

# Modélisation numérique, outil indispensable pour mieux comprendre les matériaux

Hélène Zapolsky et Denis Ledue

GPM, UMR 6634, Université de Rouen, France

[helena.zapolsky@univ-rouen.fr](mailto:helena.zapolsky@univ-rouen.fr)

[denis.ledue@univ-rouen.fr](mailto:denis.ledue@univ-rouen.fr)

**Discipline**

Engineering

Materials Science

Chemistry

Physics

electronic

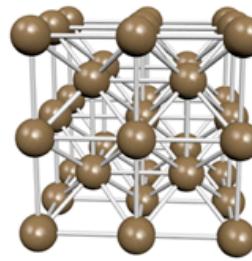
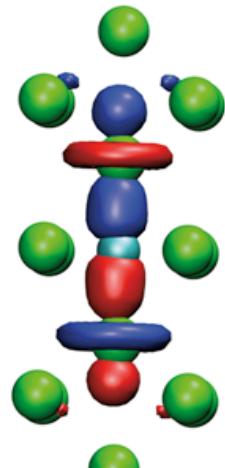
nm

μm

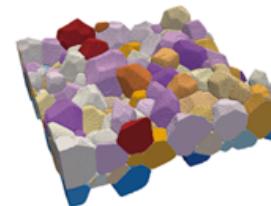
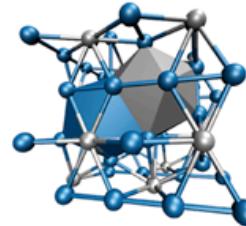
mm

m

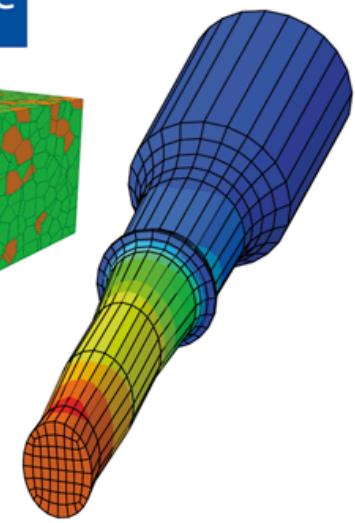
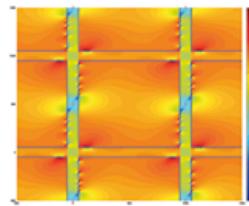
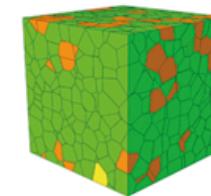
**Length Scale**



atomistic

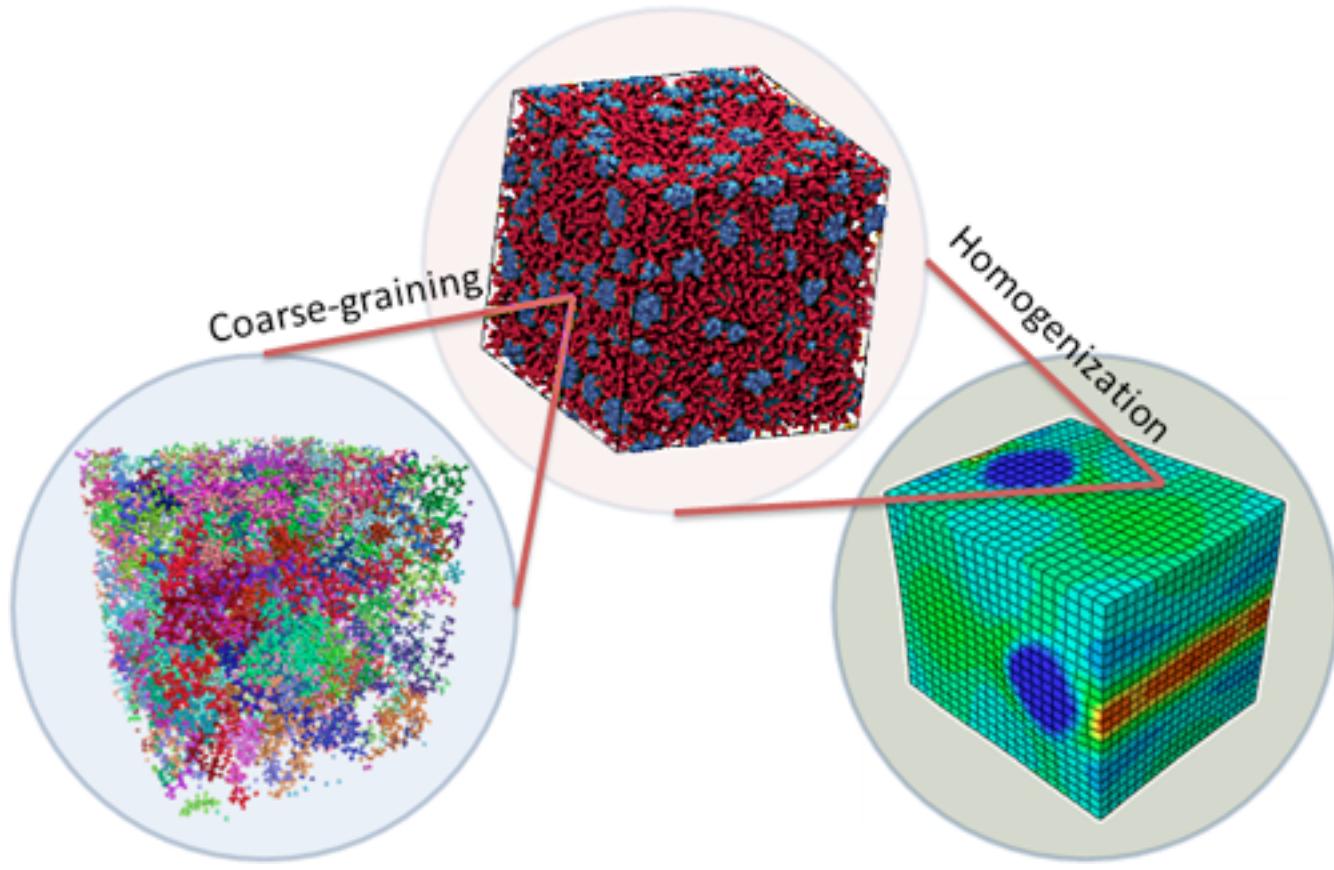


microstructure



macroscale

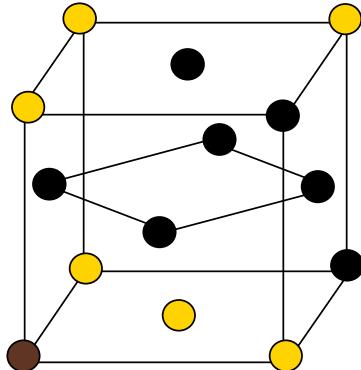
## Champ de Phases



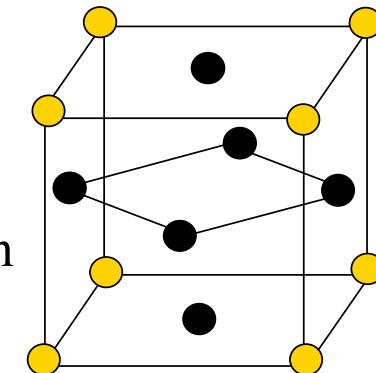
Champ-moyen  
Monte-Carlo

Eléments finis

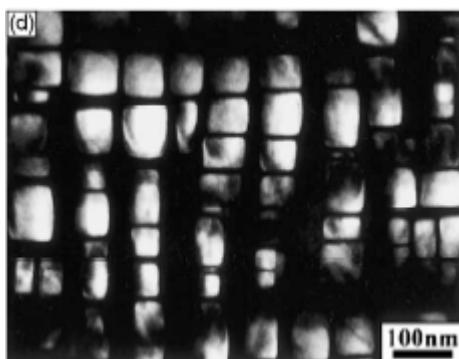
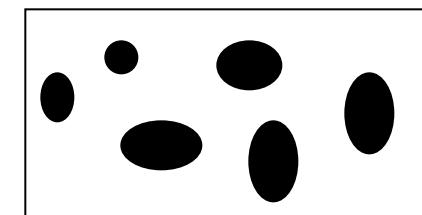
# Vieillissement des alliages



