{\rho}_A = 0.07$

$r_B = 3.5dx$

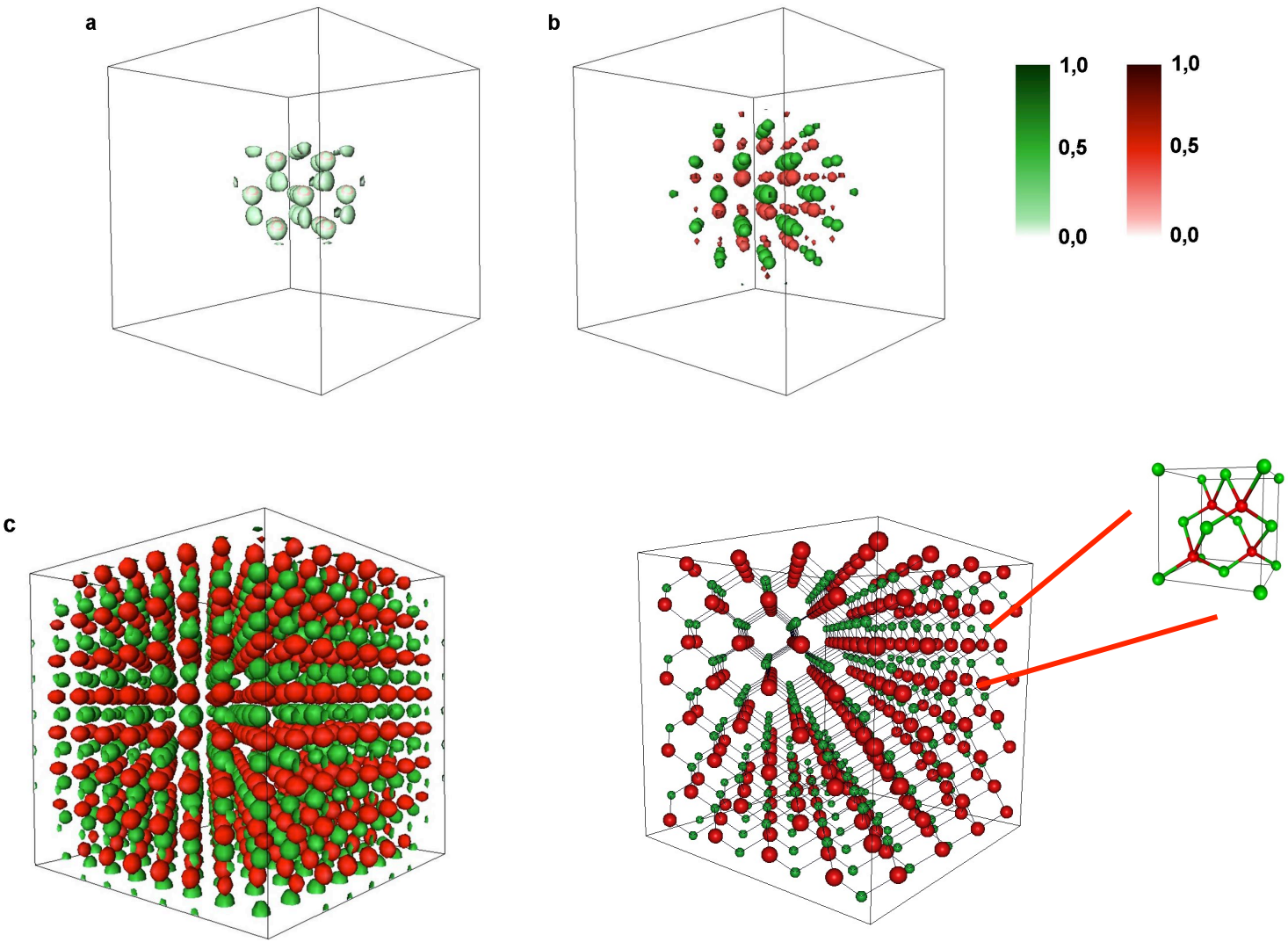
$W_{1B} = -0.062$

$W_{2B} = 0.0124$

$\bar{\rho}_B = 0.045$

$W_{1AB} = -0.048$

Self-assembling of random distribution of two-component liquid into zinc-blende structure

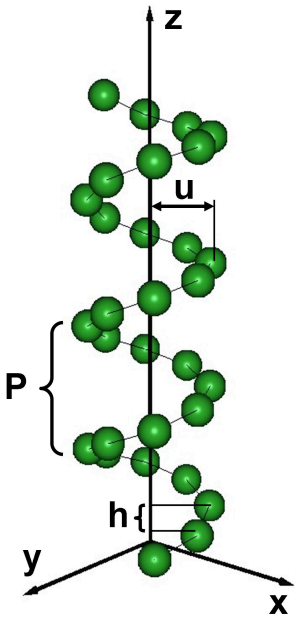


Self-assembling of random distribution of fratons in helix structure

- **Long range potential :**
  - $i_{\alpha\beta}$: structural cluster is the star of bonds indexed by $j_{\alpha\beta}$

    $j_{\alpha\beta}, k$) : thermodynamic and mechanical property of each bond (~ length, directions and rigidity of the bonds)

    $r_{j\alpha\beta}$: atomic sites in the one pitch P



Cluster

$$\widetilde{\Omega}_H(\mathbf{k}) = \left(2 + 2\cos\left(hn_0k_z\right)\right)\left(6 + 2\sum_{n>m=0}^{n_0-1}\cos\left(\phi(n,m)\right)\right)$$

