Contribution to the FEMS meeting on « Precipitation Hardening »

Prepared by the SF2M-MECAMAT « Phase transformation » working group

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Contribution to the FEMS meeting on « Precipitation Hardening »

- Experts who have been interviewed so far:
  - Philippe Maugis (Steel) philippe.maugis@im2np.fr
  - Jean-Marie Welter (Copper Alloys) jean-marie.welter@pt.lu

Objectives of the Meeting

- « to identify the needs of industry for R&D&I in the field of precipitation and to influence Horizon 2020 with an opinion white paper ».

- « particular focus on precipitation hardening in alloys (Fe, Al, Cu, Ti alloys, etc.) »

- « to identify subtopics and to prioritized them»

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What is at stake

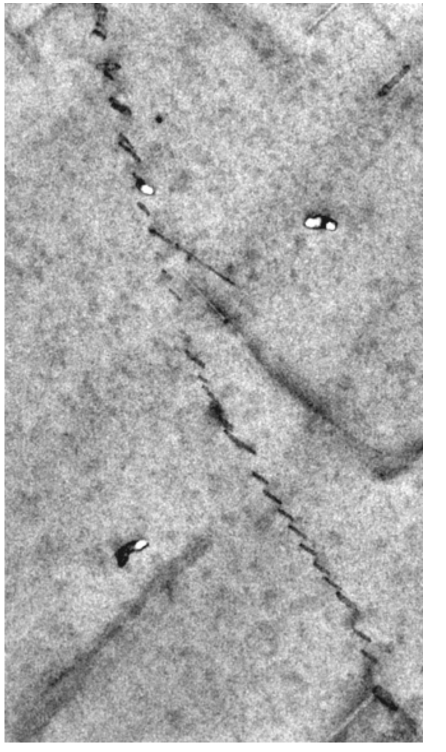
- Acceleration of new light materials developpement to improve energy consumption
- Replace elements which could be critically available (rare earth) or expensive (with a fluctuating price Mo, Ni, Ag) for Europe
- ….
- USA has launched the MATERIALS GENOME INITIATIVE & Europe must have an ambitious project to accelerate the development of new materials and maintain a top level in material science.

4 themes identified

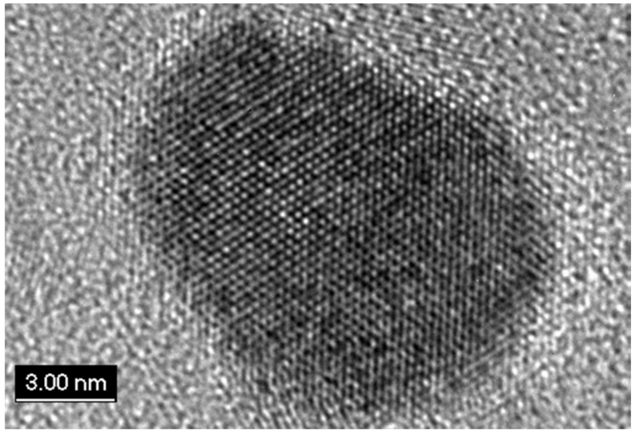
- First stages of precipitation/natural ageing
- Coarsening resistance / heat resistant alloys
- Dynamics of reconstructive phase transformations
- From microstructure description to stress-strain curves calculation

THEME 1.a

- First stages of precipitation/natural ageing
  - Very small clusters (including their free energy),
  - Solute vacancy interactions,
  - Solute-solute & solute-vacancy elastic interactions,
  - Elastic field generated by precipitates
  - At least 2 solute elements (for example Al-Mg-Zn, Al-Mg-Si, Fe-Nb-C-N, Cu-Ni-Si, Cu-Ni-Sn)
  - Competition between phases,
  - Homogeneous nucleation
  - Heterogeneous nucleation on grain boundaries and dislocation
  - Impact on subsequent precipitation kinetics .