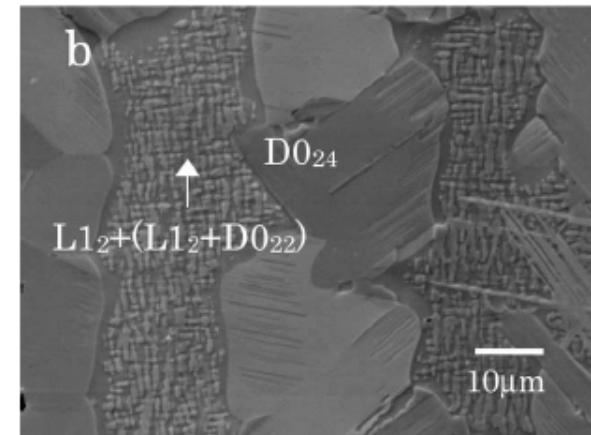
Order-disorder phase transition



Phase separation



microstructure



Ni-8%Al-6%Ti aged at 800°C during 45h

Ni-7.5%Al-15%Ti-2.5%V aged at 1100°C during 5 days

# Applications des superalliages



- Disques de compresseur et de turbine HP élaborés par métallurgie des poudres (MdP)
- Aubes et distributeurs de turbine HP élaborés par solidification monocristalline

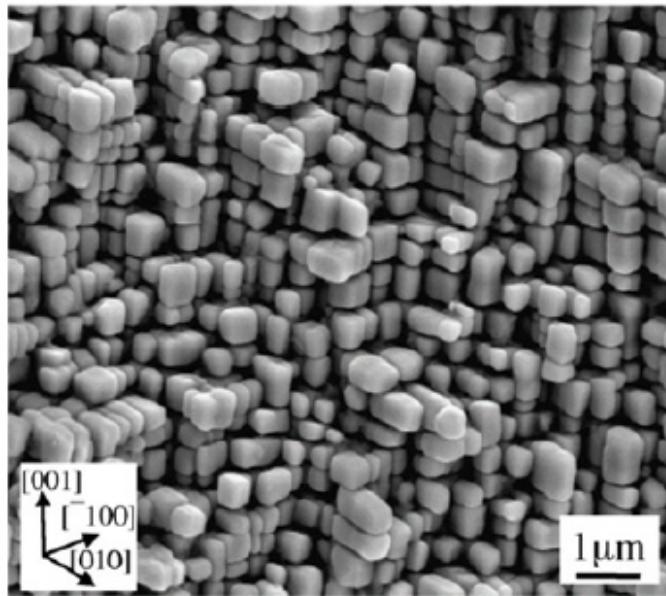


Aubes monocristallines de turbine HP pour hélicoptères

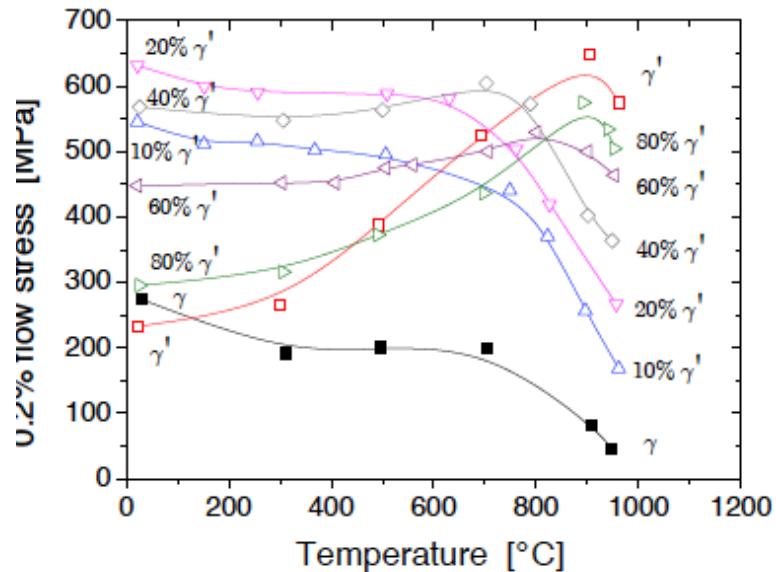


# Précipitation dans les superalliages

(collaborations: ONERA, ArcelorMittal et Aubert&Duval)

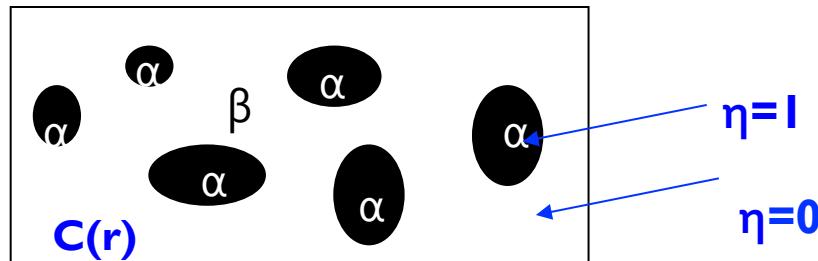


Les particules de la phase  $\gamma'$  ( $\text{Ni}_3\text{Al}$ )



# Phase Field equations (mesoscopic description)

**Phase field variables:**  
**Concentration  $c(r)$**   
**Order parameter  $\eta(r)$**



- Time dependent Ginzburg-Landau equation for the lro parameters

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

Cahn-Hilliard equation for the concentrations

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

M – mobility .

