Modeling Alloys under irradiation: *open questions*

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- Limitations of classical approaches

- “Local” successes

- Some suggestions

Microstructural evolution under irradiation : background

- Engineering alloys =

major components *(e.g. Fe Cr Ni Mn C…)*

+ *minor elements* *(C N S P…)*

Microstructural evolution under irradiation : background

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- Most (≈ 90%) modeling of

microstructural evolution under irradiation :

book keeping of point defects and of minor elements

⇒ *Defect and solute-defect clusters*

⇒ *Dislocation climb*

+ *effective medium approx^{tion} for major components*

=> swelling, hardening, segregation of minor elements…

Limitations of the classical approach

- Drawbacks of *effective medium* approx^{ion}

(concentration dependant properties):

- ? Irradiation induced segregations
(e.g. Cr in Austenitic and ferritic steels)?

-? Phase separation (e.g. Nb, O in Zaloys…)?

- ? Concentration dependent p^{pties} of dislocation cores
(e.g. sink efficiency as a function of SFE,
stability of Frank loops vs unfaulting…)?

e.g. (Austenitic steels)

$\Rightarrow$ Incubation dose for swelling?

$\Rightarrow$ Early dose recovery of the dislocation network?

$\Rightarrow$ …

Stability criteria for alloy phases under irradiation?

Counterpart to the industrial skill with Calphad, Dictra…??

- Competition ballistic / thermally activated atomic jumps

=> Stationary rather than equilibrium state(s)

- Dienes… 50's : order disorder transitions (*stationary LRO, homogeneous*)

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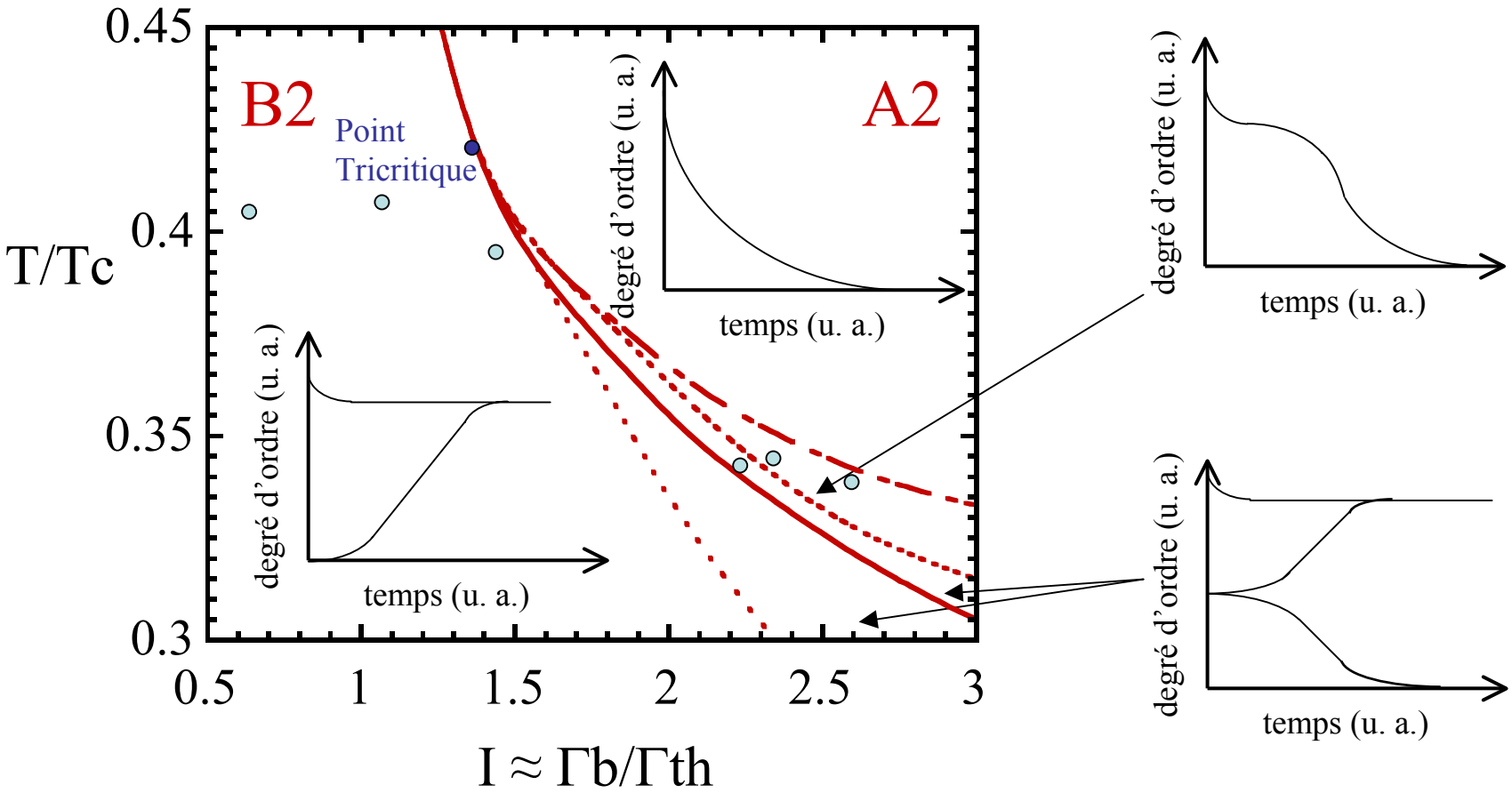
- Vaks et al 94 : Effective Hamiltonian $V_k^{eff} / k_BT = V_k\, f_k(\Gamma_b/\Gamma_{th}) / k_BT$
  (*binaries, interstitial relocation*)