Al-Mg-Si-Cu, STEM, T. Epicier (MATEIS, Lyon) & C. Cayron (CEA Grenoble)

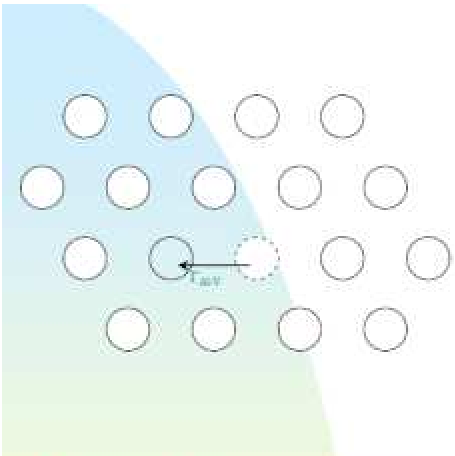


NbC in stell, HRTEM + nano EELS, <u>*E. Courtois*</u> *(GEMPPM Lyon)*

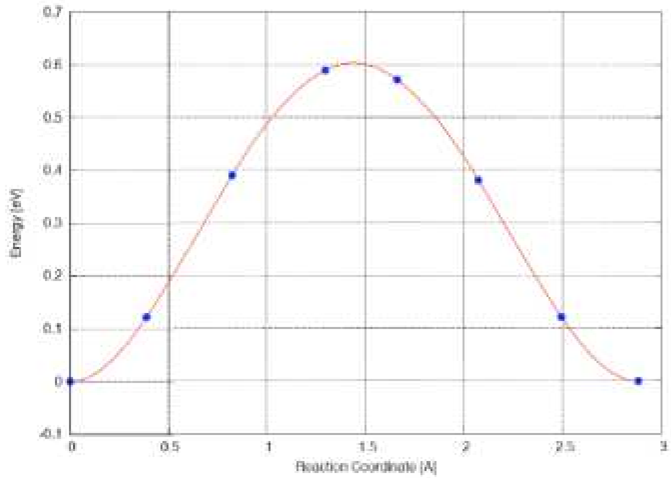
Al – Sc –Zr alloy, Al3(Zr,Sc) E. Clouet & M. Nastar, CEA Saclay

Theme1.a/modeling tools

- Ab-initio T=0K:
  - Solute-solute, solute-solvant & solute-Va chemical interaction (unrelaxed cluster enthalpies),
  - Free-stress eigenstrains of clusters,
  - Elastic constants of pure solvant,
  - Saddle points and kinetic paths (-> solute mobilities).
  - Interaction solute –dislocation and GB