L – kinetic coefficient describing the motion of the interface

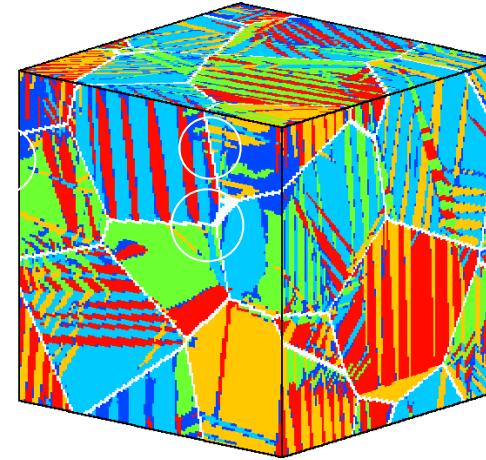
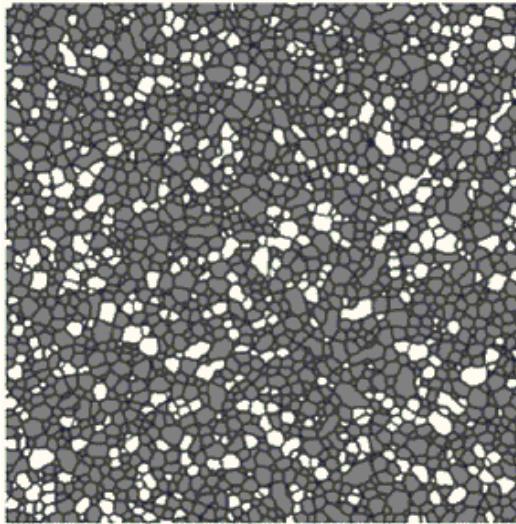
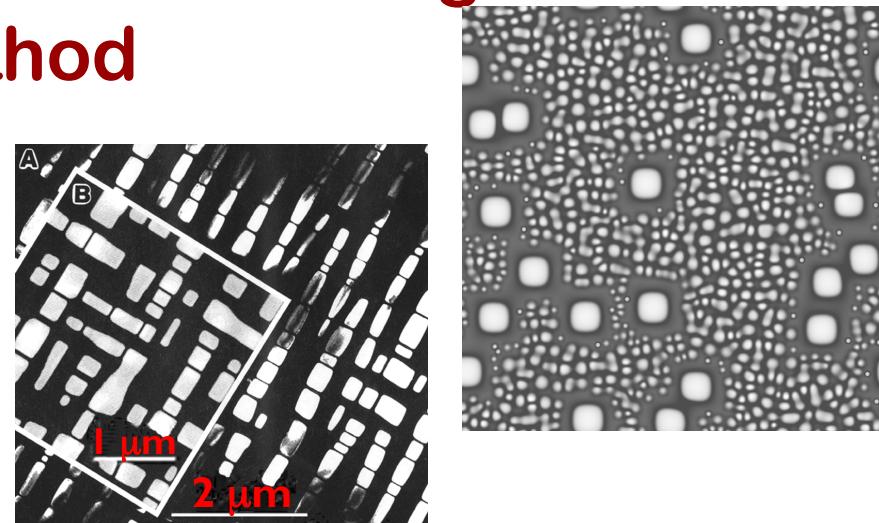
F – total free energy.  $F = F_{\text{chemical}} + F_{\text{elastic}}$

$\zeta_c(r,t)$  et  $\zeta_\eta(r,t)$  – Langevin noises.

# Advanced Microstructure Modeling using Phase Field Method

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

$$\frac{\partial \eta_p(\mathbf{r},t)}{\partial t} = -L \frac{\delta F}{\delta \eta_p(\mathbf{r},t)} + \xi_p(\mathbf{r},t)$$

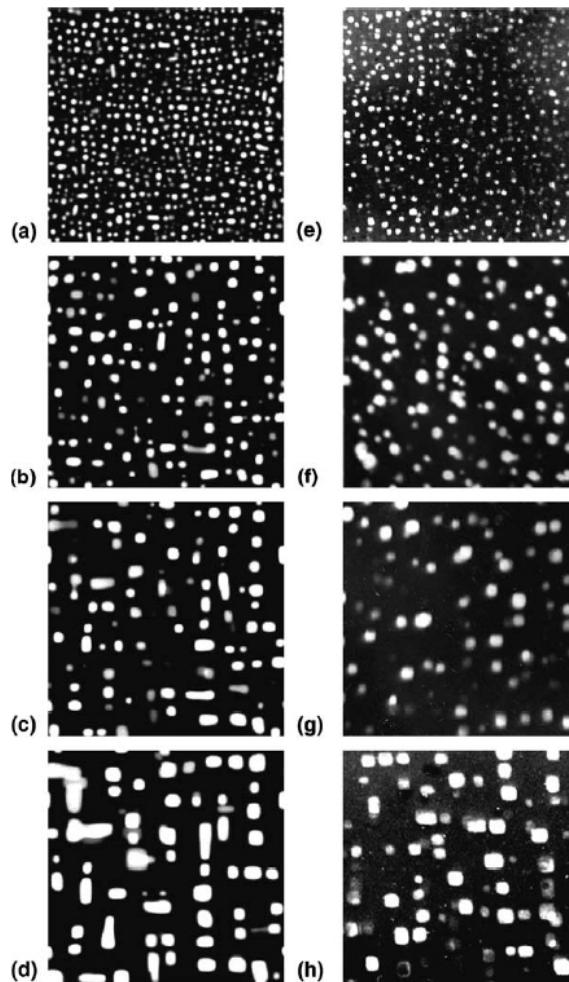


Y. Jin et. al. 2008.

The phase field method handles well arbitrary microstructures consisting of diffusionally and elastically interacting particles and defects of high volume fraction and accounts self-consistently for topological changes such as particle coalescence.