Spectacular successes (inversion of stabilities, effect of cascades size, patterning…) but limited.

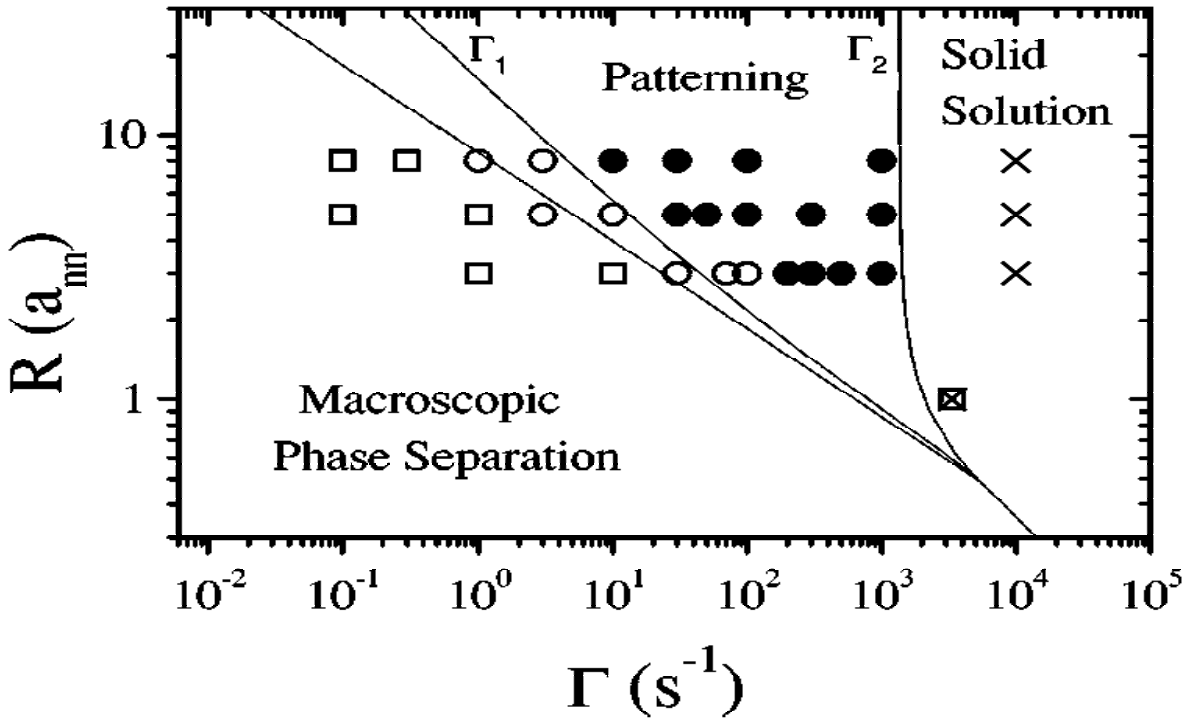
Phase diagramme for dynamical equilibrium: FeAl under ball milling

