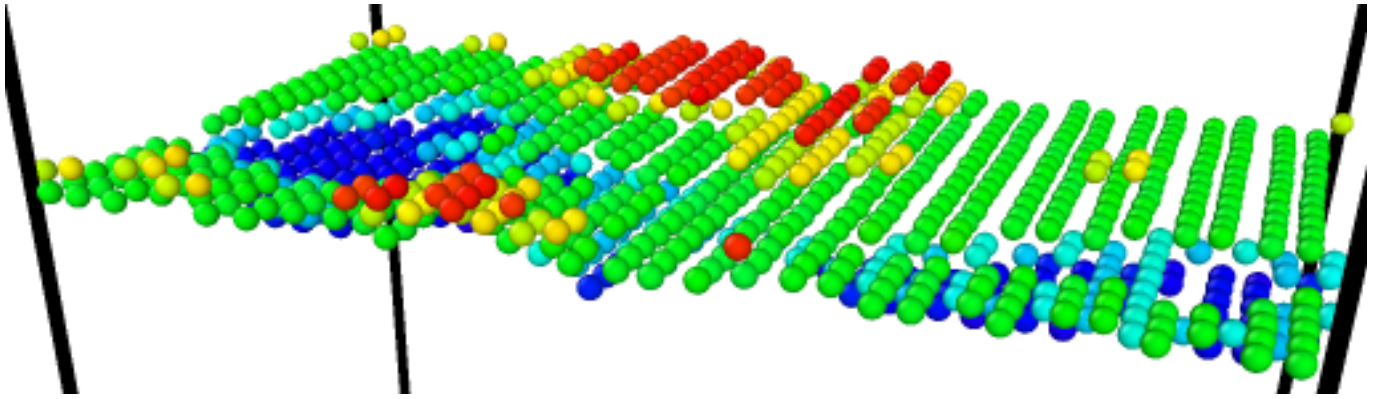
Solute effect on twinning deformation in Mg alloys

A. Luque[1], M. Ghazisaeidi[2], W.A. Curtin[1]

[1] Institute of Mechanical Engineering, École Polytechnique Fédérale de Lausanne, Switzerland

[2] Department of Materials Science and Engineering, Ohio State University, USA



Supported by ERC grant #339081 “Predictive Computational Metallurgy”, EPFL & NSF-GOALI grant #1309687.

24th International Workshop on Computational Micromechanics of Materials, 1-3 October 2014. Madrid (Spain)

INTRODUCTION – Mg & Mg Alloys

- Magnesium:
  - Excellent candidate for low-weight structural applications
  - Limited ductility due to strong plastic anisotropy
    - Twinning is one of the main deformation mechanisms

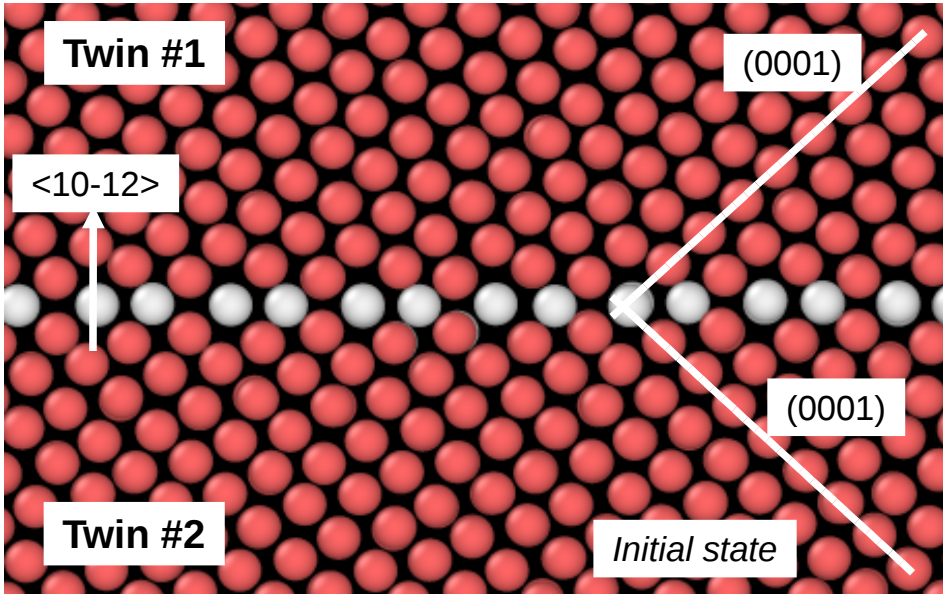
- Magnesium alloys:
  - Substitutional elements (Al, Zn...; rare-earths: Gd, Y...)
  - CRSS modification & optimization of processing route & texture
    - Improved ductility & formability

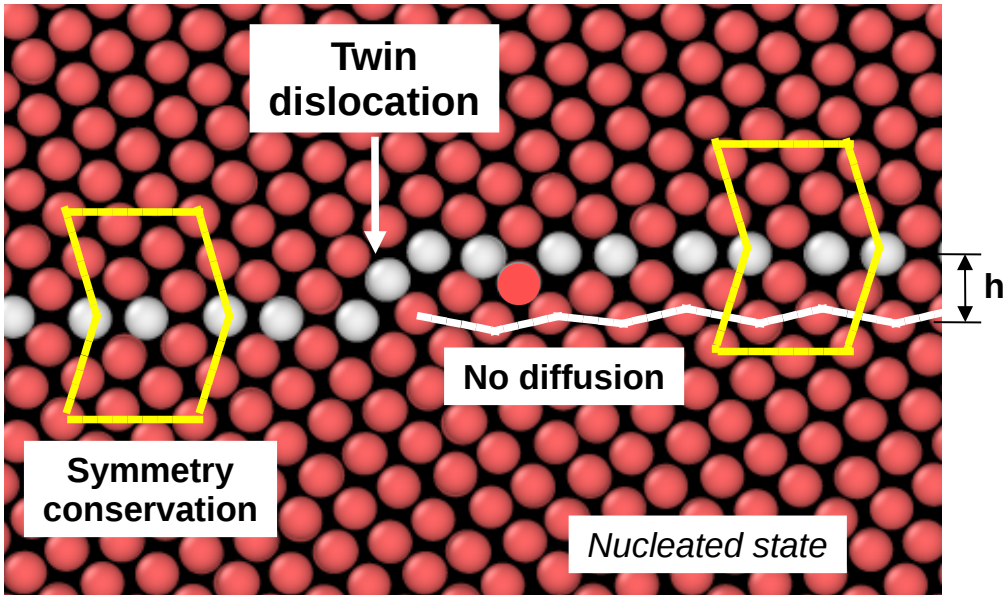
  - **Lack of understanding of the effect of solutes on**
    - Interface structures & energies
    - Solute-dislocation interactions

  - Twinning:
    - What is the intervening mechanism ?
    - What is the activation stress ?
    - What is the role of solute fluctuations ?
    - What is the effect of segregation ?
    - What are the implications in real materials ?