Ni-Al alloys

Simulation

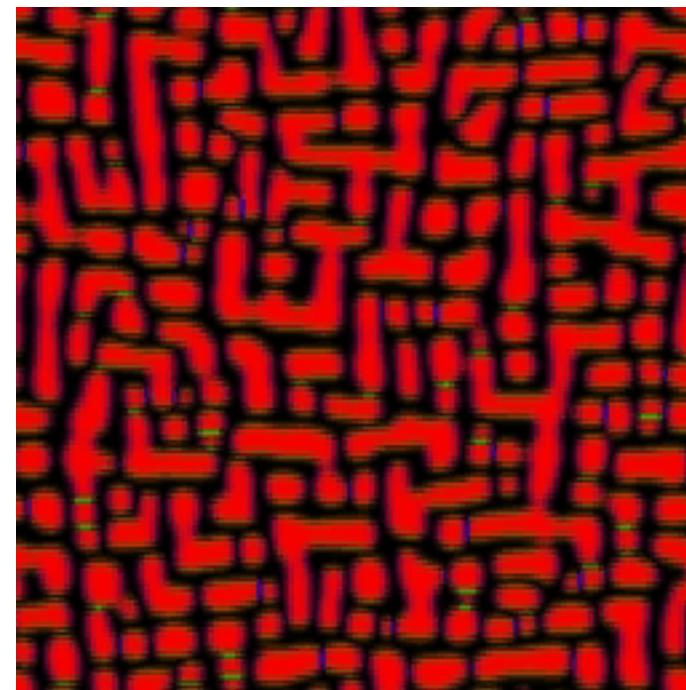


TEM images

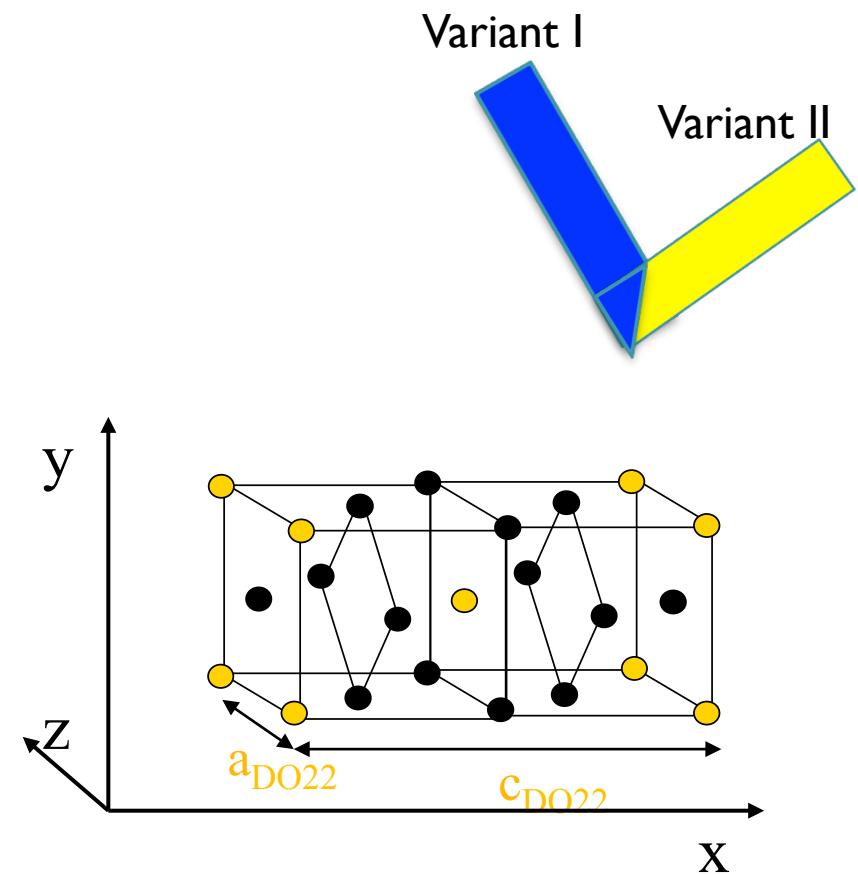
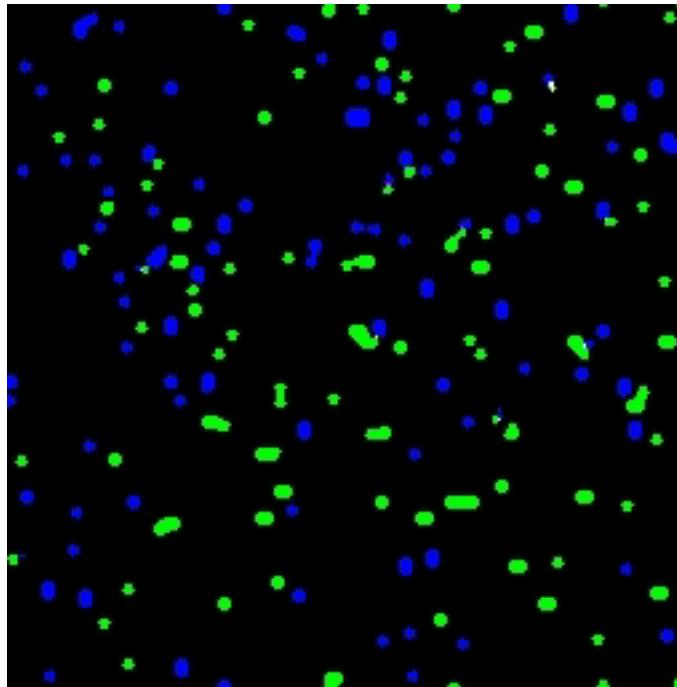
Comparison of the morphology of precipitates of the **L1<sub>2</sub>** Ni<sub>3</sub>Al phase (640Å~640 nm) obtained by phase field modeling (left column) and by TEM (right column) in the Ni—13.8at.%Al aged at 1023 K  
: (a),(e) t = 15 min ; (b),(f) t = 2 h ; (c),(g) t = 4 h ; (d),(h) t = 8 h.

**J. Boisse.H. Zapsolsky, N. Lecoq, R. Patte, Acta Mater. 2007**

## **Evolution de la microstructure dans Ni-20%Al à T=800°C**



## Evolution de la microstructure dans l'alliage Ni-20%V à T=800°C

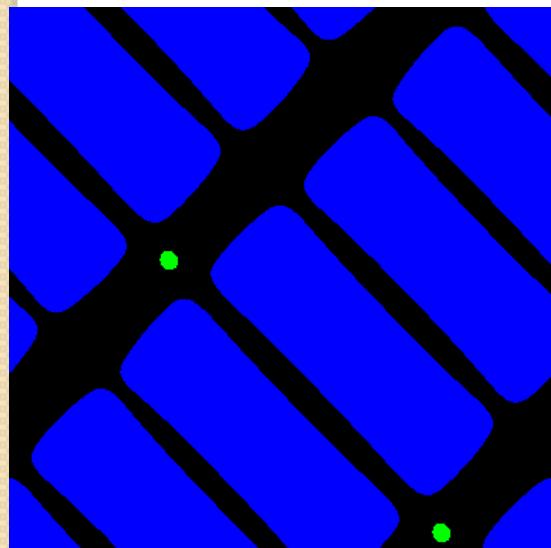
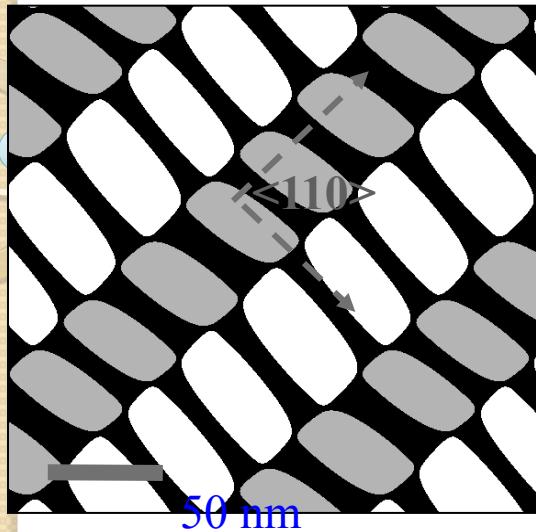


H. Zapsolsky, S. Ferry, X. Sauvage, D. Blavette, L.Q. Chen, Phil. Mag. (2011)

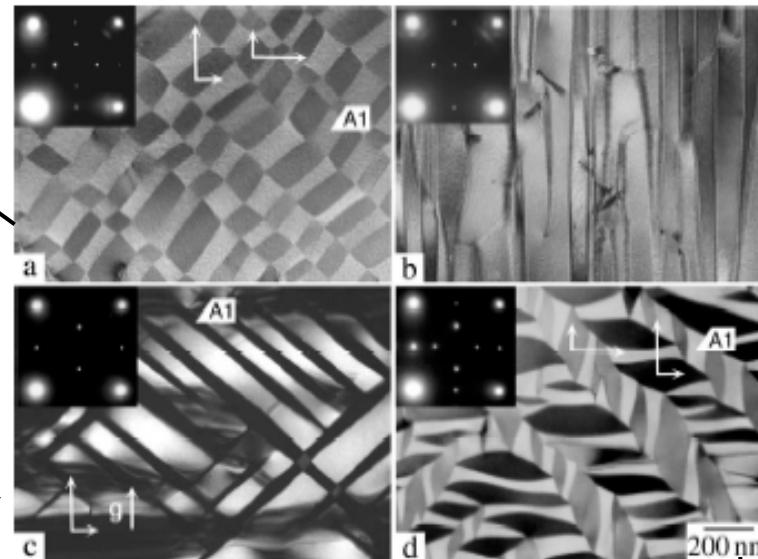
J. Boisse, H. Zapsolsky, A.G. Khachaturyan Acta Mat. (2011)

