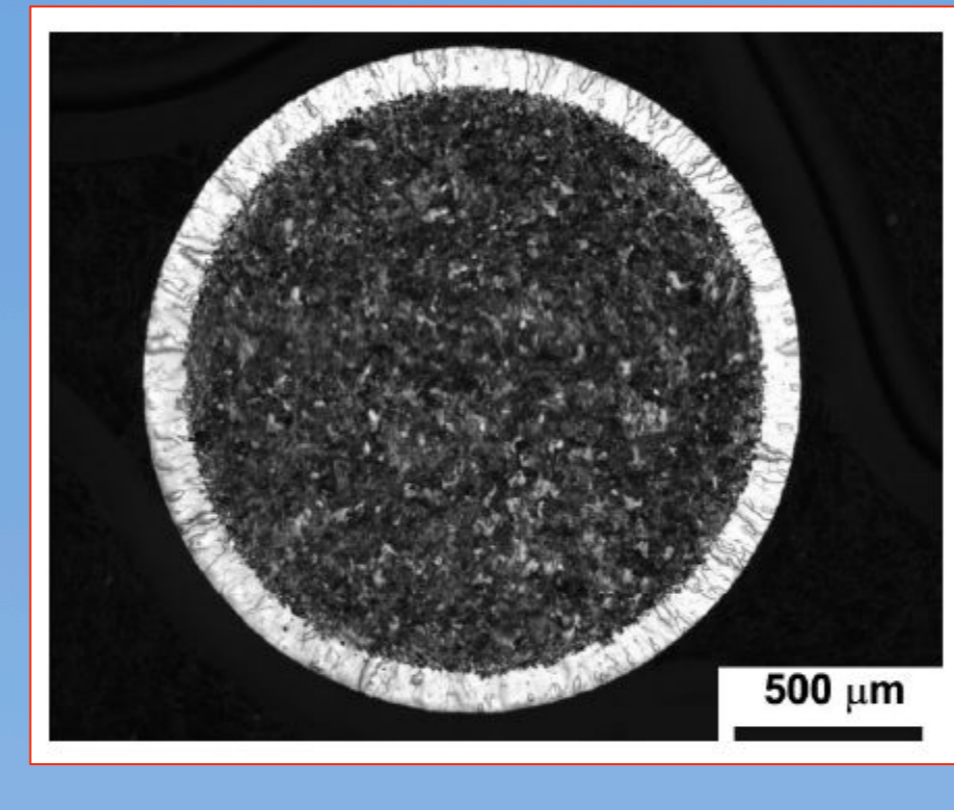
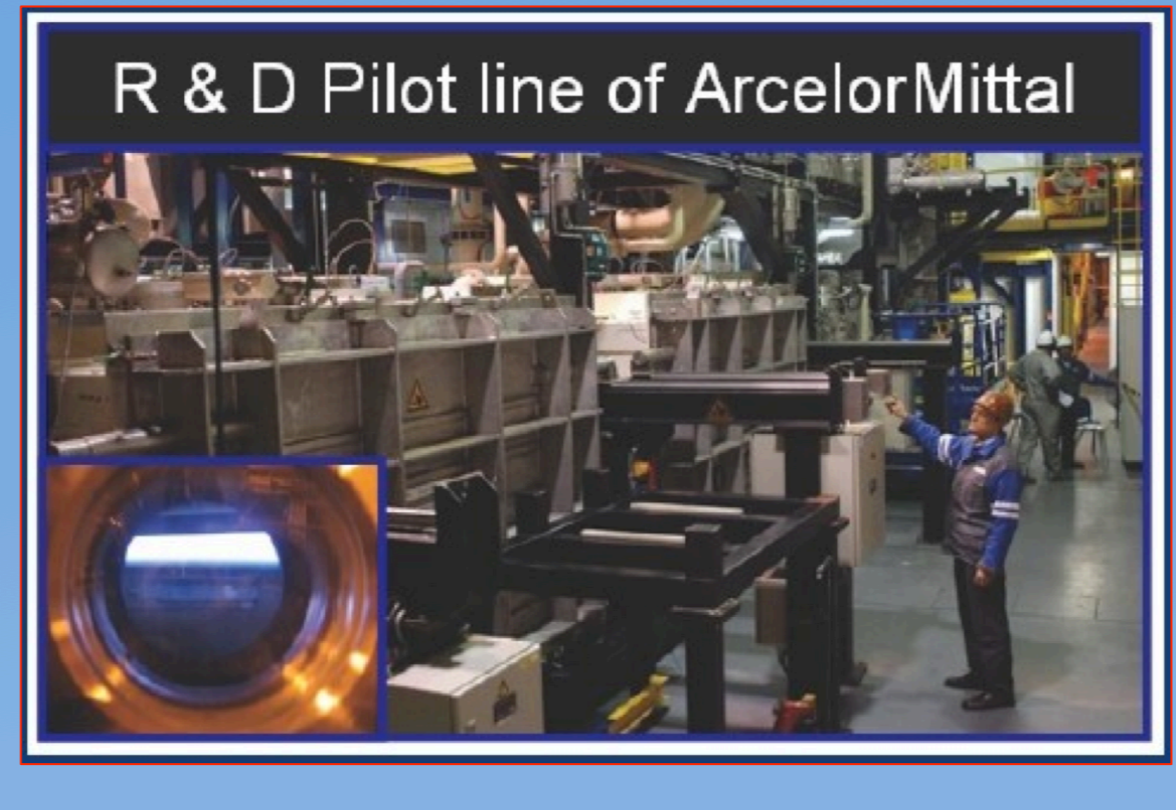