INTRODUCTION – The {10-12}<-1011> (Tension) Twin

– Twin boundary: symmetrical tilt boundary with a misorientation of ~87º
– Twinning: creation of a twinning dislocation (b_{tw} ~ 0.498 Å) with step character (h ~ 3.86 Å): **mechanism of nucleation & growth not well-established**





– We propose:
  – **A stress-driven, thermally-activated mechanism for nucleation & growth**
  – Pure Mg & Mg solid-solution alloys
  – Material parameters:
    • Twin dislocation line energy (MD)
    • Solute/twin-boundary interaction energies (DFT)

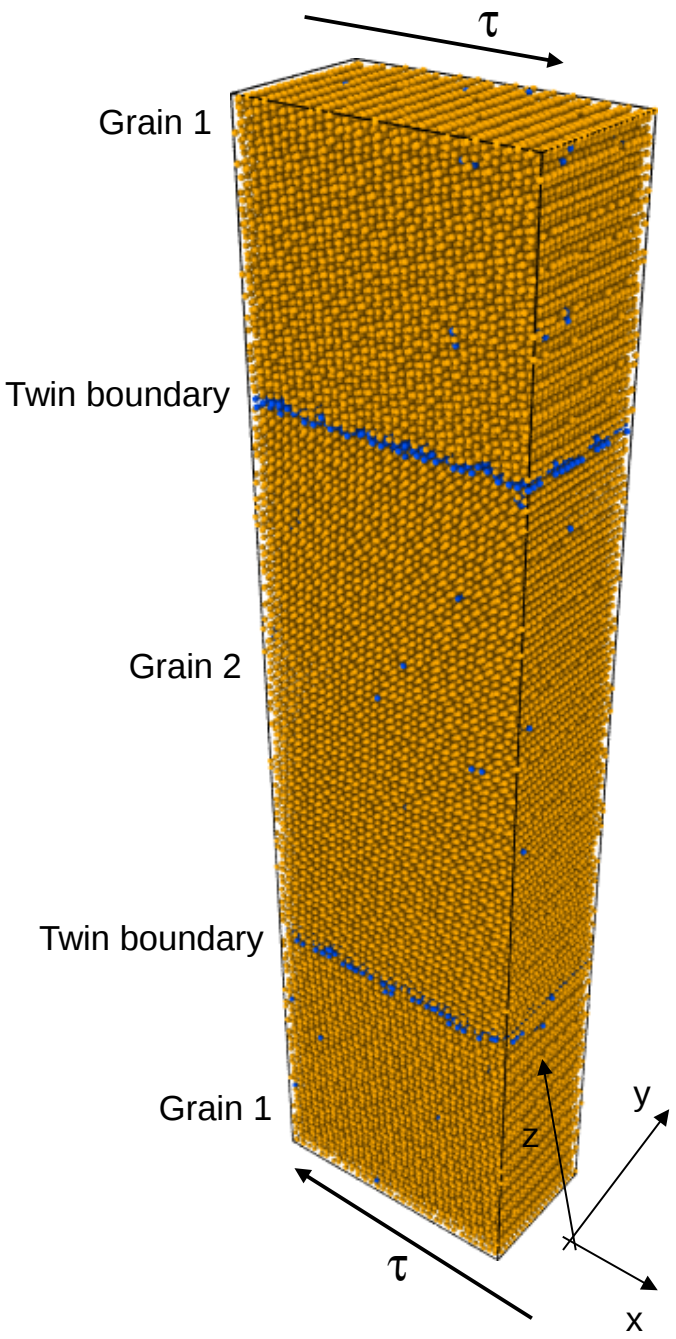
THE MODEL – MD simulations

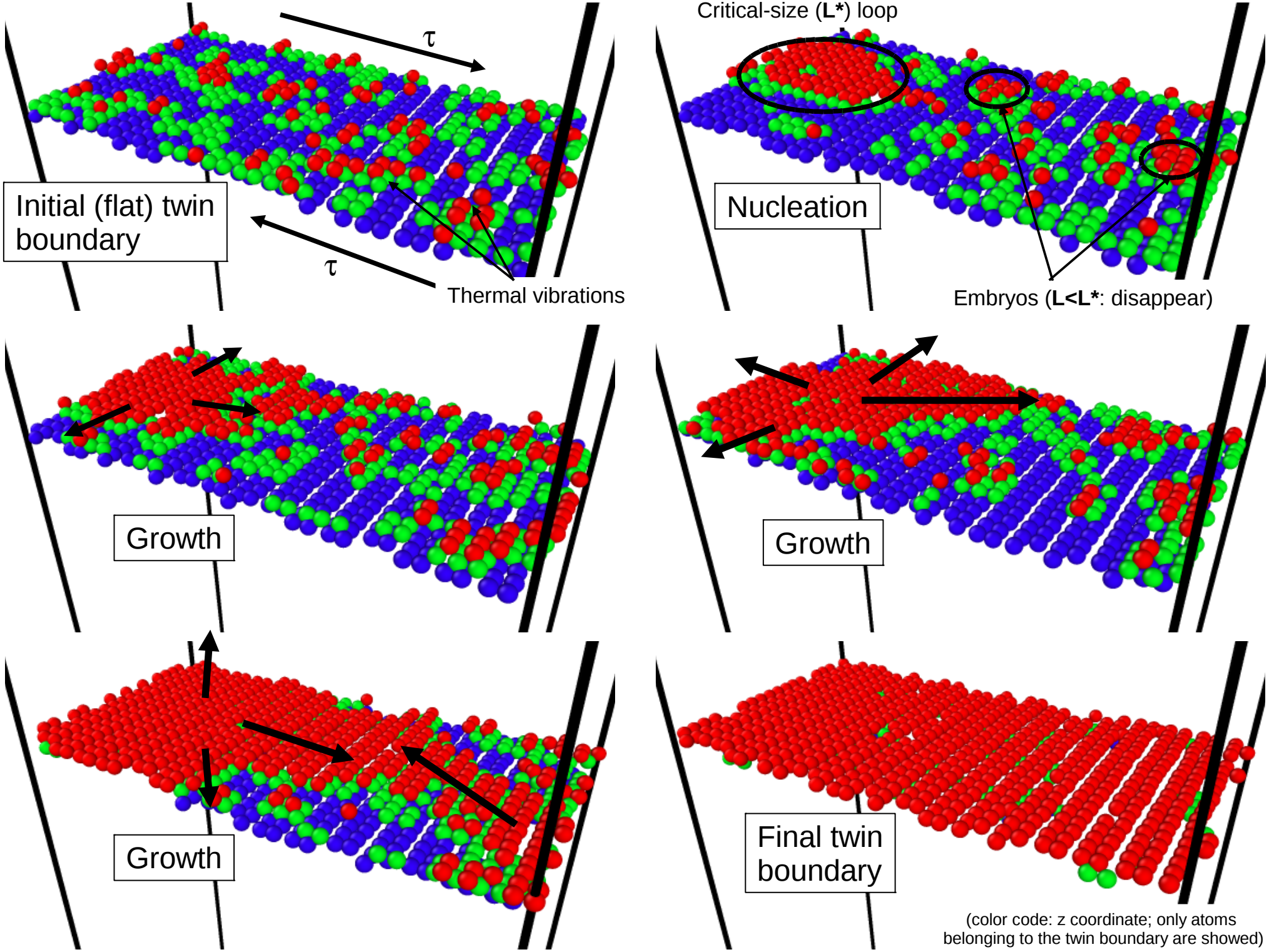
– Material:
  – Mg-Al: **a reliable EAM potential exists**