where

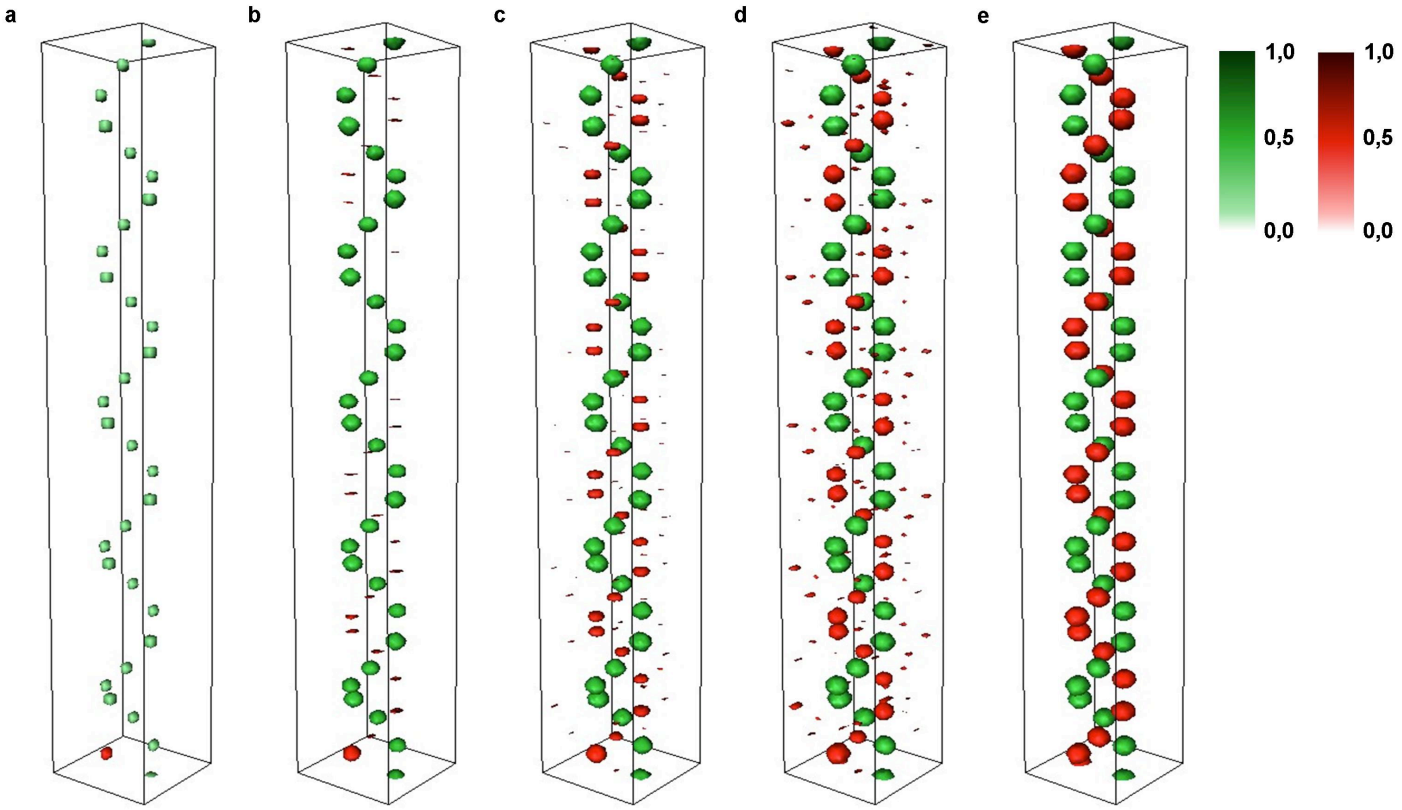
$$\phi(n,m) = k_x u\left(\cos\left(\frac{2\pi n}{n_0}\right) - \cos\left(\frac{2\pi m}{n_0}\right)\right) + k_y u\left(\sin\left(\frac{2\pi n}{n_0}\right) - \sin\left(\frac{2\pi m}{n_0}\right)\right) + k_z h(n-m)$$

Self-assembling of a double-thread helix polymer: single-thread helix in a the “soup” of monomers

$$\Psi_A^{cltr}(\mathbf{k}) = \left(1 + e^{-i\frac{n_0 h}{2}k_z}\right)\left(\sum_{n=0}^{n_0-1} e^{-i(x_n k_x + y_n k_y + z_n k_z)}\right)$$

$$\Psi_B^{cltr}(\mathbf{k}) = e^{-i\frac{n_0 h}{2}k_z}\left(1 + e^{-i\frac{n_0 h}{2}k_z}\right)\left(\sum_{n=0}^{n_0-1} e^{-i(x_n k_x + y_n k_y + z_n k_z)}\right)$$

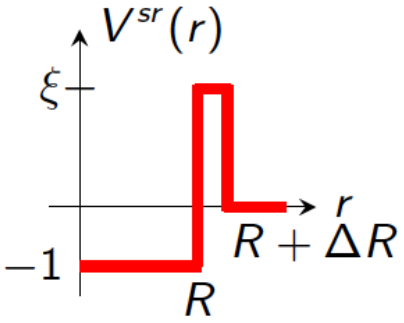
$$\tilde{\Omega}_{DH}^{AB}(\mathbf{k}) = 2\cos\left(h\frac{n_0}{2}k_z\right)\left(2 + 2\cos\left(hn_0 k_z\right)\right)\left(6 + 2\sum_{n>m=0}^{n_0-1}\cos\left(\phi(n,m)\right)\right)$$



α-Fe system

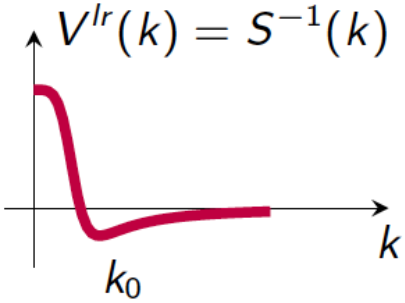
- Short range potential :

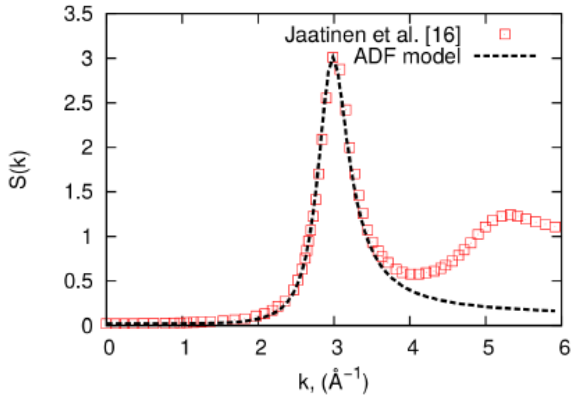
$$V^{sr}(r) = \begin{cases} -1 & \text{if} \quad r < R \\ \xi & \text{if} \quad R \leq r \leq R + \Delta R \\ 0 & \text{if} \quad r > R + \Delta R \end{cases}$$

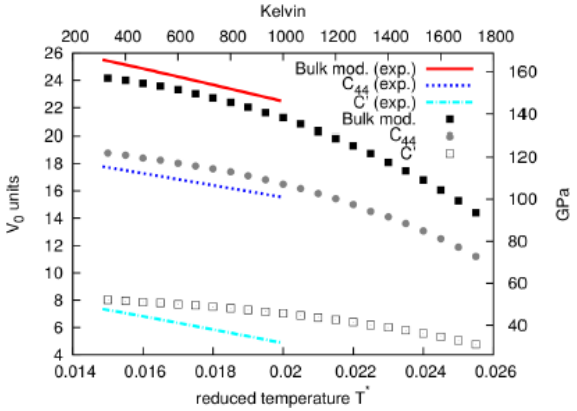


- Long range potential[1] :