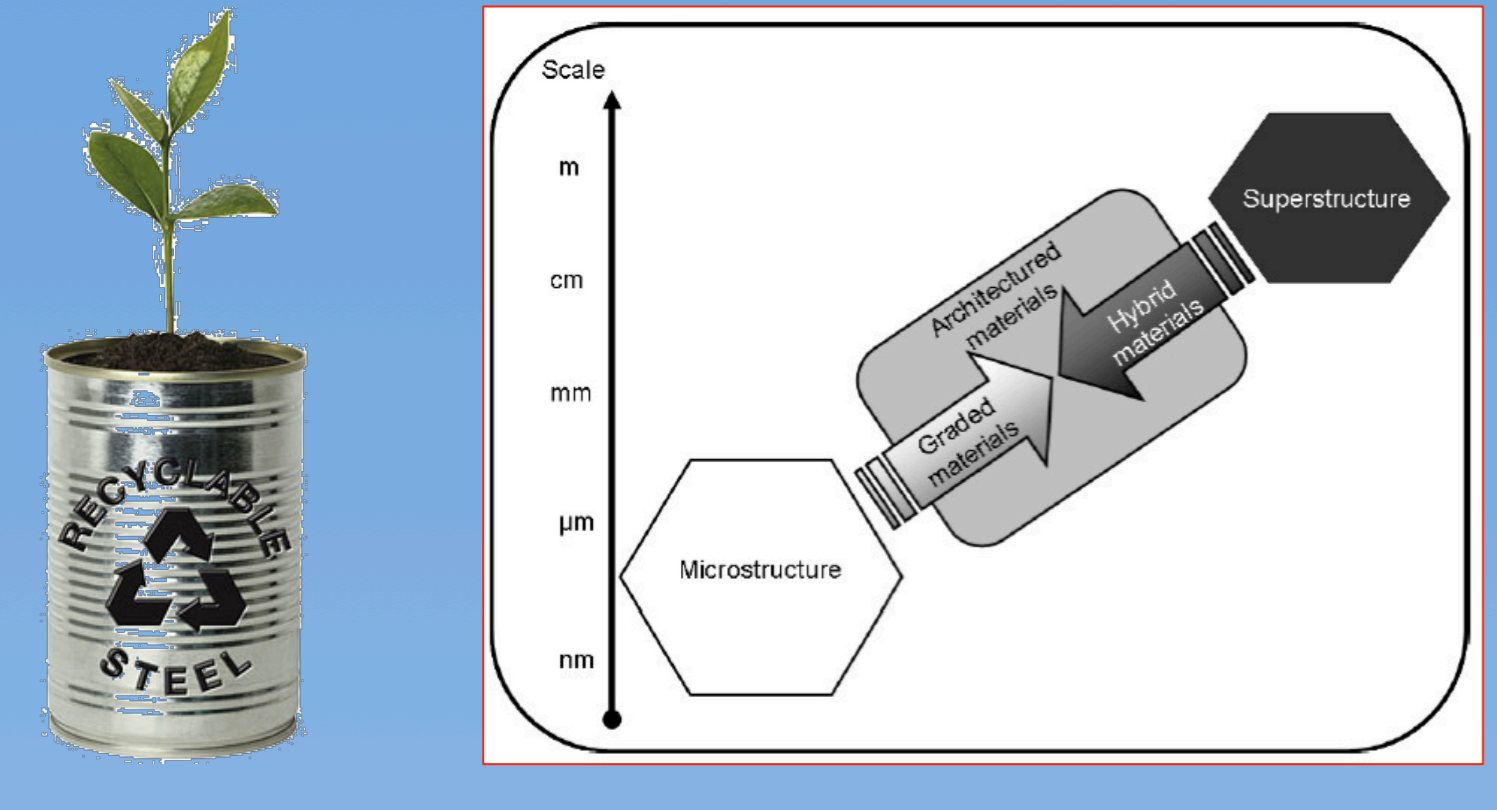