– Geometry:
  – x // <-1011>, y // <-1210> & z // <10-12>
  – L_x = 12.1 nm, L_y = 6.4 nm, L_z = 50.0 nm
  – **Size effects on nucleation energetics are accounted for:**
    • Interactions with periodic images
    • Limited fluctuations

– Boundary conditions:
  – Periodic boundary conditions along x, y & z
  – **Control of σ_x, σ_y, σ_z & τ_{xz}**
    • Elastic anisotropy of the material
    • Intrinsic interface stress
    • Individual events, long quiescent periods

– Simulation conditions:
  – T = 300 K
  – **Pure Mg & Random Mg alloy** (1, 3, 5 at.% Al)
  – Constant shear stress tests: migration rates

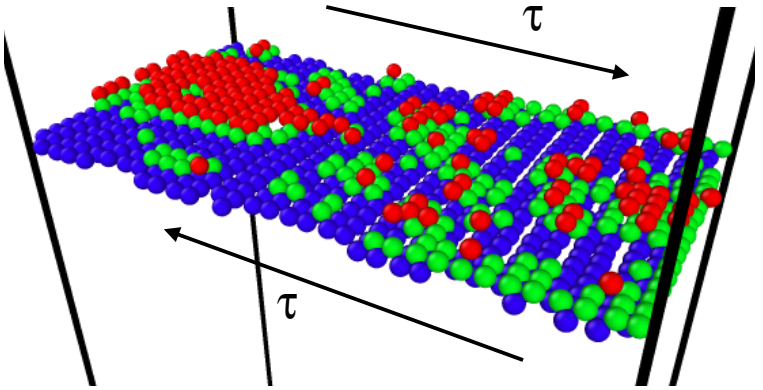


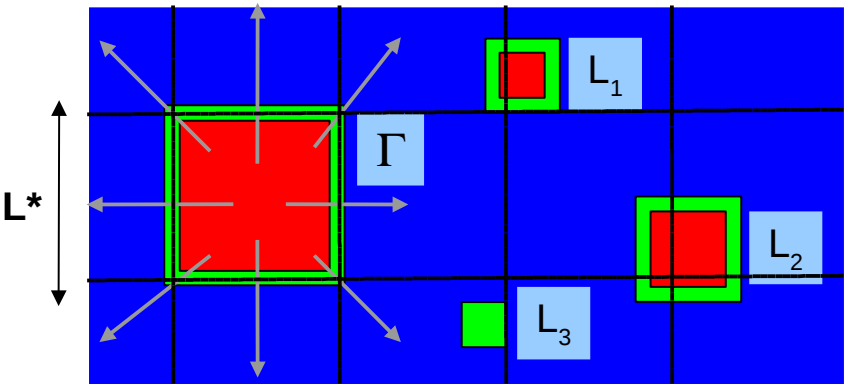

τ
Initial (flat) twin boundary
τ
Thermal vibrations
Critical-size (L*) loop
Nucleation
Embryos (L<L*: disappear)
Growth
Growth
Growth
Final twin boundary
(color code: z coordinate; only atoms belonging to the twin boundary are showed)

THE MODEL – Pure Mg

– Energy analysis (*nucleation* of loop of size L):
  – NO interface energy change
  – Mechanical driving force ~ τ
  – Dislocation line energy ~ Γ

$$\Delta E = 4\Gamma L - \tau b_{tw} L^2$$





* Critical condition:

$$\left.\frac{d\Delta E}{dL}\right|_{L=L^*} = 0$$

* Stability condition:

$$\left.\frac{d^2\Delta E}{dL^2}\right|_{L=L^*} < 0$$

*** Critical loop size:**

$$L^* = \frac{2\Gamma}{\tau b_{tw}}$$

*** Energy barrier:**

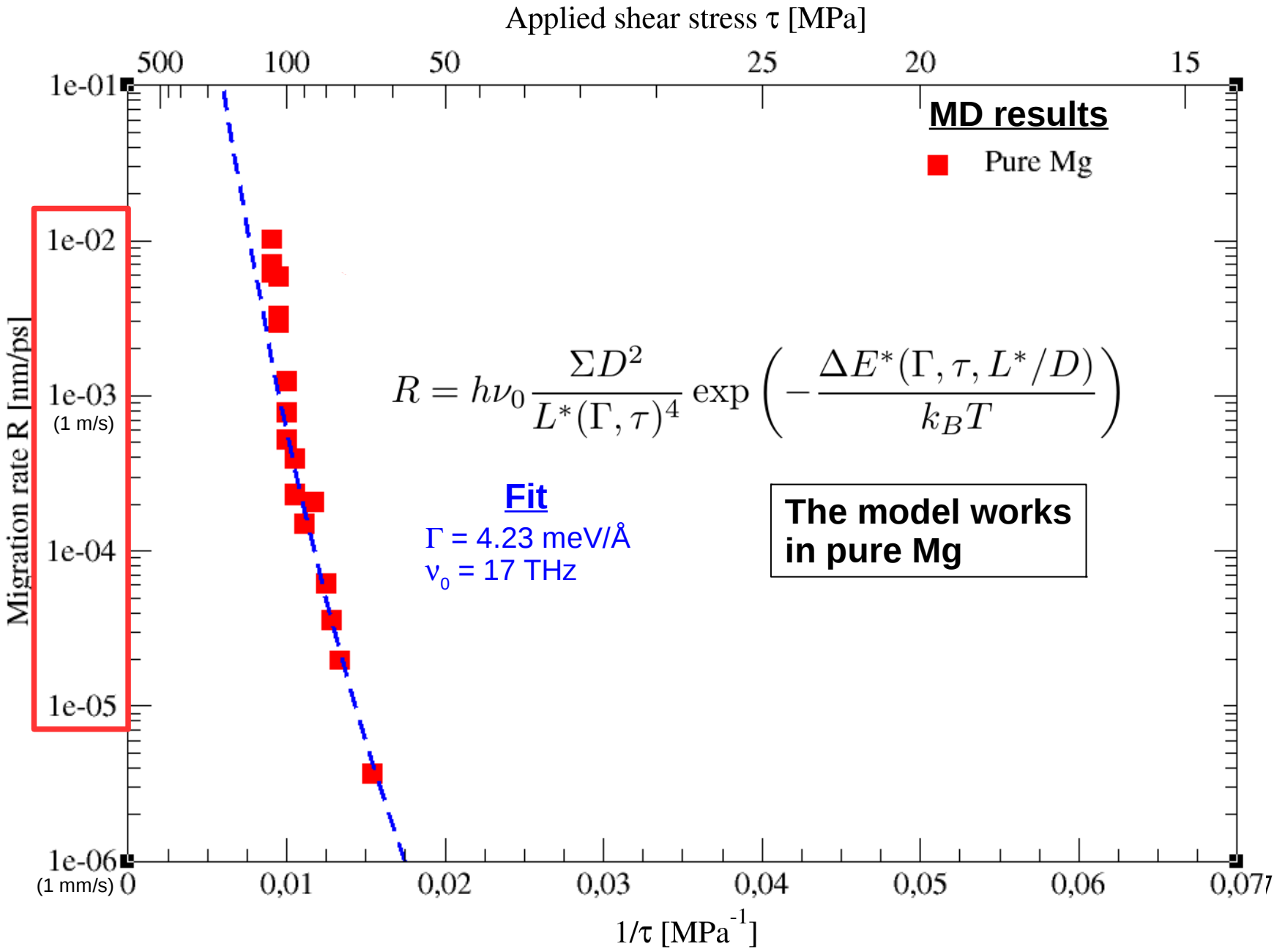
$$\Delta E^* = \frac{4\Gamma^2}{\tau b_{tw}}$$