M. Eckholm, H. Zapsolsky, A. Ruban, I. Vernyhora, D. Ledue, I. Abrikosov, Phys. Rev. Letters (2010)

# Simulations atomistiques des microstructures dans les alliages à base de Ni.

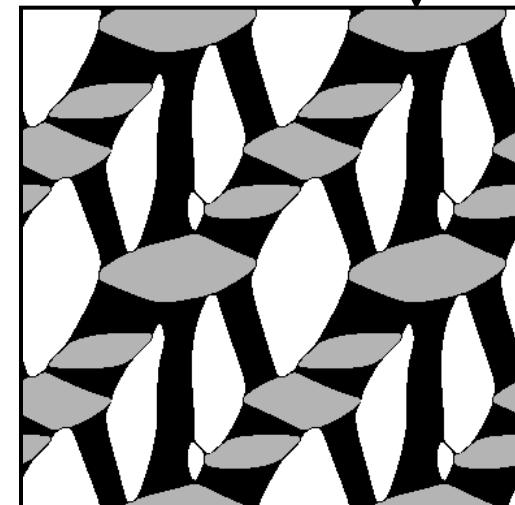


Images expérimentales obtenus en microscopie électronique  
Ni-20%V-10%Co



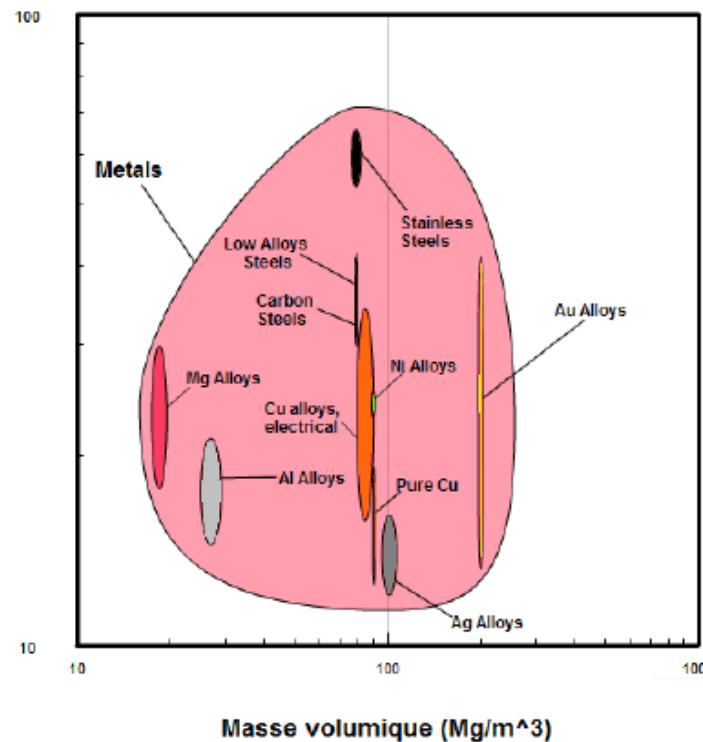
Ni-19%V-4%Fe

Ni-15%V-5%Nb

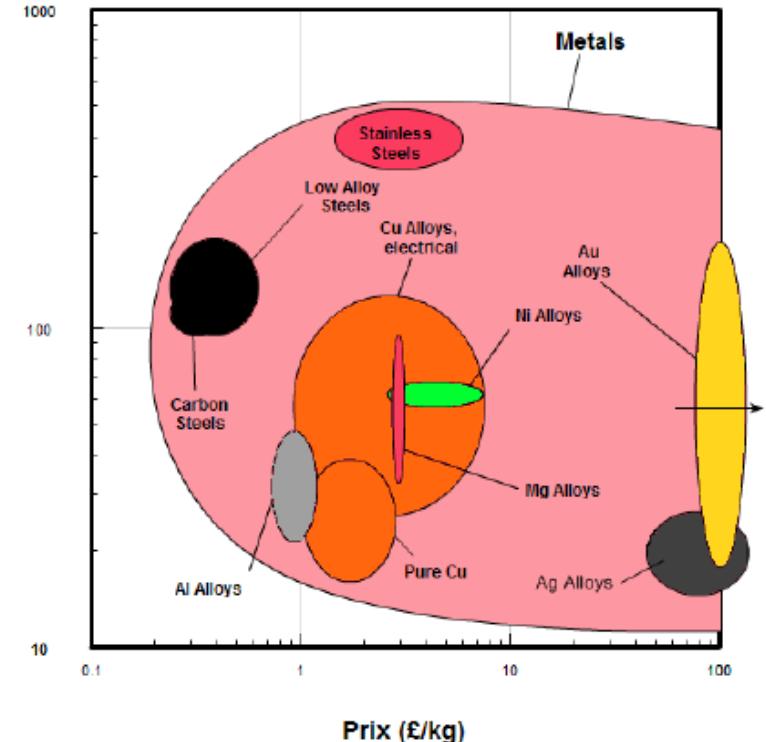


# Les alliages à base d'Al collaboration NEXANS

Résistivité électrique ( $n\Omega \cdot m$ )



Résistivité électrique ( $n\Omega \cdot m$ )



**L'objectif:** développer une nouvelle génération de câble électrique en aluminium ayant de bonne propriétés électriques et une bonne tenue mécanique à haute température