# Gradient Composite Steel design

C. Sinclair, B. Lawrence, A. Weck, P. Gosson, E. Cantergiani, X. Sauvage, A. Fillon M. Perez and C. Scott

## GraCoS

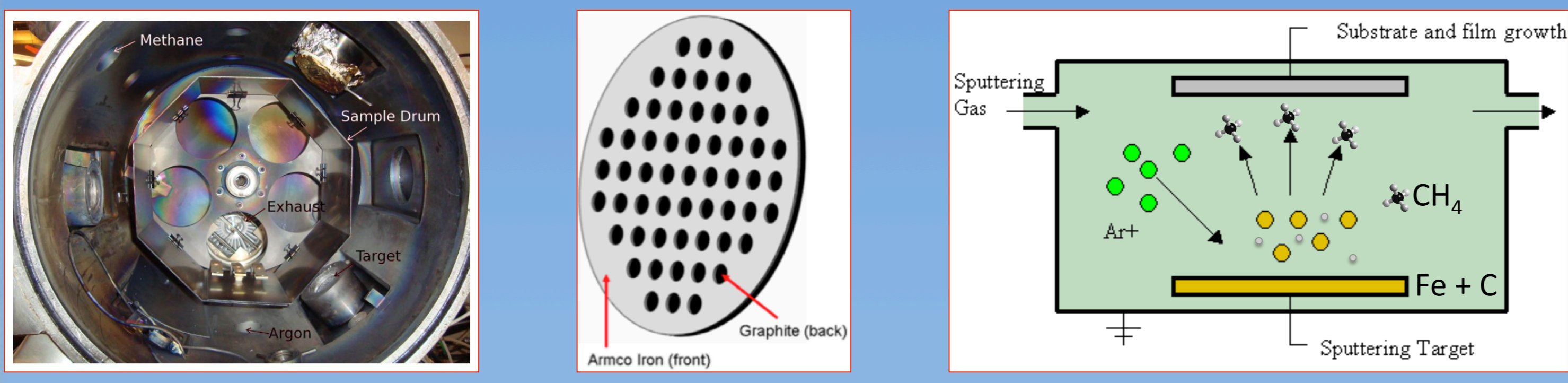
## The GraCoS project



- ✓ Low solubility but high influence of C in  $\alpha$ -iron
- ✓ PVD coating of steel sheets: carbon reservoirs
- ✓ Opportunity to develop far from equilibrium phases

C.P. Scott, C. Sinclair, and A. Weck. Amorphous  $Fe_{1-x}C_x$  coatings as carbon reservoirs for diffusion strengthening of steel sheets. Scripta Mater, 65:763-766, 2011.