*** Migration rate (Arrhenius model):**

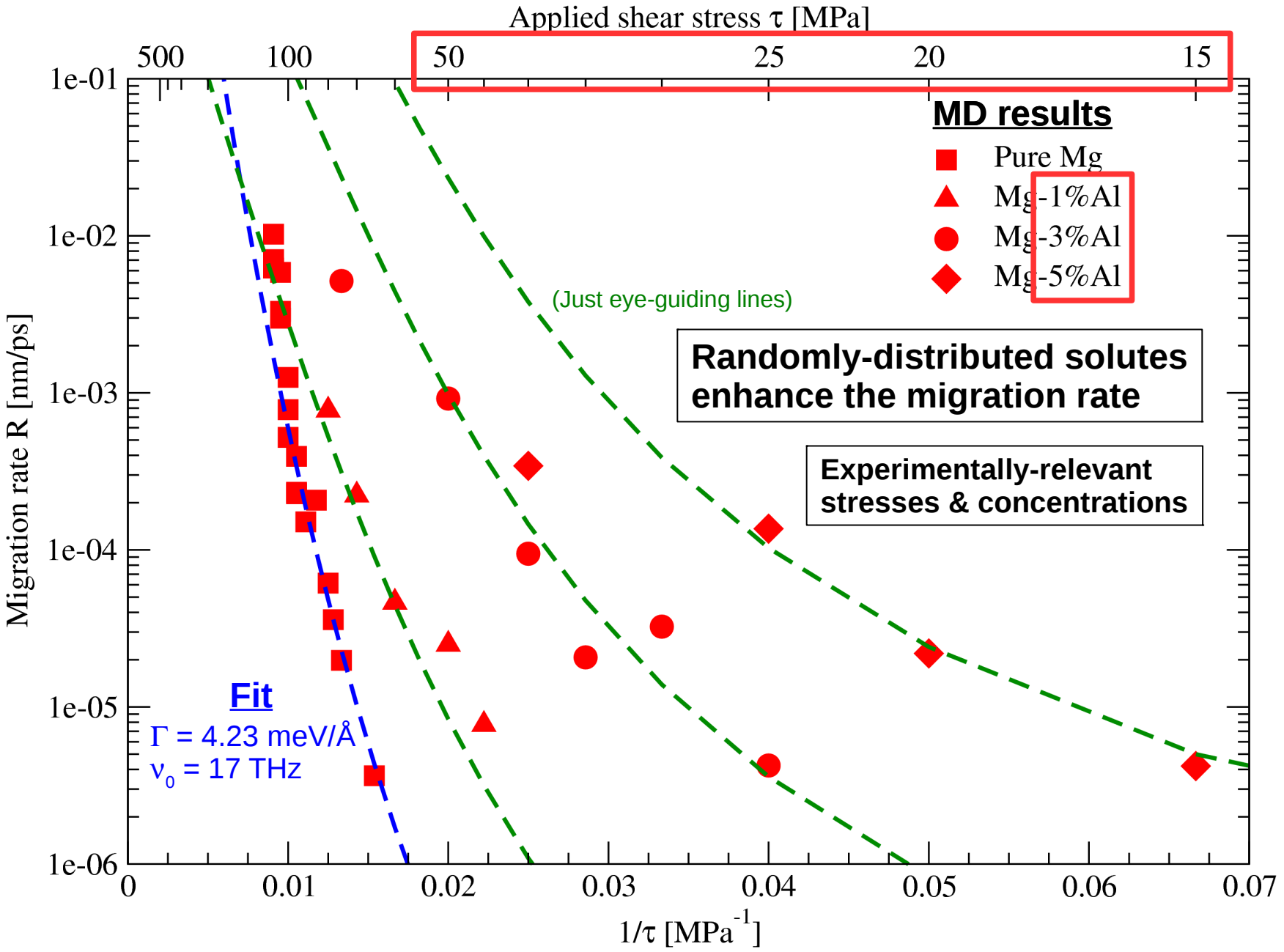
$$R = h\nu_0 \frac{\Sigma}{L^{*2}} \frac{D^2}{L^{*2}} \exp\left(-\frac{\Delta E^*}{k_B T}\right)$$