$$V^{lr}(k) = 1 - \frac{k^4}{(k^2 - k_1^2)^2 + k_2^4}$$





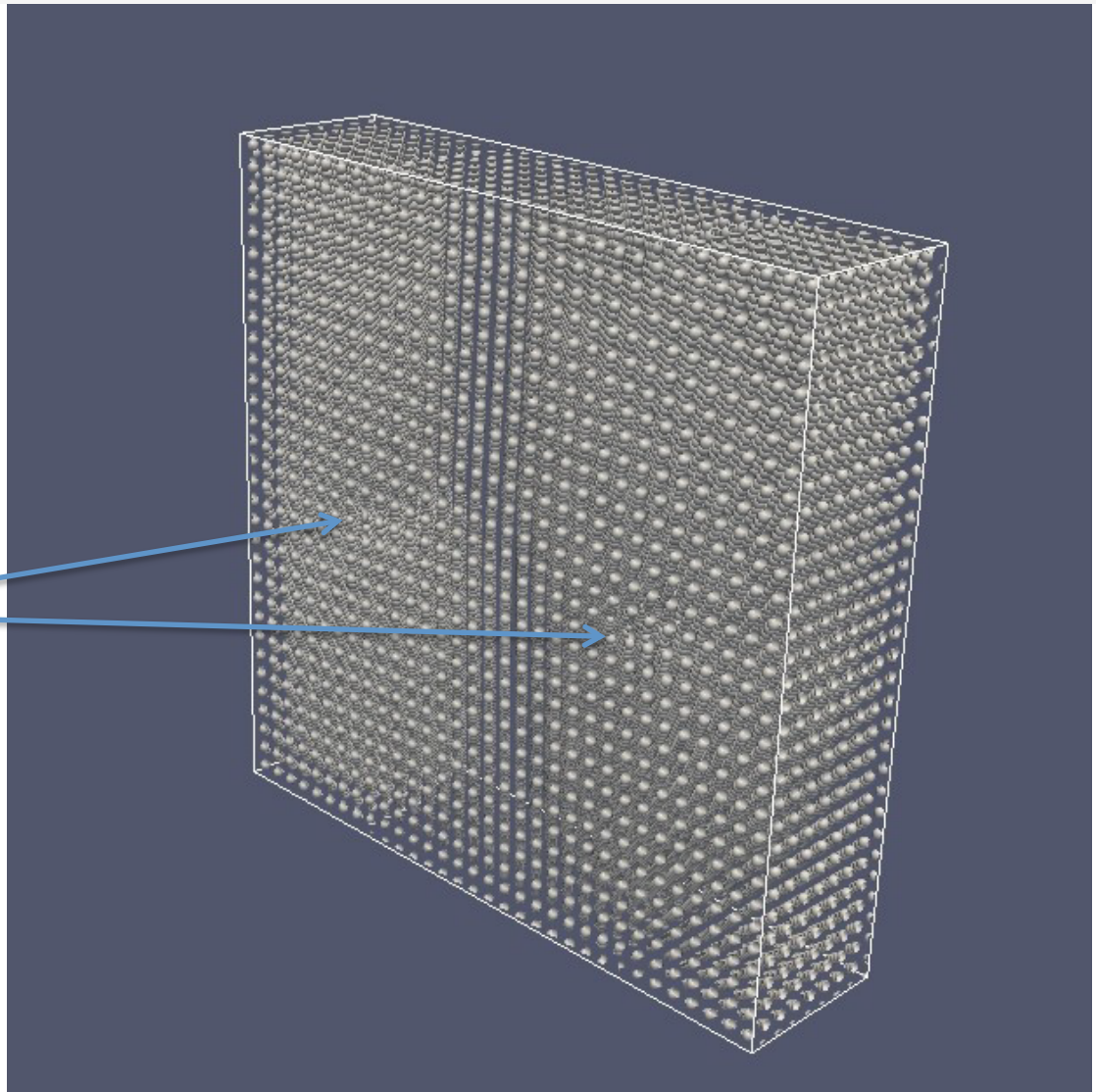


[1] O. Kapikranian, H. Zapolsky & al. Phys. Rev. B 00, 004100 (2015)

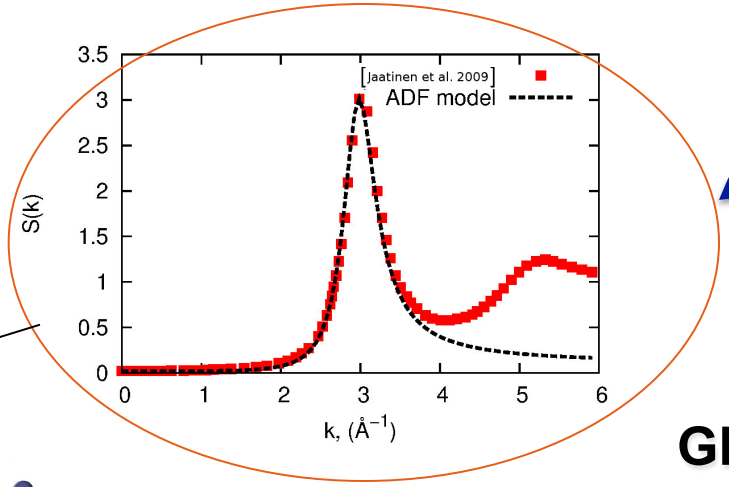
[16] Jaatinen et al. Phys. Rev. E 80 (2009) 031602

GB growth (tilt angle θ = 3.58°)

Dislocations
at GB



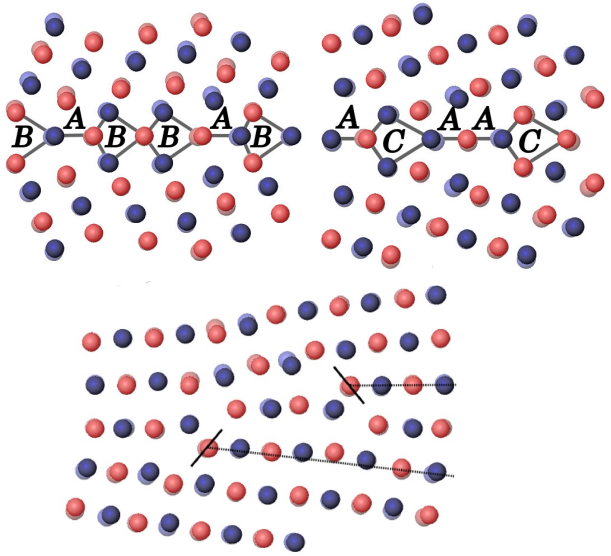
The atomic density function (ADF) model of tilt grain boundaries in α-Fe