*Pochet et al. PRB***52** (1995) 4006

FeAl B2 ⟶ A2 sol. sol. (I, T)



Cascade size effects
(*R* : range of ballistic relocation)



Comparison between KMC simulations and a Cahn-Hilliard type model
(P. Bellon and R. Enrique, PRB 2001)

Stability criteria for alloy phases under irradiation

For binaries:

Inverse Kirkendal effect (RIS & RIP)
and
ballistic forcing
$\Rightarrow$ a single common theoretical frame
(G.M. and P. Bellon SSP **50**, 1996, 189)

Higher complexity?

For the time being: brute force atomistic modeling!

Requires:

- Safe implementation of diffusion mechanisms in KMC(vacancy and self interst[al]) (Soisson et al.),
- Safer phase field type equations (Nastar et al.),
- Safer alloy models (for cascade simulations, for kinetics…).

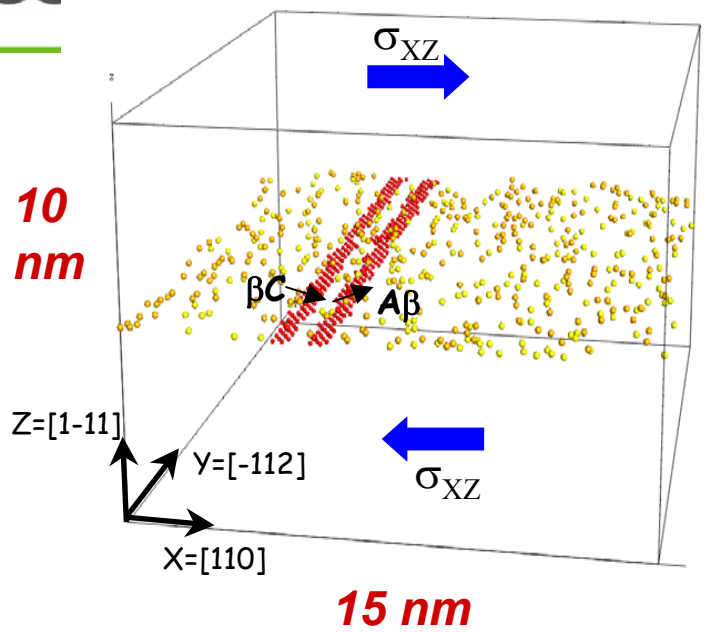
Learning from brute force atomistic simulations

-1 Chemical hardening

- 2 Fracture in oxides

- 3 Cascades in compounds

Plasticity of alloys: Solid Solution hardening



- **EAM optimized for Ni(Al), Ni_3Al**
- **Boundary conditions :**

  X,Y => periodic;

  $Z= \pm Z_{max}$ => $Z=c^t$ 2D dynamics
- $7{,}5 \leq \sigma_{xz} \leq 400$MPa

  $\mathbf{f_{ext}}$ on atoms at $\pm Z_{max}$
- **Temperature** : 300K rescaling velocities /100 time steps