## Films deposition: Reactive magnetron sputtering

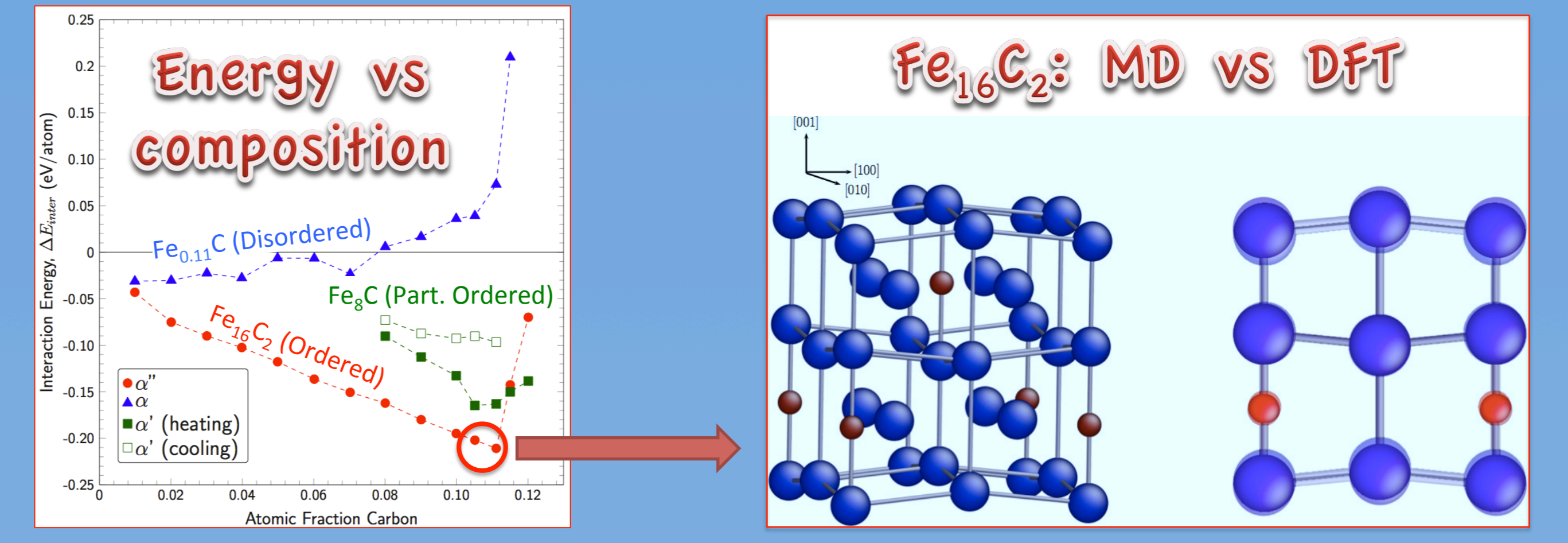


- ✓ From 0 to 40% carbon
- ✓ From 100 to 1000 nm

## Down to the atomic scale

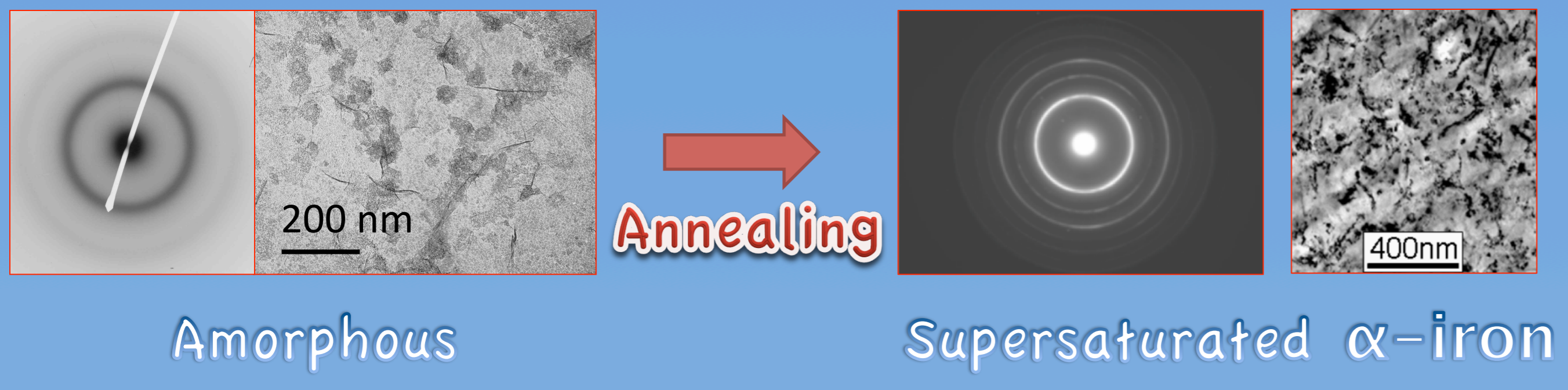
- ✓ Molecular Dynamics
  - ✓ Recently developed FeC potential
- $F = m \times a$   
force mass acceleration
- Becquart (C. S.), Raulot (J. M.), Bencteux (G.) et al., Atomistic modeling of Fe system with small C concentration, Comp. Mat. Sc., vol. 40, 2007, p. 119-129