## Précipitation dans les alliages à base d'Al

dureté des matériaux

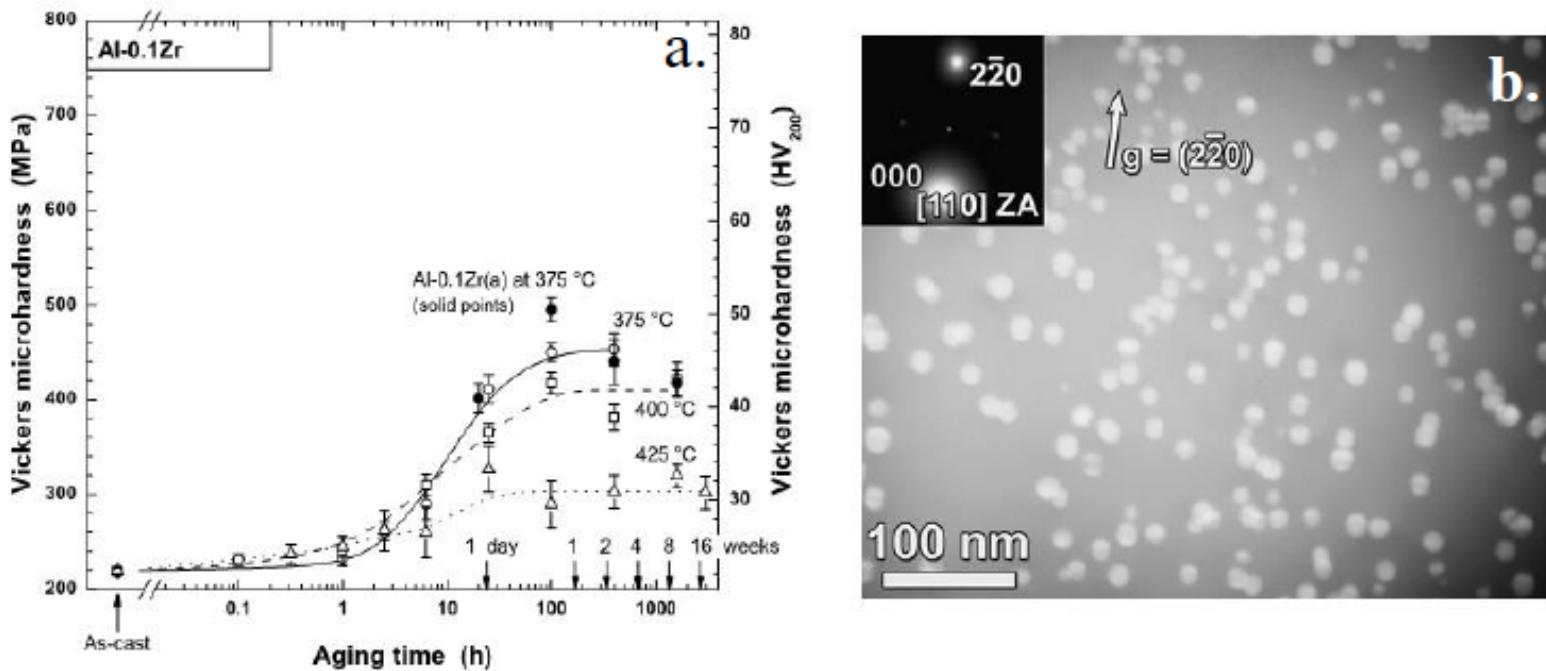
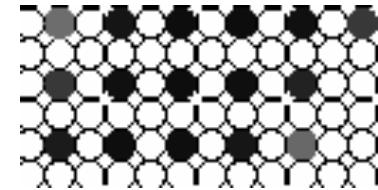


Figure 14 Mesure de dureté Vickers sur l'alliage Al-0.3%wt Zr vieillis à 375-400-425°C et Cliché MET en champ sombre de la précipitation d' $\text{Al}_3\text{Zr}$  dans une dendrite obtenu après 1600h de traitement à 425°C

$$\langle r \rangle = 10.9 \text{ nm} \pm 1.9 \text{ nm} \quad [\text{Knipling et al. 2008b}]$$

## Simulations atomistique

$P_A(r,t)$  is the probability of finding of an A atom at a given lattice site  $r$  at a given time  $t$ .

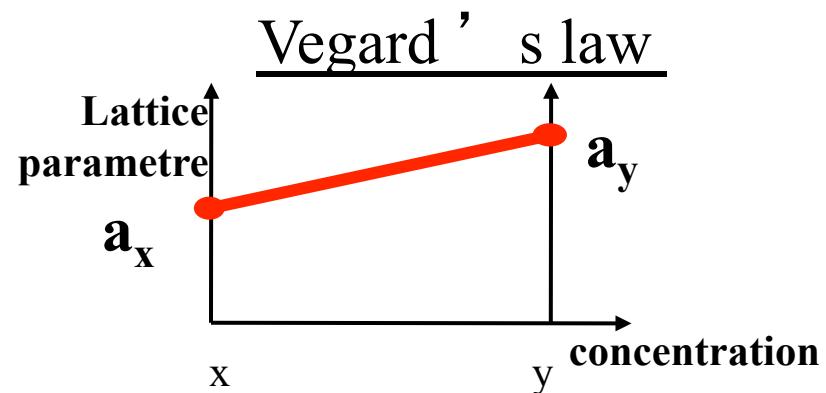
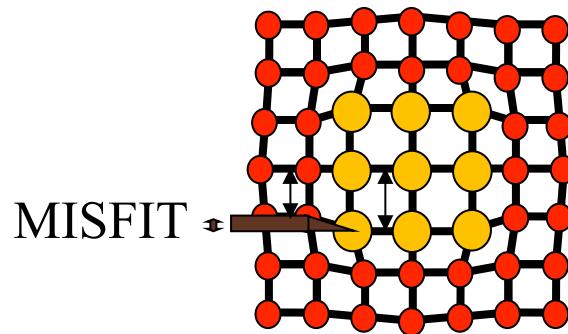


Onsager equation (equation of relaxation dynamic):

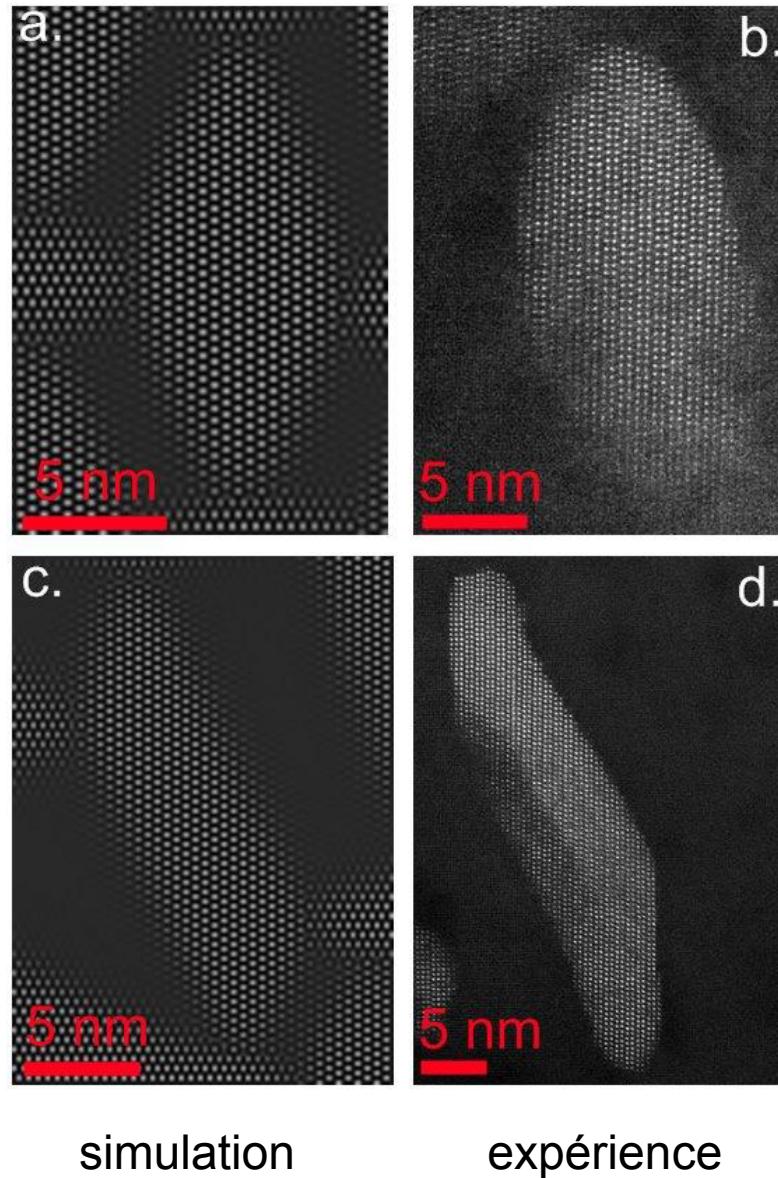
$$\frac{dP(r,t)}{dt} = \frac{1}{k_B T} \sum_{\alpha, \beta} \sum_{r'} L_{\alpha\beta}(r - r') c_\alpha c_\beta \frac{\partial F}{\partial P(r',t)}$$

$L_{\alpha\beta}(r-r')$  is a matrix of kinetic coefficients.