Σ/L^{*2}: atoms involved in nucleation; D^2/L^{*2}: possible nucleation sites

ATOMISTIC RESPONSE – Pure Mg



ATOMISTIC RESPONSE – Randomly-distributed solutes

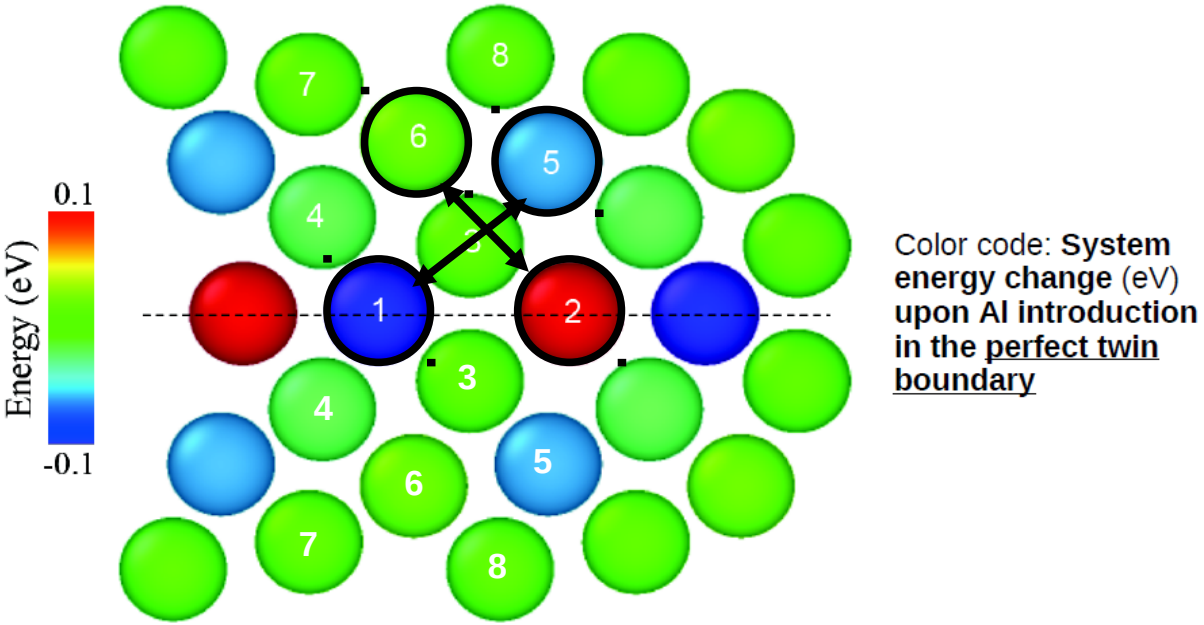


THE MODEL – Solute/twin-boundary interaction energies

– 'Structural' symmetry conservation (NO diffusion!):
  – 8 unique sites: 1 ↔ 5, 2 ↔ 6, 3 ↔ 7 & 4 ↔ 8

– Solutes interact with the twin boundary:
  – Attractive (binding) & Repulsive interaction energies
  – Solutes breaks the 'energetic' symmetry
    • **Solutes provide a driving or retarding force for migration**

Site	(eV)
1	−0.150
2	+0.105
3	−0.002
4	−0.023
5	−0.058
6	+0.020
7	+0.009
8	−0.008



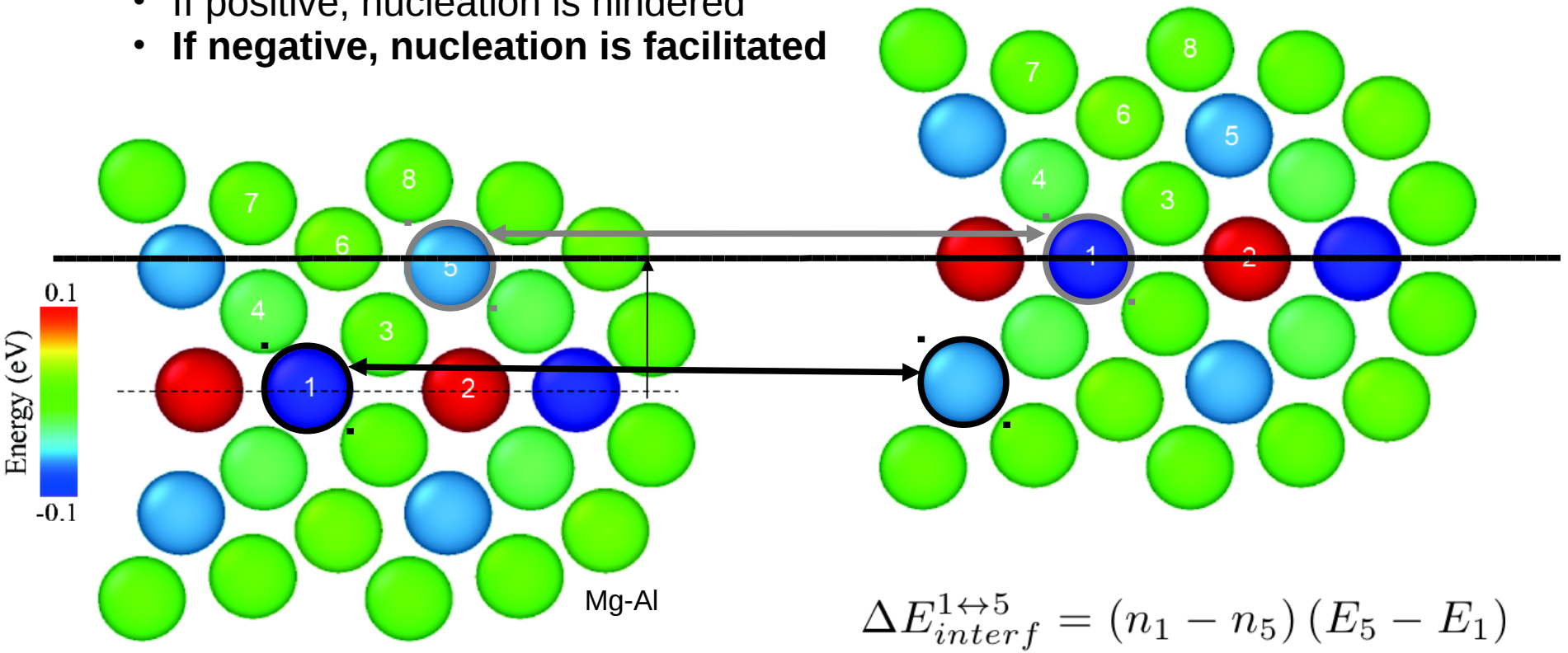
THE MODEL – Effect of solutes

– Additional energy term associated to the interface

$$\Delta E = 4\Gamma L - \tau b_{tw} L^2 + \Delta E_{interf}$$

– Consider one Al solute laying on site 1; after twin migration (no diffusion) it occupies a site 5:

  – The associated energy is $E_5 - E_1$
    - If positive, nucleation is hindered
    - **If negative, nucleation is facilitated**

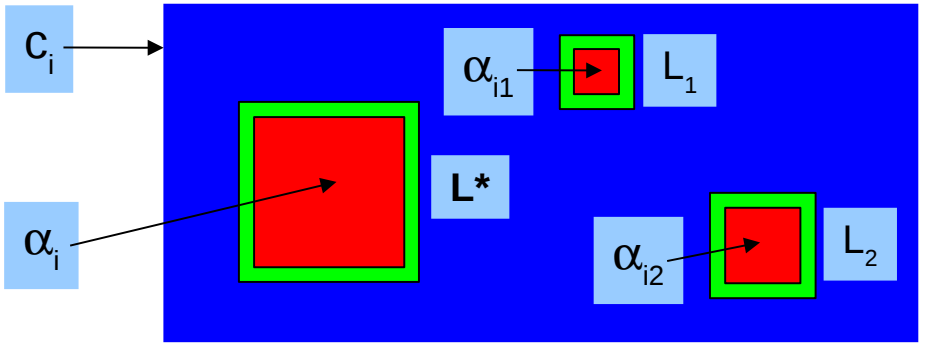


$$\Delta E_{interf}^{1 \leftrightarrow 5} = (n_1 - n_5)\,(E_5 - E_1)$$

THE MODEL – Effect of solutes

– How does this relates to concentration/segregation $\mathbf{c}_i$ & concentration fluctuations?