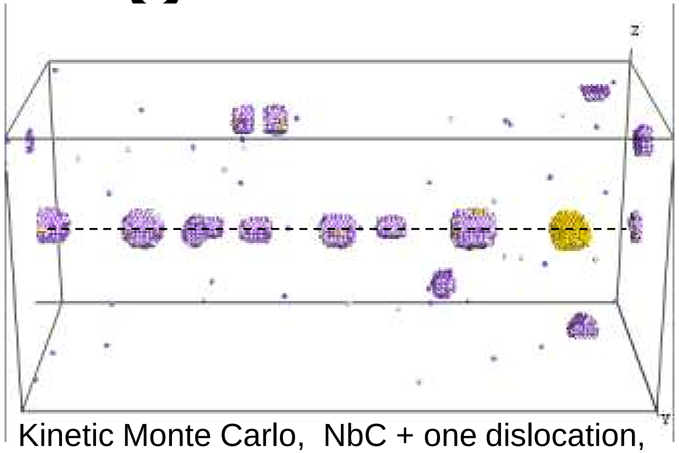
Jump into a vacancy



Activation energy barrier

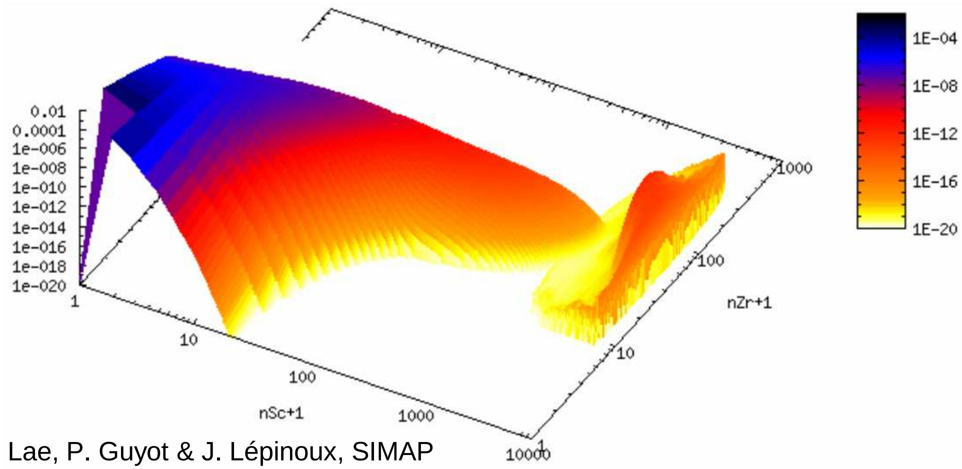
Theme1.a /modeling tools

- Kinetic Monte Carlo:
  - Several solutes,
  - Long range elastic interactions (lattice statics),
  - Out-of-equilibrium vacancies.
  - Grain boundary, dislocation



Kinetic Monte Carlo, NbC + one dislocation,
Céline Hin & F. Soisson, CEA Saclay

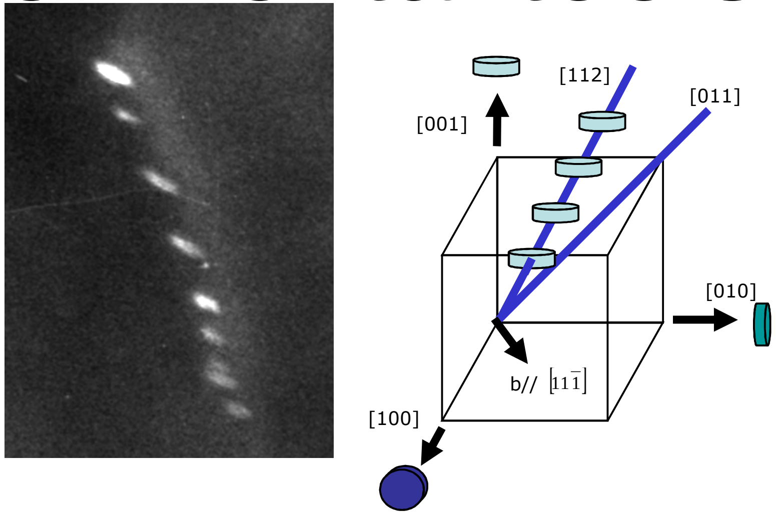
- Upscaling towards meso- & macro-models (at least for the coarsening stage).
  - Cluster Dynamics
  - Phase field modelling
  - Size distribution macro model