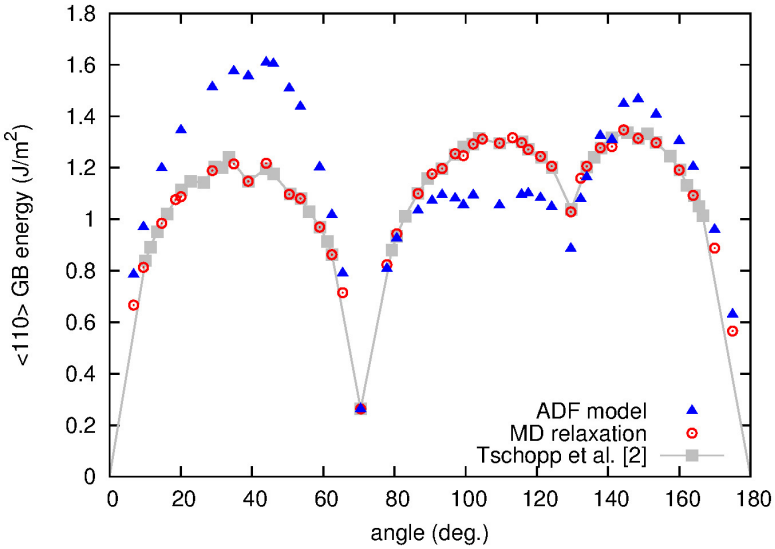
$V_{LR}(k)$

$T=0.9T_m$

Atomic configurations

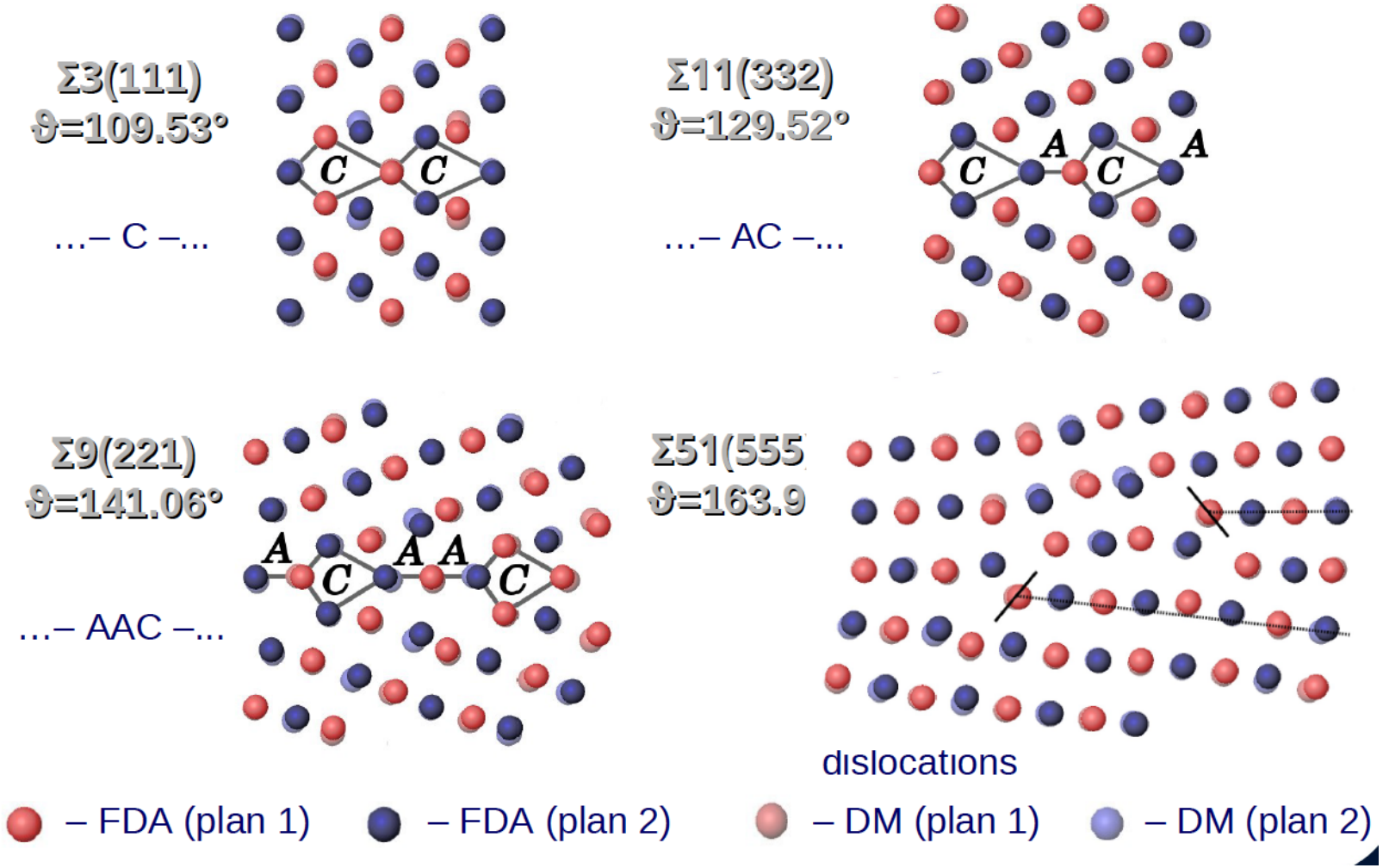


GB energy

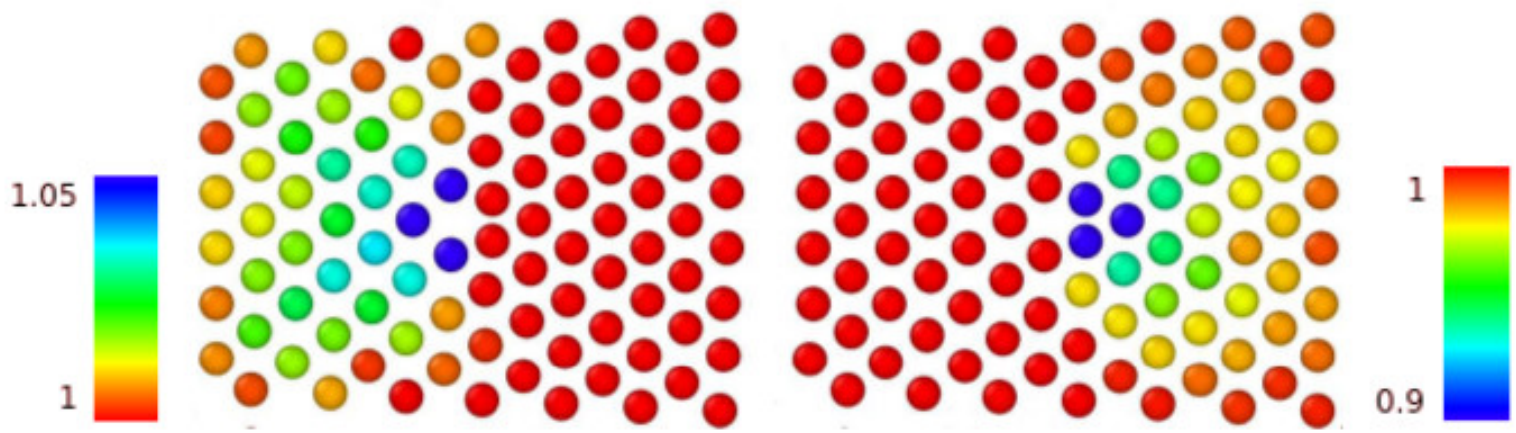


A. Kapikranyan, H. Zapolsky, C. Domain et al., Phys.Rev. B., 89, 014111, 2014.

Configurations of grain boundaries in the bcc Fe



Elastic field around dislocation at grain boundary



expansion **compression**

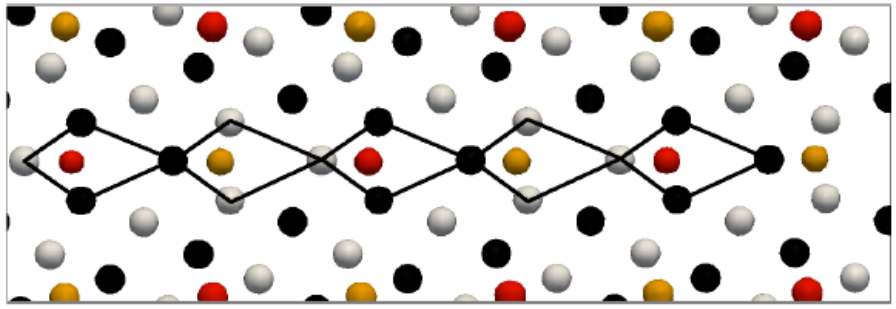
$$\int_{voronoi} d^3r\ \rho(\mathbf{r})/\Omega\rho_0 > 1 \qquad \int_{voronoi} d^3r\ \rho(\mathbf{r})/\Omega\rho_0 < 1$$