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



## Les précipités ordonnés avec la structure DO<sub>22</sub> dans l'alliage Al-Zr



# Spinodal decomposition in Fe-Cr

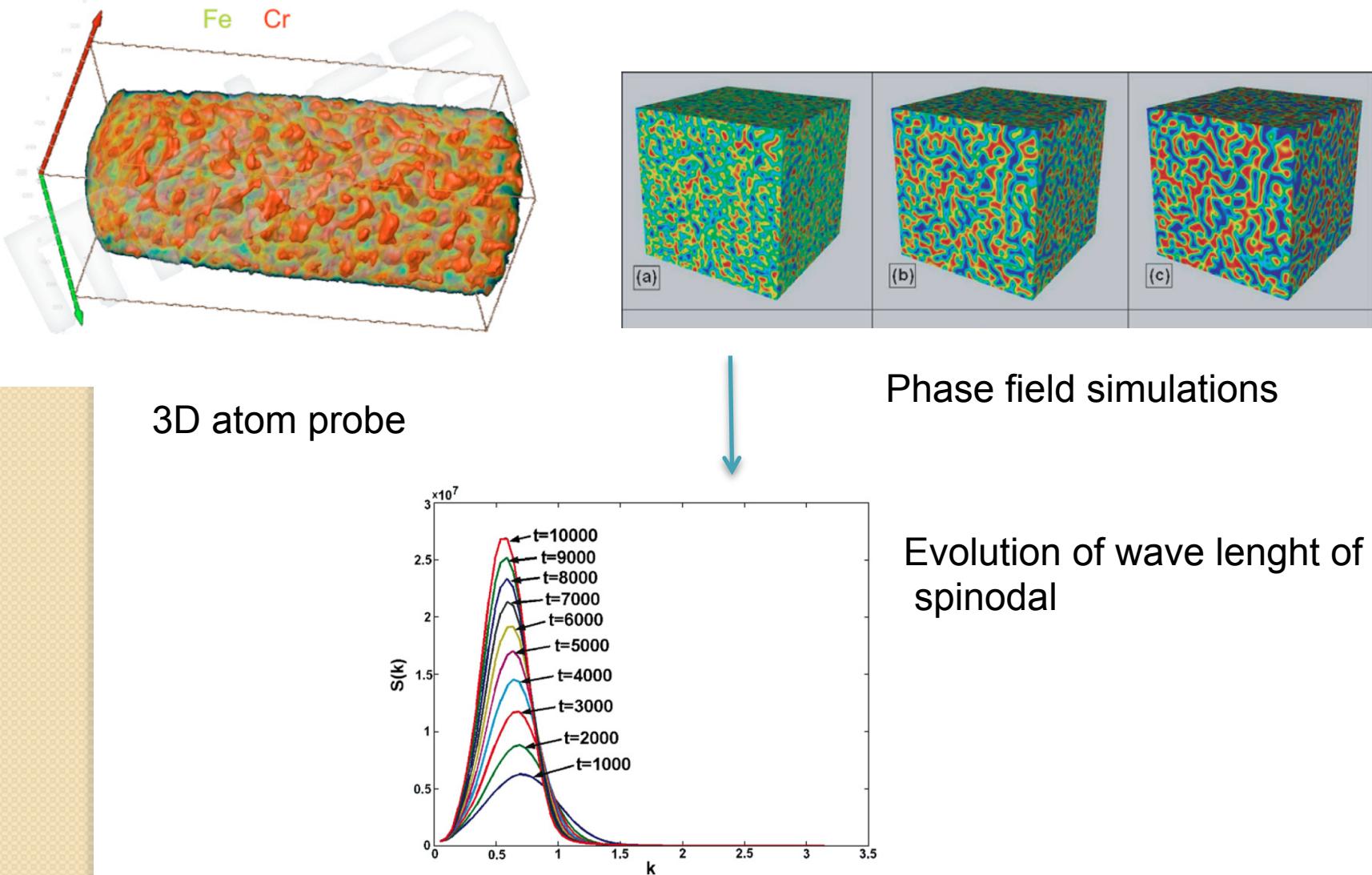


Fig. 2. Evolution of the equal time structure factor in spinodal decomposition as predicted by Eqs. (12) (13) and Cahn-Hilliard parabolic numerical equation (11) with  $\tilde{\tau}_D = 0$  and  $\tilde{e}_c^2 = 1.0$ . Numbers at the curves show number of time steps in units of  $\tau_D$ .

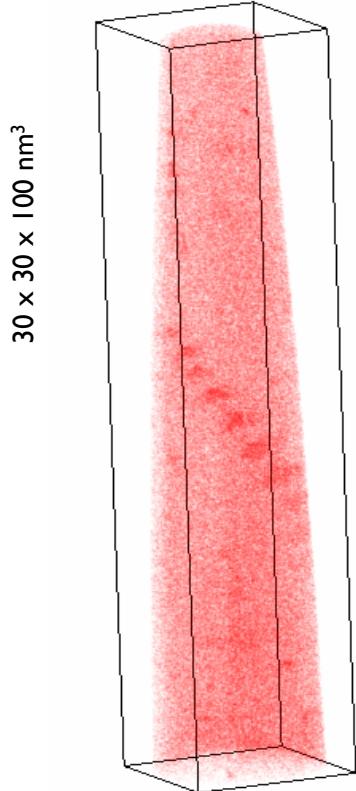
# Segregation at grain boundaries in irradiated materials