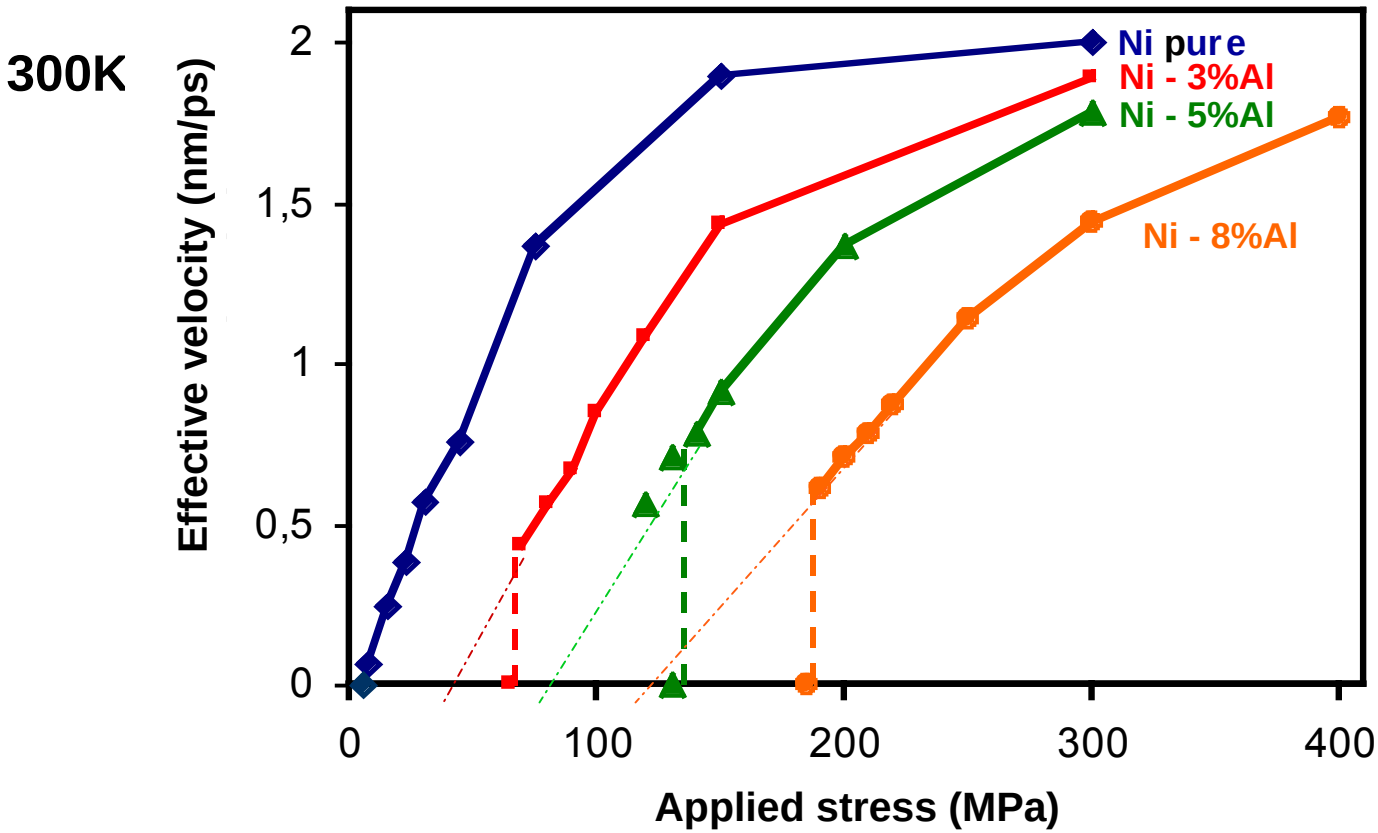
- **2.3 10^5 atoms ;**
- **t ≤ 700ps** ($\delta t=2.10^{-15}$ s)

$$(N,V,T,\sigma_{appl}) = c^t$$ *(Rodary et al. 2004)*

Glide of an edge dislocation : ***random*** solid solution 3 at% Al, **70**MPa (300K)

QuickTime™ and a Cinepak decompressor are needed to see this picture.

Effective dislocation velocity = f(applied stress)



$$\text{static}\ and\ V \qquad C_{sound} \qquad then V \qquad \frac{b \qquad \text{dynamical}(c)}{B(c)}$$

From glide velocity $v(\sigma;c)$ ➔ to stress strain curves $\sigma(\varepsilon)$

$$\text{static} \quad \textit{and} \quad V \qquad C_{sound} \qquad \textit{then } V \qquad \frac{b \qquad \text{dynamical}(c)}{B(c)}$$

Can be implemented in models of :

- DDD,

with appropriate mobility law;