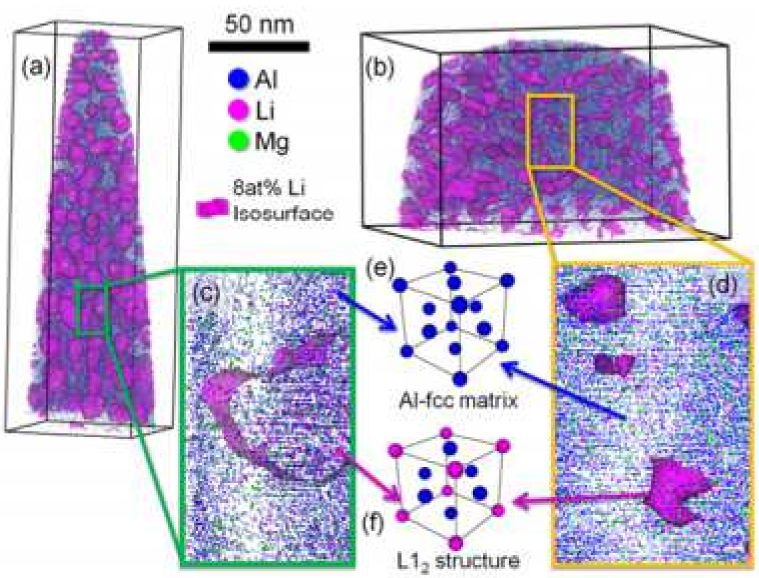
Cluster Dynamics, L. Lae, P. Guyot & J. Lépinoux, SIMAP

Theme1.a/experimental tools

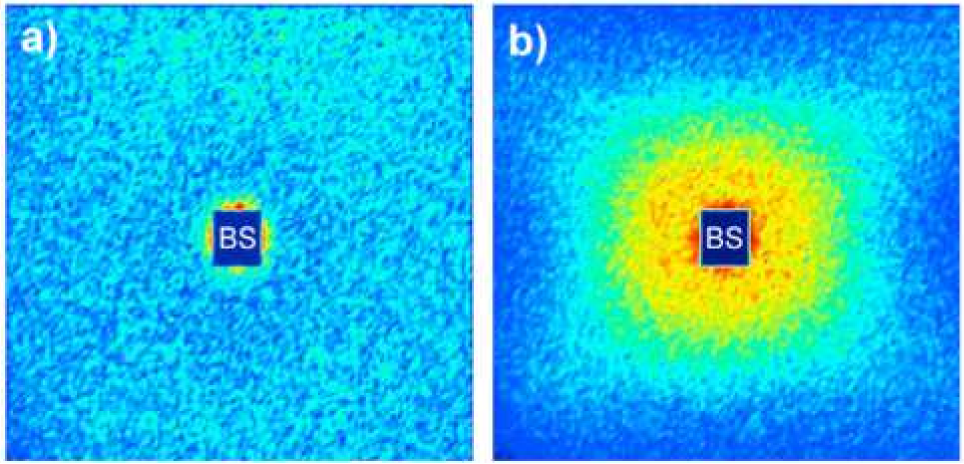
- DSC, resistivity, dilatometry, SAXS, SANS
- Positron Annihilation,
- Atom probe tomography,
- In-situ measurement of lattice parameter by X rays,
- MET HAADF.



NbC aligned on a dislocation, TEM DF, F. Perrard CEA Saclay



Atom Probe, B. Gault, Sydney



SAXS of GP zones in Aluminum, A. Dechamps, SIMAP

Theme 1.b / coarsening resistance

- At stake: heat resistant alloys,
  - Modification of the nature of the precipitate
  - Modification of solute mobilities

- Example of some heat resistant alloys:
  - Cu-Cr, Cu-Ni-Si,
  - AlCuLi, AlCuMg

Theme 1.b / Modeling tools

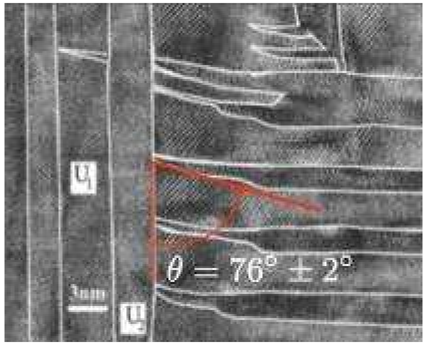
- Ab-initio+ Statistical Physics (T>0K):
  - Interfacial energies
  - Interfacial & bulk mobilities
  - Free energy of phases
- Meso- & macro- models
  - Cluster Dynamics
  - Phase field modelling
  - Size distribution macro model