- **Average number** of occupied sites *i* is $\bar{n}_i = c_i N = \frac{c_i L^2}{2\Sigma}$
- **Standard deviation** in the number of occupied sites *i* is $\Delta n_i = L\sqrt{\frac{c_i(1-c_i)}{2\Sigma}}$
- **Current number** of occupied sites *i* is $n_i = \bar{n}_i + \alpha_i \Delta n_i$



Magnitude of fluctuations associated with site *i*

(if N large, α_i Gaussian)

– Therefore, energy change associated with sites 1 and 5:

$$\Delta E_{interf}^{1\leftrightarrow 5} = (n_1 - n_5)(E_5 - E_1)$$

$$= \underbrace{L^2 \frac{(c_1 - c_5)}{2\Sigma}(E_5 - E_1)}_{\text{Segregation}} + \underbrace{L\left[\alpha_1\sqrt{\frac{c_1(1-c_1)}{2\Sigma}} - \alpha_5\sqrt{\frac{c_5(1-c_5)}{2\Sigma}}\right](E_5 - E_1)}_{\text{Statistical fluctuations}}$$

THE MODEL – Effect of solutes

– When it comes to energy maximization & determination of L*:

– **Concentration/segregation**, related to the state of the entire twin area
  – **Fluctuations** vary from place to place (favorable fluctuations)

– The critical condition yields, for $\tau > \tau_{pin}$ (stability condition):

*** Critical loop size:**

$$L^* = \frac{2\Gamma}{(\tau - \tau_{pin})b_{tw}}$$

*** Energy barrier:**

$$\Delta E^* = \frac{4\Gamma^2 - 2\Gamma|\Delta\Gamma|}{(\tau - \tau_{pin})b_{tw}}$$

where

$$\tau_{pin} = \frac{1}{2b_{tw}\Sigma}\left[(c_1 - c_5)(E_5 - E_1) + (c_2 - c_6)(E_6 - E_2)\right]$$

and

$$|\Delta\Gamma| = \frac{|E_5 - E_1|}{\sqrt{2\Sigma}}\left[|\alpha_1|\sqrt{c_1(1-c_1)} + |\alpha_5|\sqrt{c_5(1-c_5)}\right]$$

$$+\frac{|E_6 - E_2|}{\sqrt{2\Sigma}}\left[|\alpha_2|\sqrt{c_2(1-c_2)} + |\alpha_6|\sqrt{c_6(1-c_6)}\right]$$

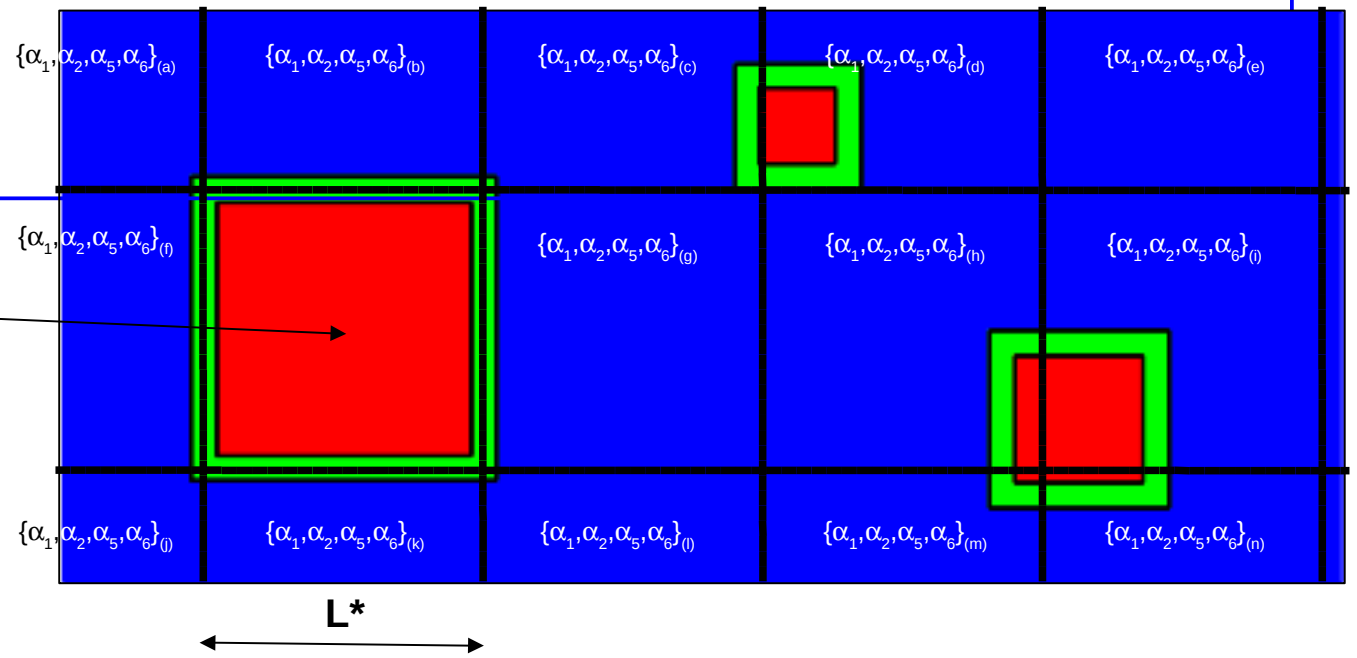
THE MODEL – Effect of solutes

– Statistical analysis provides fluctuations accurately:
  – **α_i gets the *largest probable* value so $|\Delta\Gamma|$ is maximum**