- crystalline plasticity,

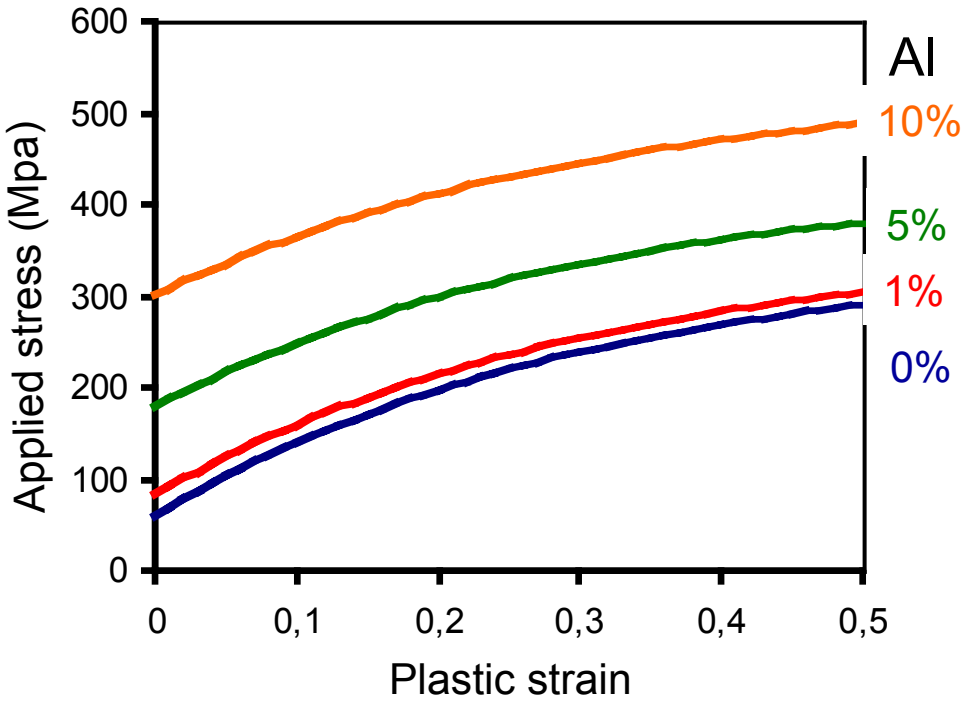
with $\sigma > \sigma_{\text{yield}}$ instead of $\sigma > \sigma_{\text{static}}$:

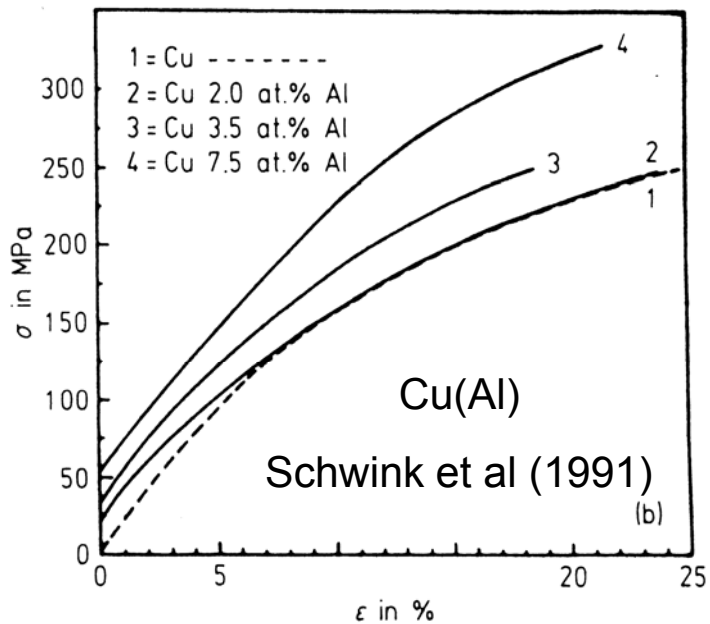
$$\textit{yield} \qquad \textit{static} \qquad b\sqrt{}$$

From nano to macro scale?

σ_{yield} *and* v C_{sound} *then* V $\dfrac{b}{B(c)}$ **dynamical** (c)

Y_p $b\,V$ $\dot{Y}$ $\dot{Y}_p$ $A\sqrt{\ }$ D





¥ $_{flow}$/ c= 25 (MPa/at%) (vs 10 exp.) ; **missing strain hardening (c%) : A(c), D(c)**

Learning from brute force atomistic simulations

-1 Chemical *hardening*

results from solute-solute interaction,

(rather than from solute-dislocation interaction)

- 2 Fracture of oxides

- 3 Cascades in compounds

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Fracture of complex compounds; SiO_2 cristobalite vs glass

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Van Brutzel et al
2002

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Learning from brute force atomistic simulations

-1 Chemical hardening

- 2 Fracture in oxides:

Fracture of SiO2 glass proceeds by cavitation;

can be tuned by adjusting % of network modifiers.