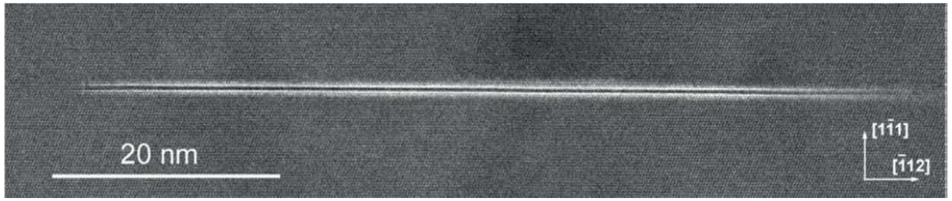
Theme1.b / experimental tools

- DSC, dilatometry, SAXS, SANS
- Atom probe tomography,
- TEM, SEM.
- Room temperature and Hot Tensile test

THEME 2

- Dynamics of reconstructive phase transformations
  - *without solute long range diffusion*
    - Massive transformation (Fe-Cr alloys),
    - Martensitic transformation (shape memory alloys)
  - *with solute long range diffusion*
    - Precipitation in Aluminum Alloys: Effect of cold deformation on nucleation on stacking faults and growth of Al_2CuLi (fcc->hcp),
    - Precipitation in Titanium Alloys: beta (cc) to alpha (hcp)





Al2CuLi, TEM HAADF

Theme 2/modeling tools

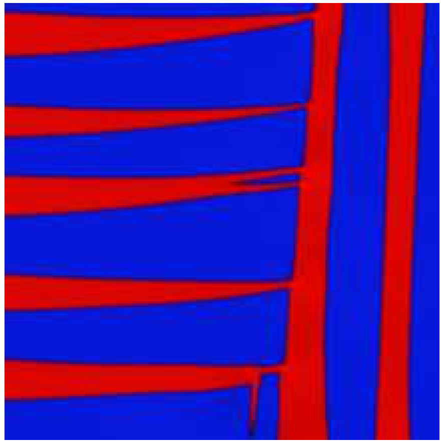
- Ab-initio T=0K:
  - Free-stress eigenstrains of second phase,
  - Elastic constants of matrix.

  - Partial dislocation / stacking fault enthalpy including effects of solute segregation along stacking faults)

- Ab-initio+ Statistical Physics (T>0K):
  - Interfacial energies
  - Interfacial mobilities
  - Free energy of phases
  - Stacking fault energy

Theme 2/modeling tools

- Continuous modeling (phase field type):
  - Generalized Landau free energy modeling describing:
    - phase transformation,
    - associated shear modes,
    - dislocations in matrix & precipitates.



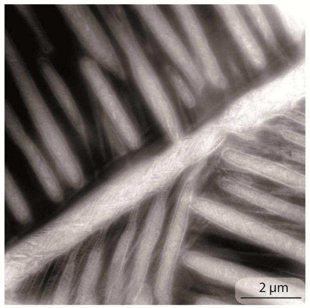
Phase field, U. Salman & A. Finel, LEM/Onera

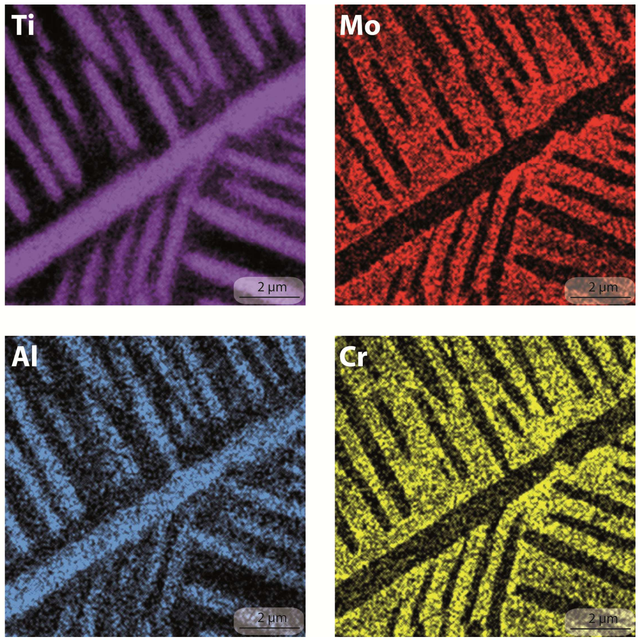
  - Model should allow large deformations