*** Migration rate**:

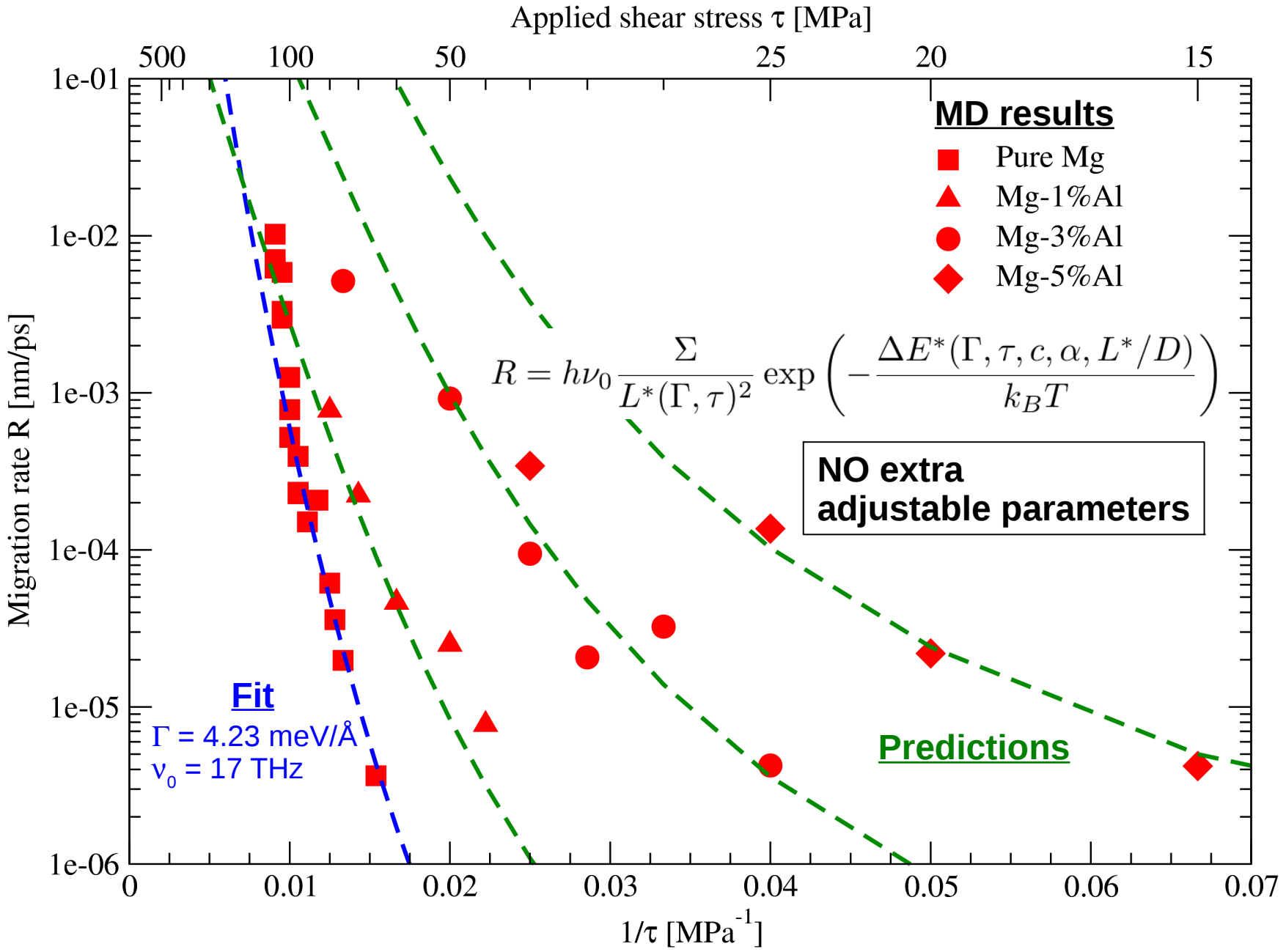
$$R = h\nu_0 \frac{\Sigma}{L^{*2}} \exp\left(-\frac{4\Gamma^2 - 2\Gamma|\Delta\Gamma|}{k_B T(\tau - \tau_{pin}) b_{tw}}\right) \quad \text{with} \quad |\alpha_i| \sim \sqrt{4 \ln\left(\frac{2D}{\pi L^*}\right) \frac{c_i(1-c_i)}{\sum c_j(1-c_j)}}$$

– If $c_i = c$:
  - $\tau_{pin} = 0$
  - $\alpha_i = \alpha \sim 2\text{-}2.5$



Nucleation occurs where the largest *favorable* fluctuations can be found

VALIDATION OF THE MODEL – Random solutes



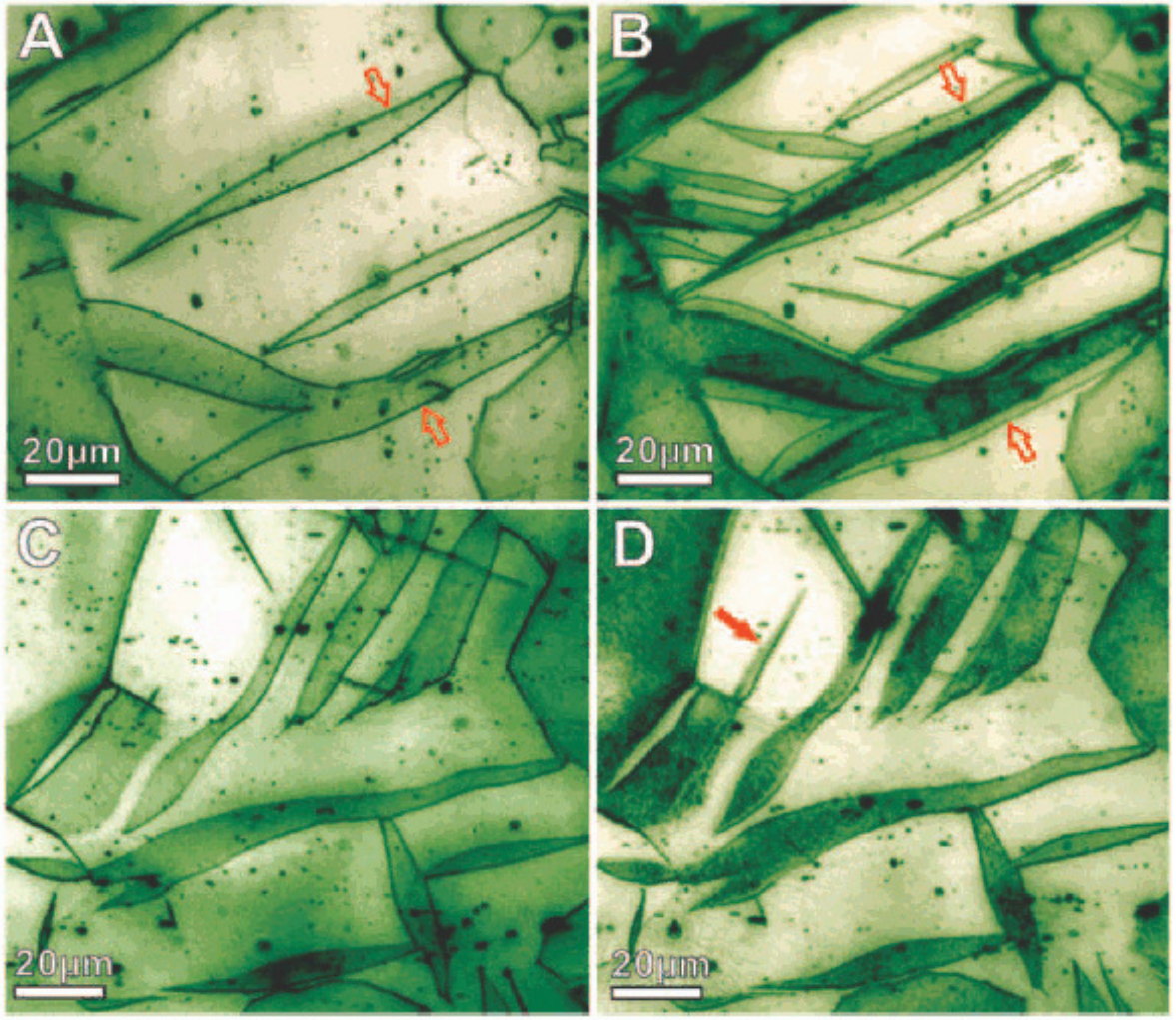
IMPLICATIONS FOR REAL MATERIALS – Segregation