Dilated (a) and compressed (b) regions near the edge dislocation of a 4.24 [110] GB, as given by the local atomic density normalized to its bulk value

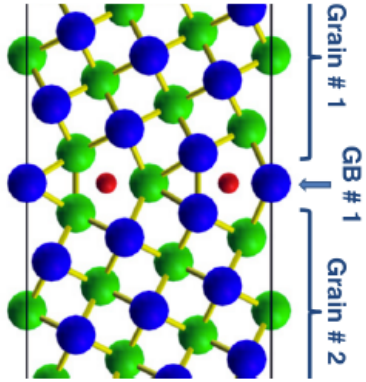
Intersticial segregation : $\langle 100 \rangle$ symmetric tilt GB in α-iron

$R1/R2 = 1.14$.

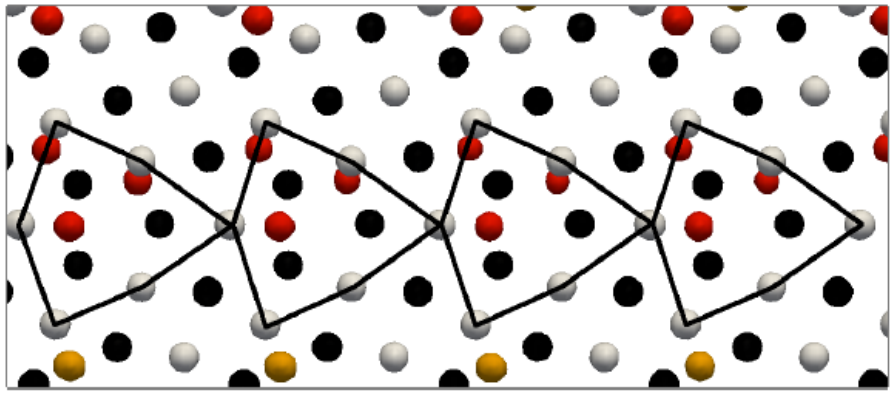
$\Sigma 5(310)$, $\theta = 36.87$, $|B.B|$



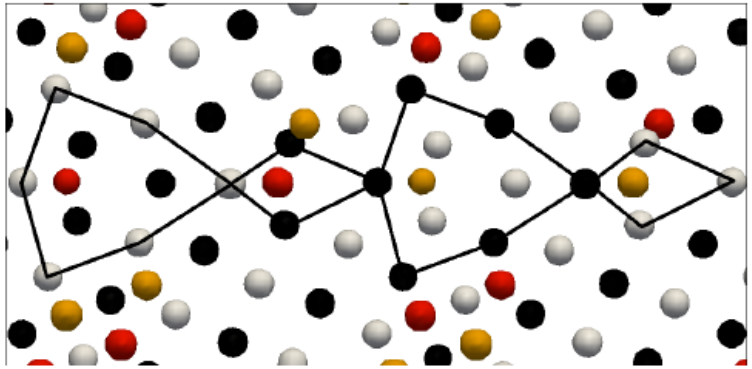
$\Sigma 5(310)$, **Ab initio**[1]



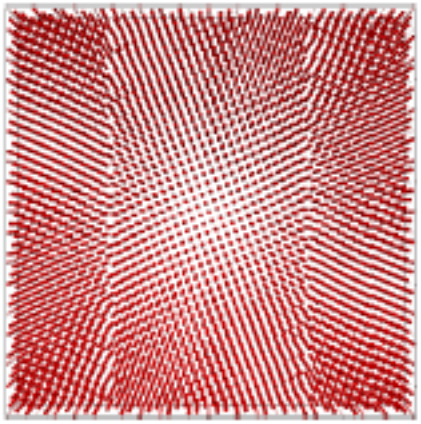
$\Sigma 5(210)$, $\theta = 53.13$, $|C|$