- 3 Cascades in compounds

Learning from brute force atomistic simulations

-1 Chemical hardening

- 2 Fracture in oxides:

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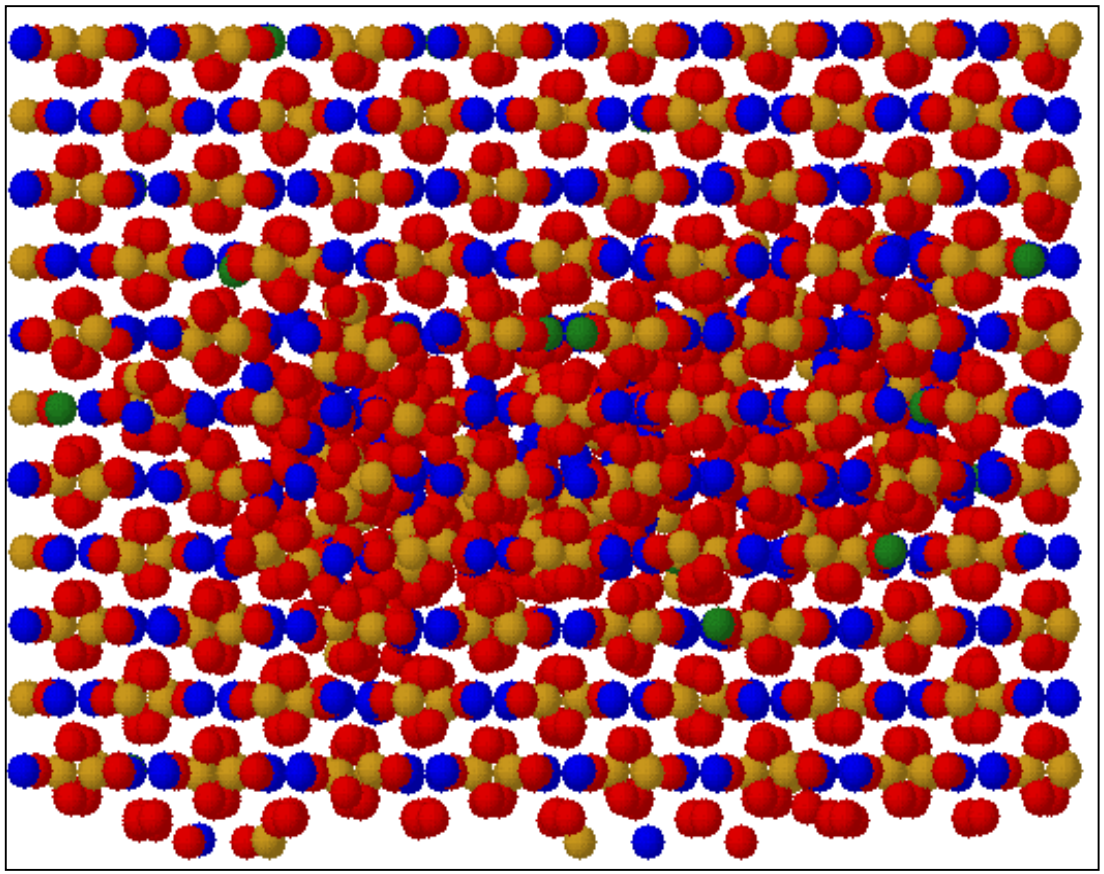
Zircon ($ZrSiO_4$)

Crocombette et al. 2002

- Direct amorphization

Zr Si O U



Learning from brute force atomistic simulations

-1 Chemical hardening

- 2 Fracture in oxides:

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Systematic: the more covalent the easier to amorphize

For the time being:

Nothing as versatile as Calphad, Dictra…

Calphad, Dictra can be taken advantage of (e.g. for RIS), provided

the appropriate Mobility matrix is implemented;

Need for basic developments:

theory + experimental

(wishful thinking? combining appropriate skill and support!)

Atomistic simulations +

integration in multiscale m^{dlg} schemes

do teach a lot + several *successful "niche applications".*