– Segregation: $$\tau_{pin} = \frac{1}{2b_{tw}\Sigma}\left[(c_1 - c_5)(E_5 - E_1) + (c_2 - c_6)(E_6 - E_2)\right]$$

- Nie *et al. 2013 Science 340*: polycrystalline Mg-0.2%at. Gd samples
  - Annealing conditions (150 ºC, 3h): c_2=0.76, c_6=0.01, c_1=c_5=0 ⇒ τ_{pin} = 2.1 GPa

As-cast, compressed (2.5%): **nucleation of twins**

(τ ~ 25 MPa)



As-cast, recompressed (4.5%): **growth of the existing twins & nucleation of new twins**

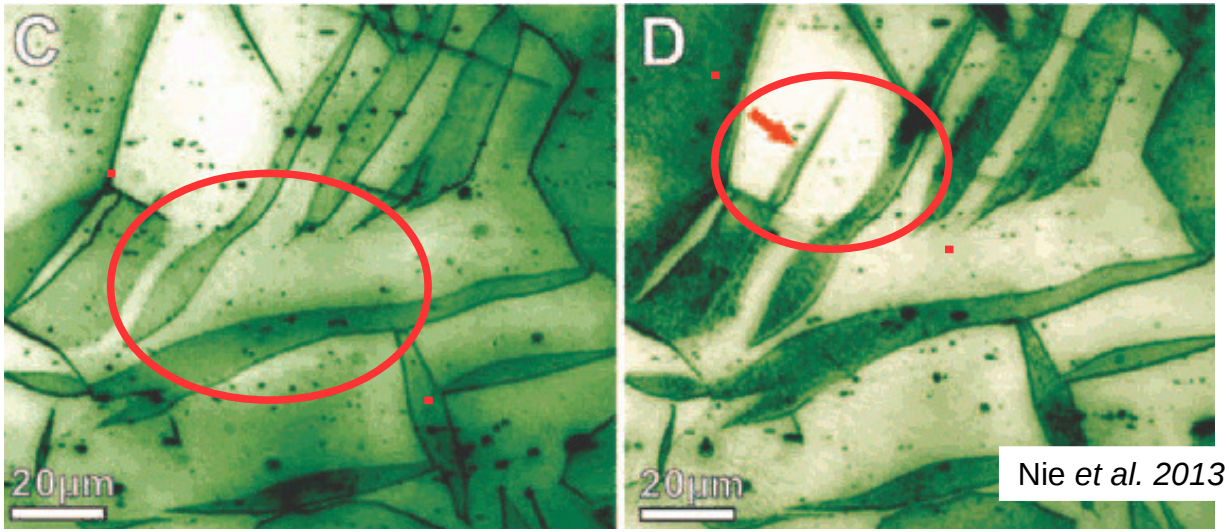
Annealed & recompressed (4.5%): **nucleation of new twins**

(τ ~ 40 MPa)

CONCLUSIONS

– We propose a new mechanism for the thickening of an existing twin
  – Energetic model based on:
    • Solute/twin interactions & dislocation line energy
    • Segregation & concentration fluctuations (*statistical analysis*)
  – Validated by means of carefully-controlled MD simulations

– We successfully apply it to evaluate several observations in Mg alloys:
  – **Randomly-distributed solutes enhance the migration process** (*detwinning*)
  – **Segregation of solutes inhibits the migration process**



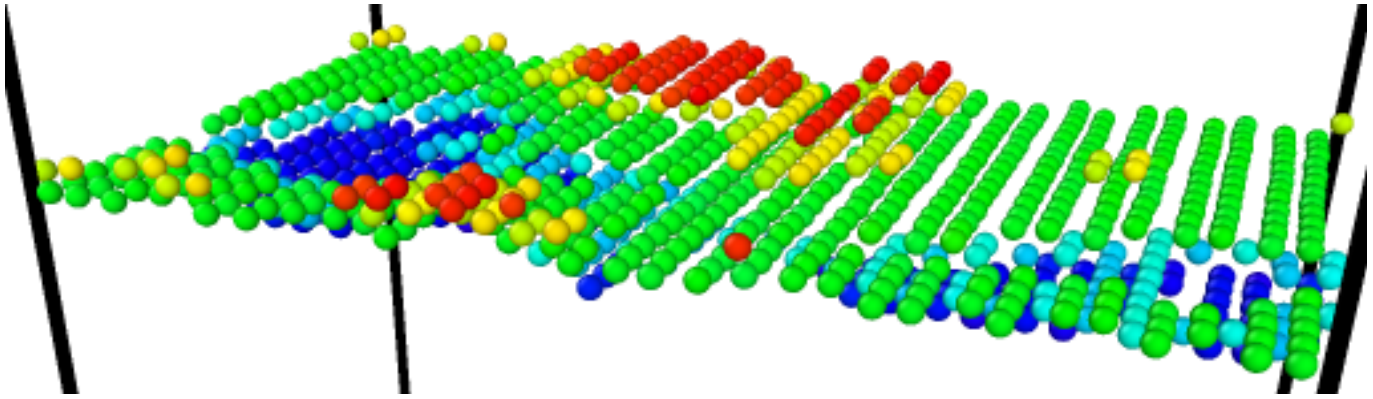
Nie *et al. 2013 Science 340*

Solute effect on twinning deformation in Mg alloys

A. Luque[1], M. Ghazisaeidi[2], W.A. Curtin[1]

[1] Institute of Mechanical Engineering, École Polytechnique Fédérale de Lausanne, Switzerland

[2] Department of Materials Science and Engineering, Ohio State University, USA



Supported by ERC grant #339081 “Predictive Computational Metallurgy”, EPFL & NSF-GOALI grant #1309687.

24th International Workshop on Computational Micromechanics of Materials, 1-3 October 2014. Madrid (Spain)