$\Sigma 29(730)$, $\theta = 46.40$, $|BC.BC|$

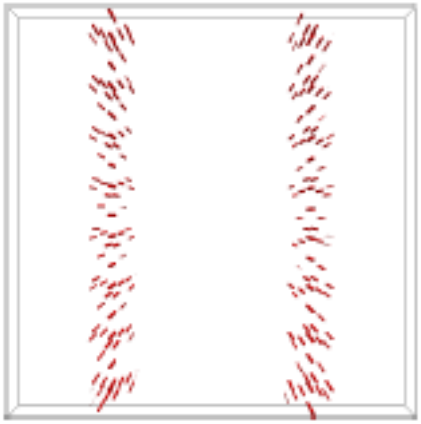


Segregation of P at <100> grain boundary, θ=46.40°



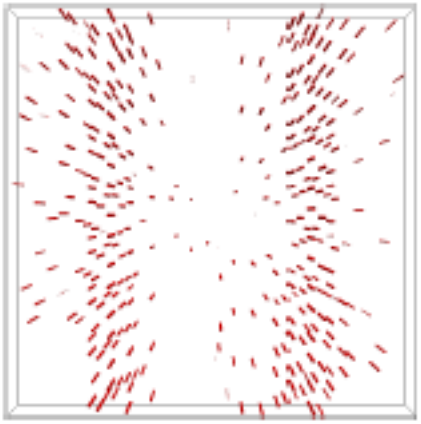
t*=0

Isoconcentrations: 0.05



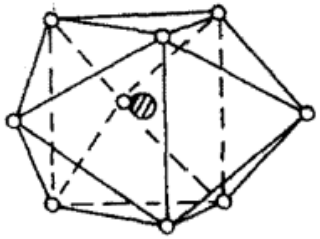
$t^*=10^5$

0.8

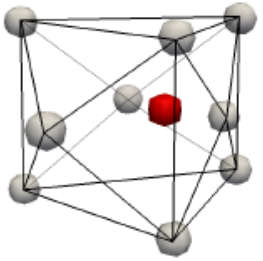


$t^*=2\ 10^5$

0.8



MD

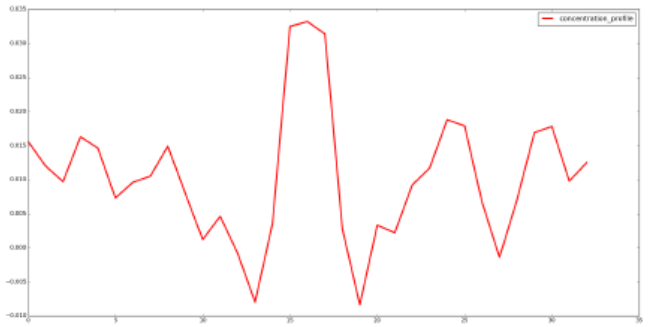


QP

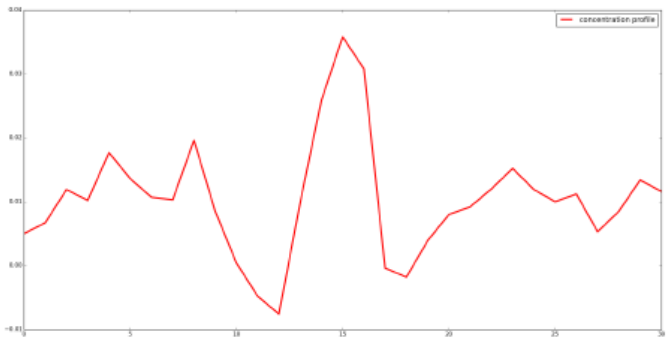
Atomic configuration around P atom situated at GB

Interstitial segregation : Concentration profile

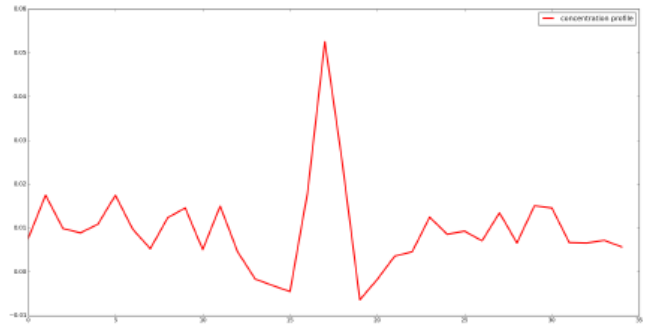
$\Sigma 17(410),\ \theta = 28.07$



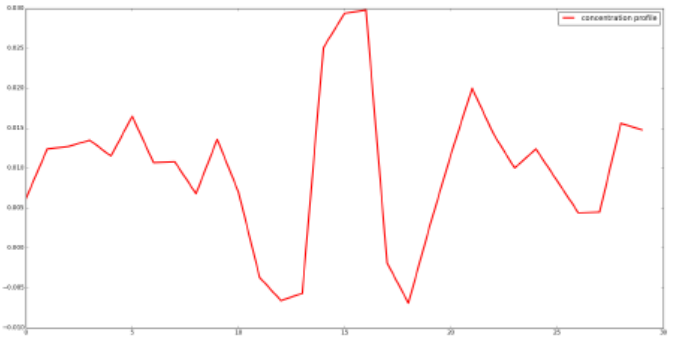
$\Sigma 29(730),\ \theta = 46.40$



$\Sigma 5(310),\ \theta = 36.87$



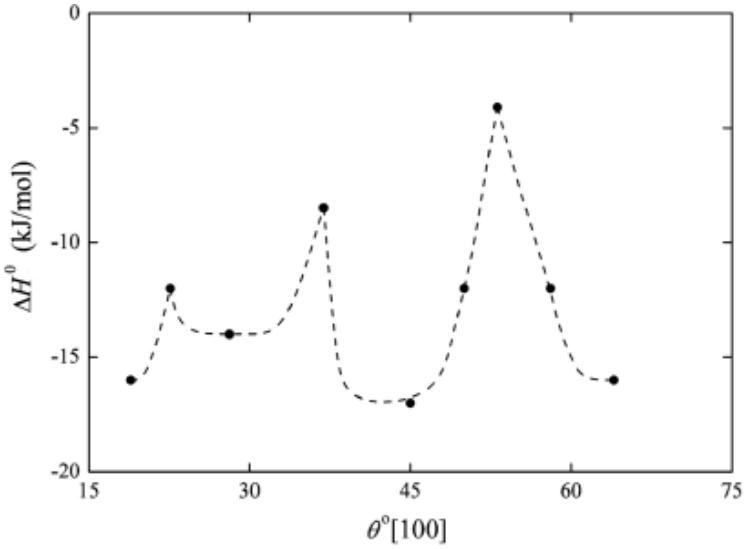
$\Sigma 5(210),\ \theta = 53.13$



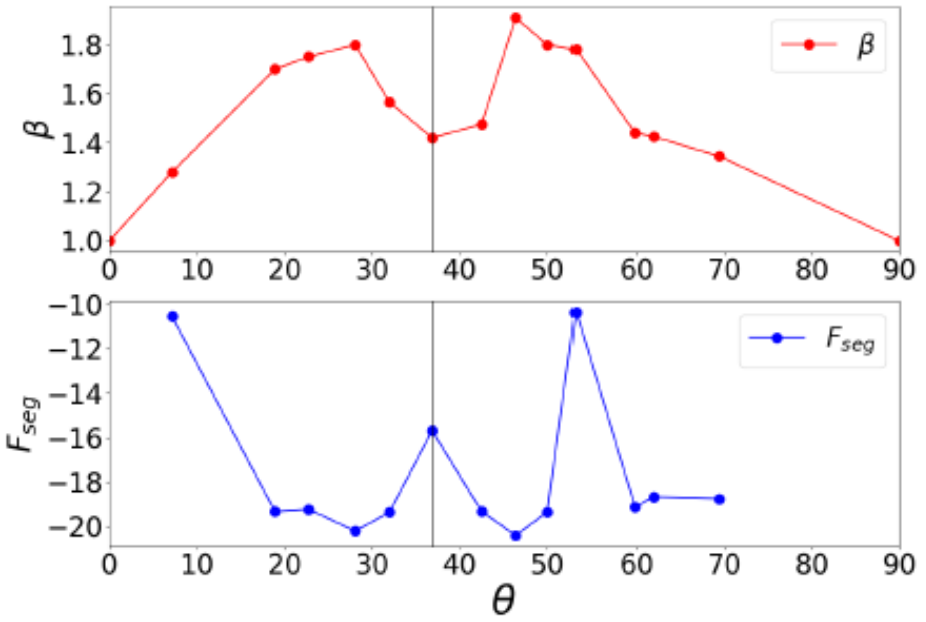
Comparison with Mc Lean theory

Enrichment factor $\beta = \frac{concentration\ \ at\ GB}{concentration\ in\ bulk} \propto \exp(-\frac{\Delta G^{GB}}{RT})$