## Collaboration EDF-GPM

- Structural and chemical analysis: APT - TEM

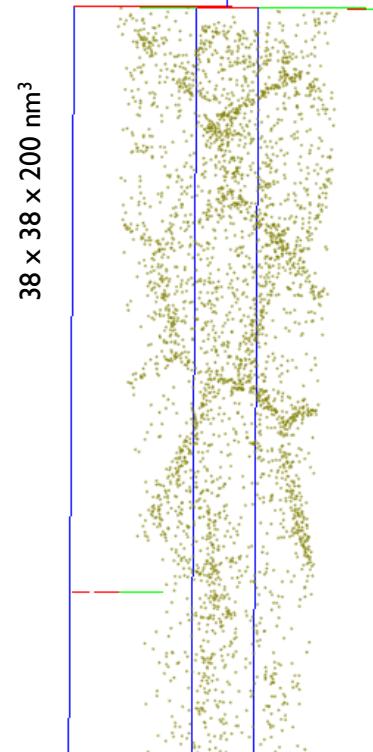
*Irradiated*

Fe-9Cr



Cr ●

RPV steel



P ●

Courtesy B. Radiguet

# Atomic density function modeling of atomic structure of grain boundaries

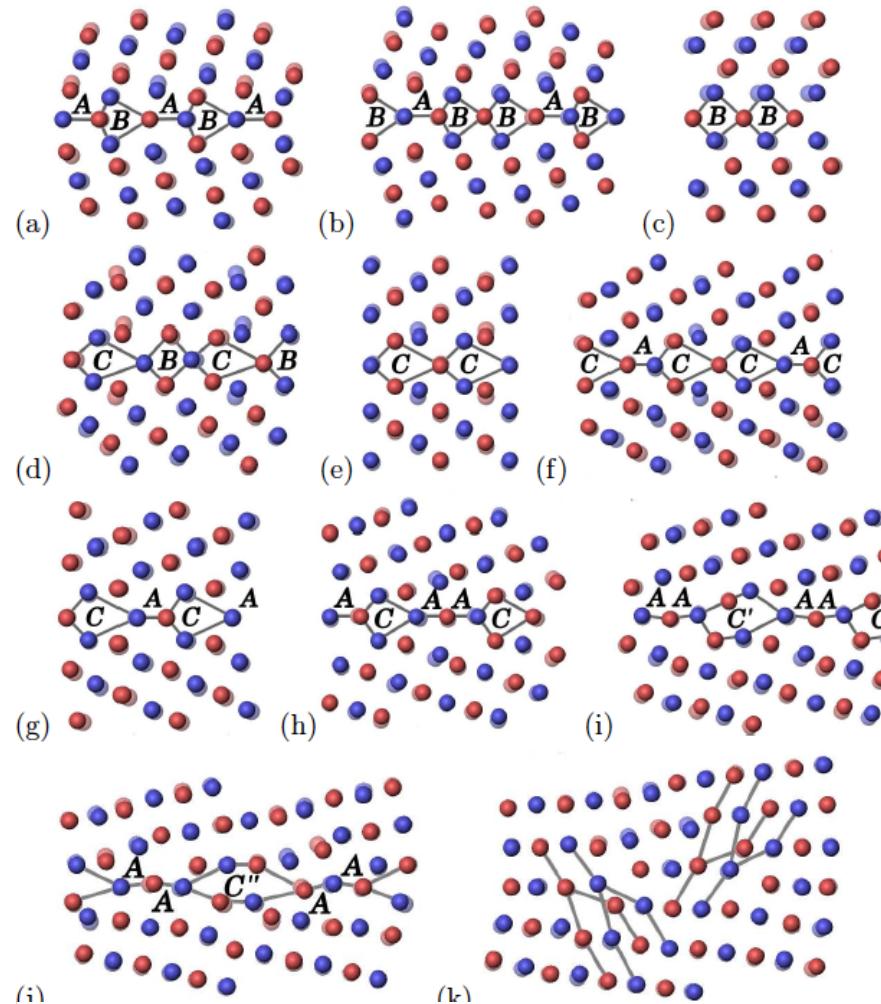
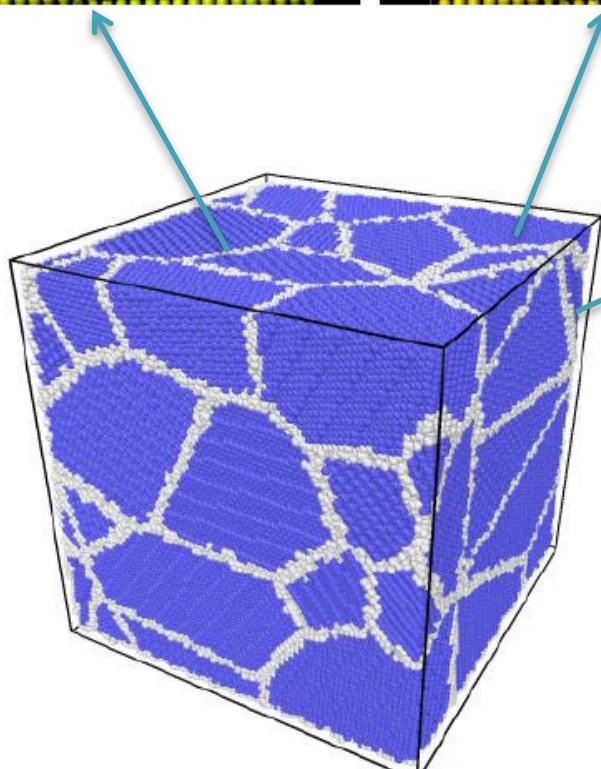
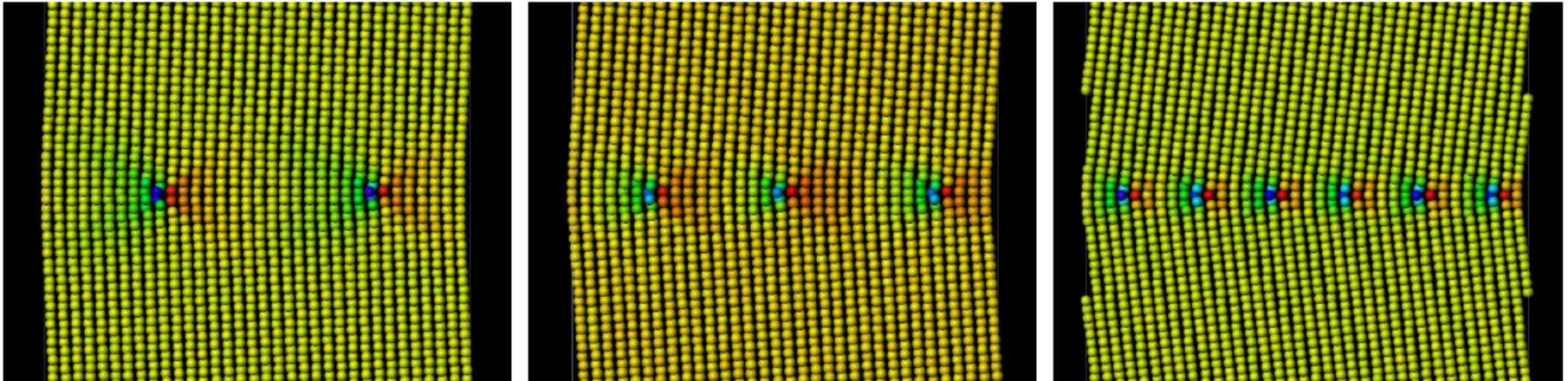


Figure 2: The structural units in  $\langle 110 \rangle$  GBs modeled by the ADF: a)  $38.94^\circ, \Sigma 9(114)$ ; b)  $50.48^\circ, \Sigma 11(113)$ ; c)  $70.53^\circ, \Sigma 3(112)$ ; d)  $93.37^\circ, \Sigma 17(334)$ ; e)  $109.53^\circ, \Sigma 3(111)$ ; f)  $121.01^\circ, \Sigma 33(554)$ ; g)  $129.52^\circ, \Sigma 11(332)$ ; h)  $141.06^\circ, \Sigma 9(221)$ ; i)  $148.41^\circ, \Sigma 27(552)$ ; j)  $153.47^\circ, \Sigma 19(331)$ ; k)  $163.9^\circ, \Sigma 51(551)$ . The equilibrium atomic positions after a relaxation by MD simulation are indicated in the background with faded colors; different colors refer to two adjacent atomic planes. The last image represents dislocations.

## Champ élastique des dislocations



Boîte de simulation de dimensions de  $2048^3$  mailles correspondant à des dimensions physiques d'environ  $40 \times 40 \times 40 \text{ nm}^3$

**La modélisation numérique est un outil très utile à la maîtrise de l'élaboration et à la prédition des propriétés physico-chimiques des matériaux.**