## Phases stability: $Fe_{16}C_2$ vs $\alpha$ -iron



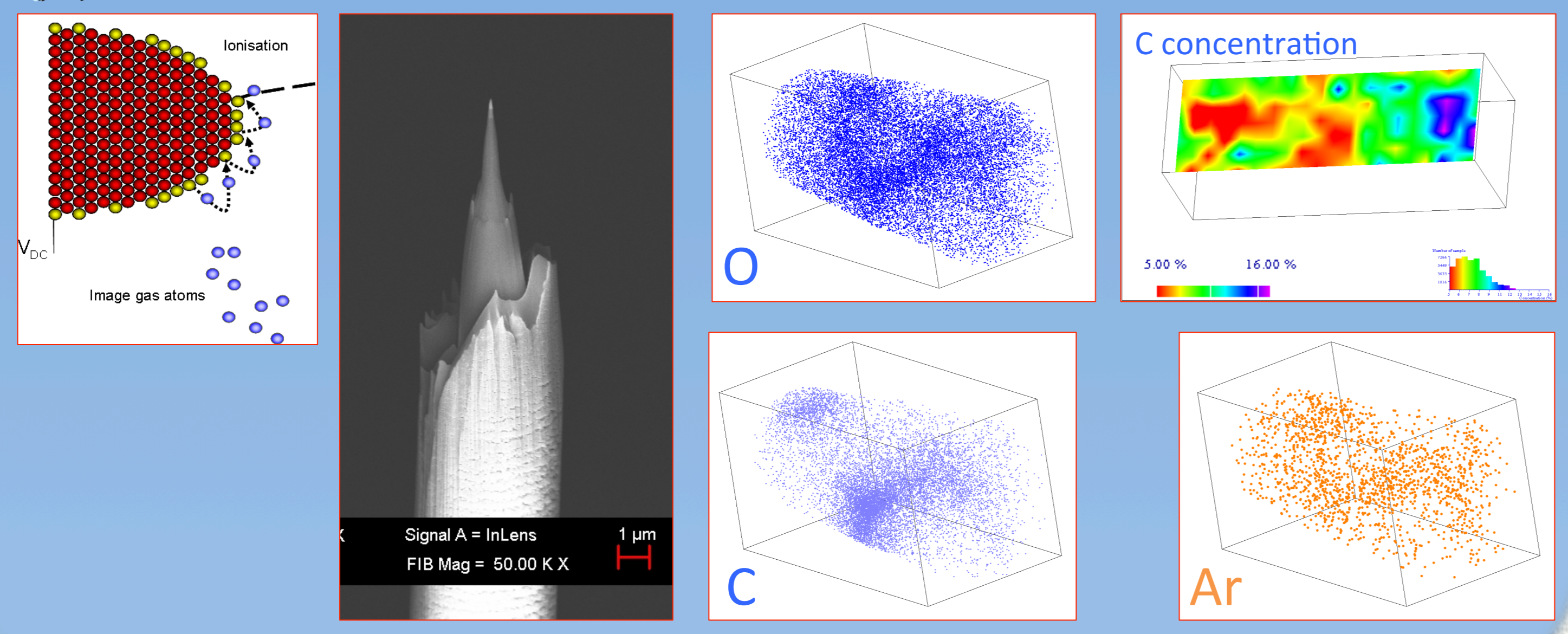
## Films characterization

### Electron Microscopy



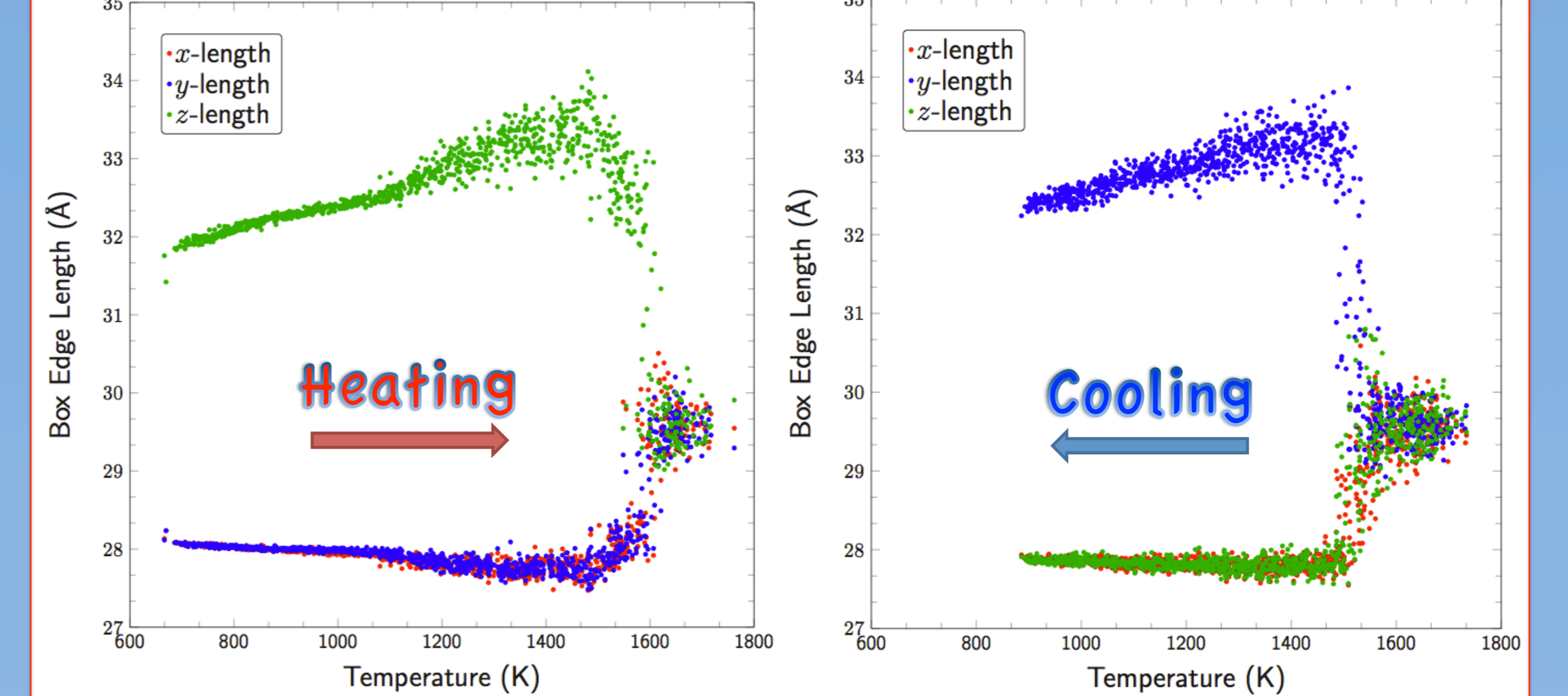
- ✓ Stability of 10% C (solid solution) in  $\alpha$ -iron?

### Tomographic Atom Probe



- ✓ Inhomogeneous repartition of C

## Tetragonal distortion vs temperature



Sinclair (C. W.), Perez (M.), Veiga (R. G. A.) and Weck (A.), Ordering of Carbon in Highly Supersaturated  $\alpha$ -Fe: A Molecular Dynamics Study, Phys. Rev. B, vol. 81, 2010, 224204.

## Diffusion of C $FeC_x$ (MD simulations)