Phase field, A. Settefrati & E. Gautier, IJL

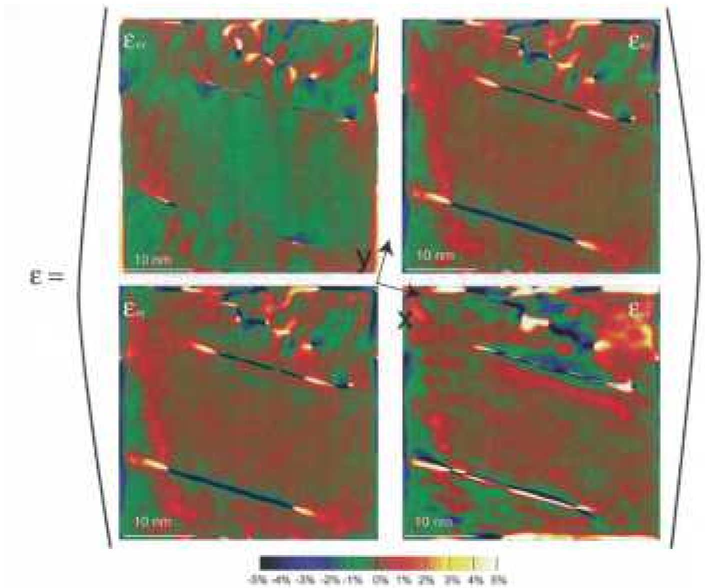
Theme 2/experimental tools

- In situ SAXS,
- SANS
- In situ X ray diffraction,
- Atom Probe,
- HAADF-STEM,
- 3D TEM, SEM
- Strain Field Measurement by HREM





β-metastable titanium alloy, TEM EDS, M. Dehmas, IJL



Strain Field Measurement by HREM in AlCuLi alloy, M. LeFournier & J. Douin, CEMES .

THEME 3

- From microstructure description to stress-strain curves calculation:
  – Interaction dislocations<->precipitates,
  – Interaction dislocations-solid solution.

  Examples:
  - Mechanical properties of Martensite
  - Solute dislocation interactions in Fe-Al Alloys
  - Bauschinger effect in steels
  - Al-Mg-Zn, Al-Mg-Si

Theme 3/modeling tools

- Ab-initio T=0K:
  - Antiphase boundary energies,
  - Core dislocation morphology energy,
  - Effect of solute elements with dislocation & on staking faults.
- Ab-initio+ Statistical Physics (T>0K):
  - Interfacial energies
  - Free energy of phases
  - Segregation on defects (dislocations, staking faults)

Theme 3/modeling tools

- Microstructure <-> Mechanics interactions:
  - Coupling of microstructure evolutions
    - Phase field,
    - Macro description,

  with:

  - dislocations:
    - Dislocation Dynamics,
    - Continuous plastic strain fields (Generalized Continuum Mechanics).

- Or new integrated approaches.

Theme 3/experimental tools

- Tensile, compression & bending tests ,
- Confocal microscopy (macro),
- SEM EBSD (stress mapping, GND density mapping),
- TEM (ex- or in- situ),
- X Ray diffraction -> elastic deformations,
- Synchrotron Radiation Tomography,
- Time resolved Synchrotron X Ray diffraction,
- in situ tensile test in MEB EBSD.
- Neutron diffraction