Experimental data

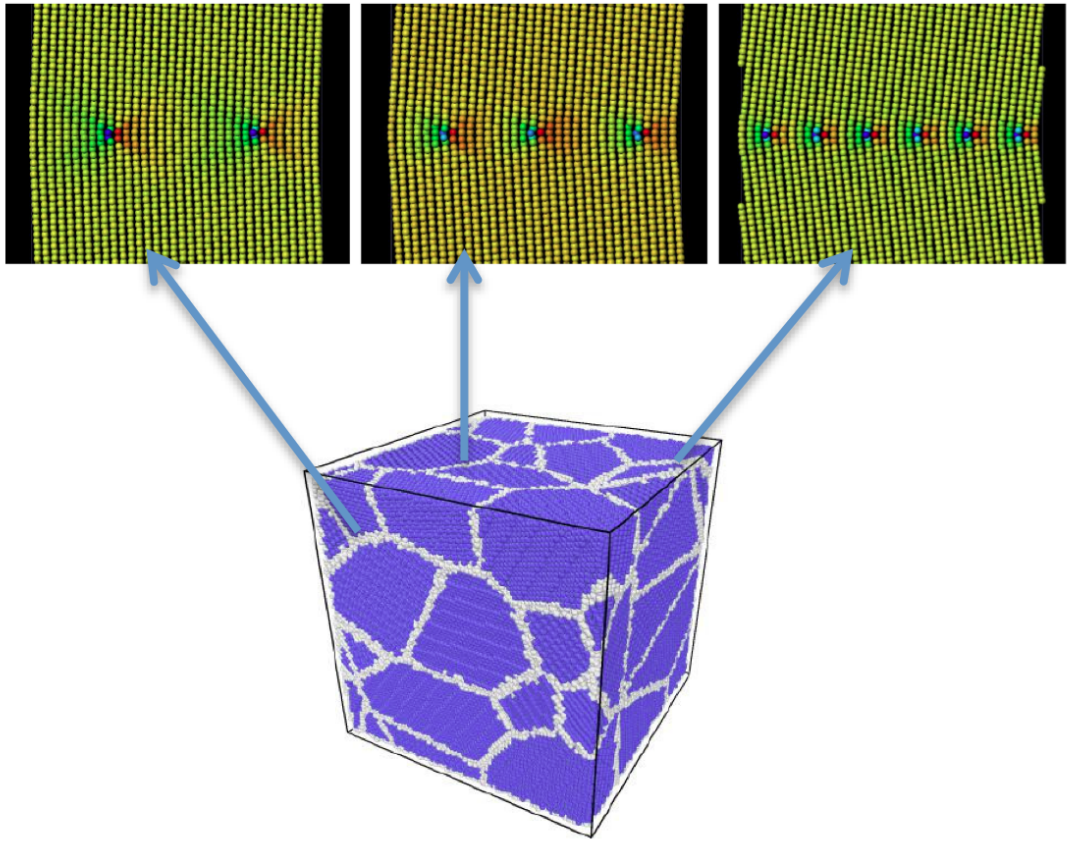


modelling



The dependence of segregation enthalpy of phosphorus in α-Fe

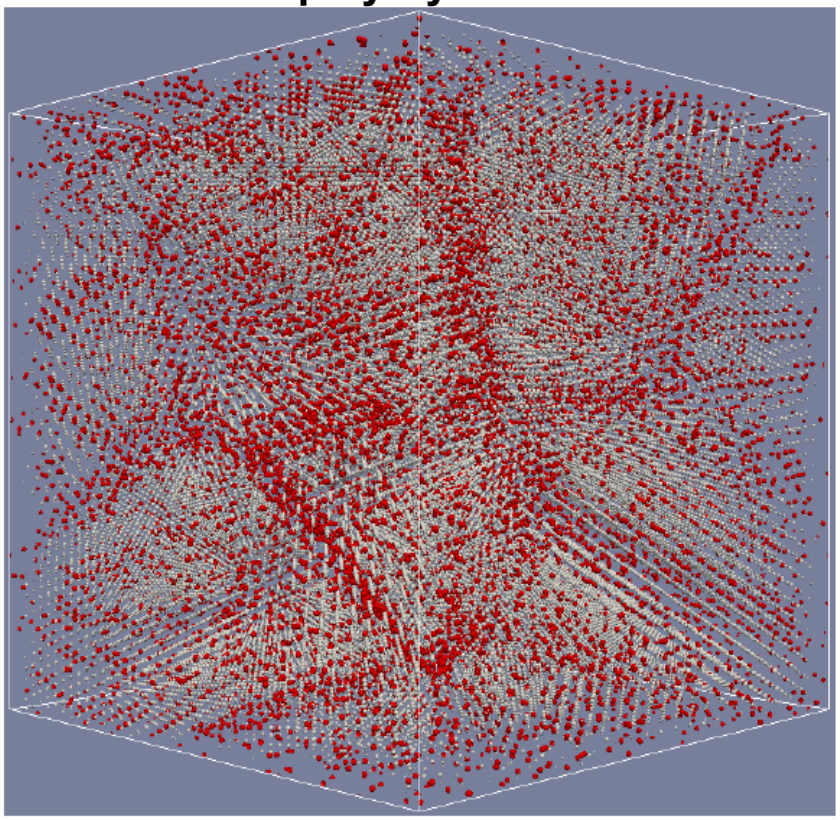
P Lejček, S Hofmann - Critical Reviews in Solid State and Material, 1995

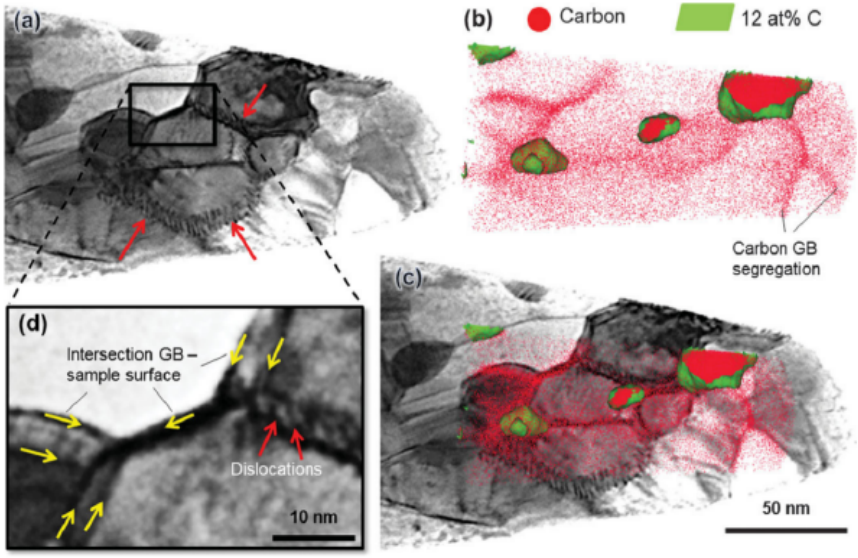


Simulated polycrystal. The grain boundaries are indicated in white. The dislocation structure and associated elastic field around each dislocation at three different grain boundaries are shown.

Segregation in polycristal

Fe-C polycrystal





Segregation of C atoms in duplex steels

Simulation box $= 512^3$

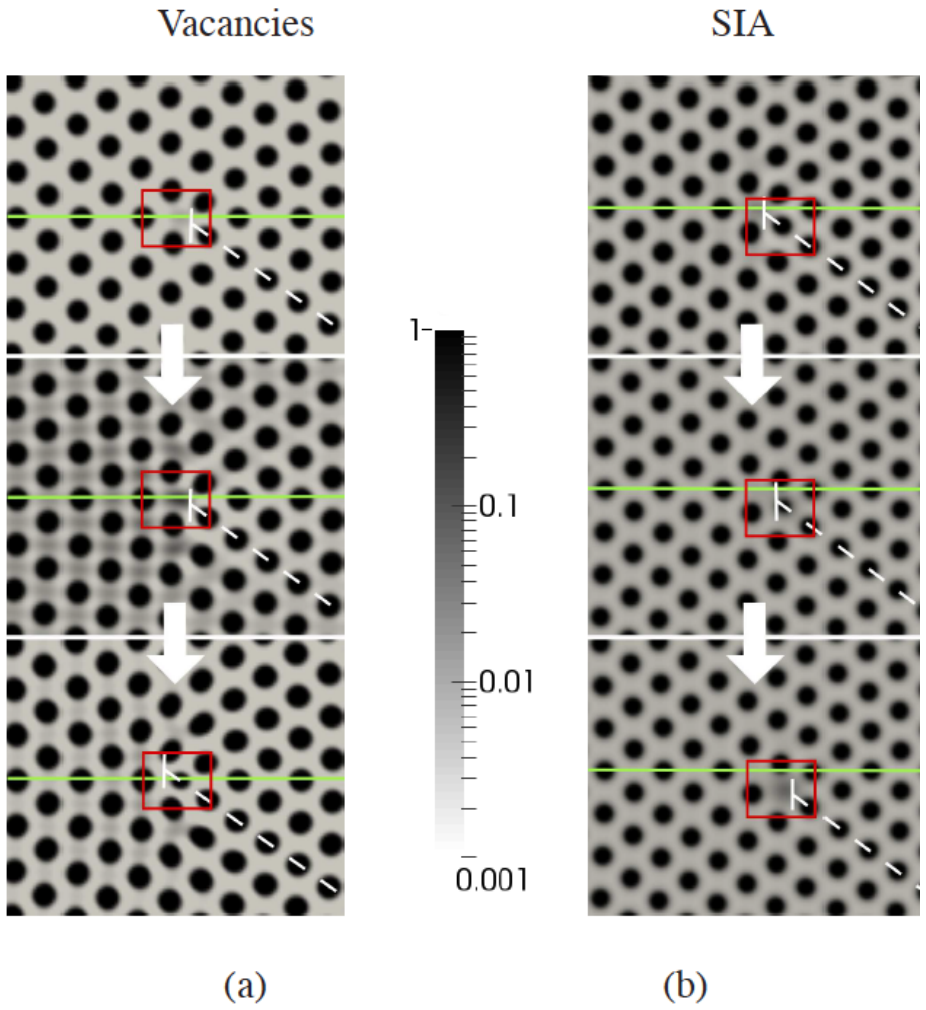
$a_{lattice1} = 16$, $a_{lattice2} = 14$

10 germes

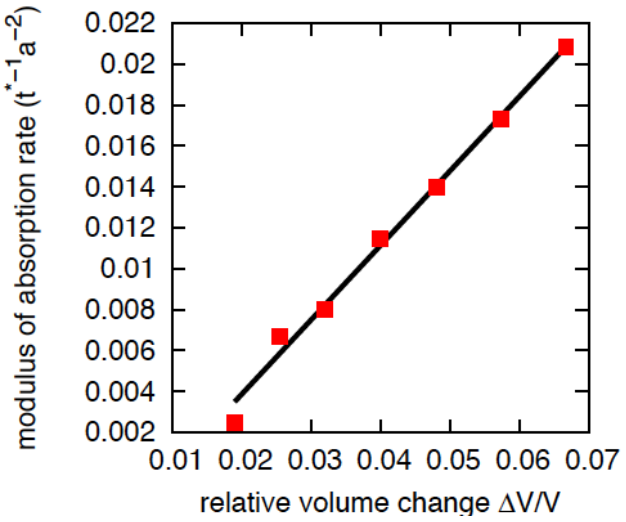
[1] M. Herbig, D. Raabe, Y. J. Li, P. Choi, S. Zaefferer, S. Goto
Physical review Letter 112, 126103 (2014)

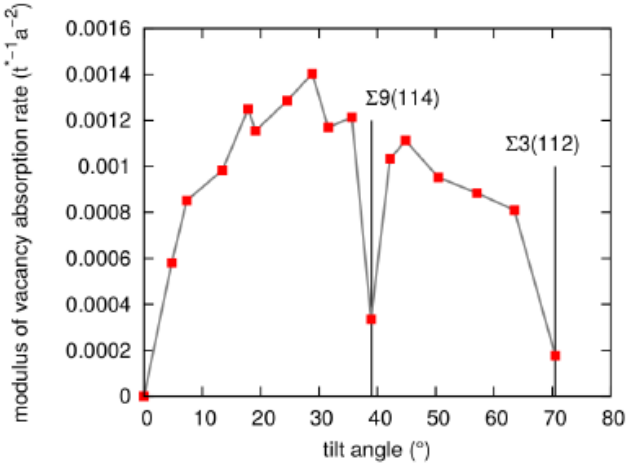
GPM Groupe de Physique des Matériaux

Segregation of vacanacies at <110> GB in α-iron



Point defect absorption kinetics at a [110] edge dislocation (indicated with white dashed lines) in a system with (a) vacancy and (b) self-interstitial supersaturation. The dislocation is part of a GB which plane is highlighted with green color. The [110] cross-sections of the atomic density function profile are given in logarithmic gray scale in order to make visible the variations of the ADF in between the atomic peaks. The time axis is pointing downwards.





O. Kapikranyan et al, Phys.Rev.B, 92, 2015

CONCLUSIONS

1. ***Quasiparticle approach opens a way to answer numerous outstanding questions concerning the atomistic mechanisms of the defects formation, the formation of polymers due to aggregation of monomers in their solution, crystalisation soli-solid phase transformations and etc.***

2. ***Two new ideas in Quasiparticle method:***

- the configuration of the system is defined by fraton density function.

-the interatomic interaction is defined by structural cluster

Thanks for your attention