An atomistic investigation of the interaction of dislocations with Guinier-Preston zones in Al-Cu alloys

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OUTLINE

A) Motivation

1 – VIRMETAL PROJECT

2- Atomistic simulation and modeling of Al-Cu alloys

3 - Al-4%Cu alloy precipitation sequence

B) Atomistic simulations of dislocation Guinier-Preston zones interaction

1 - Atomistic Setup

2 - Simulation methodology

3 - Results

Transition state theory with direct Molecular Dynamics

Nudged elastic band method

Thermodynamics of Dislocation-GP zone

Predictions of flow stress based on atomistic results

C) Conclusions

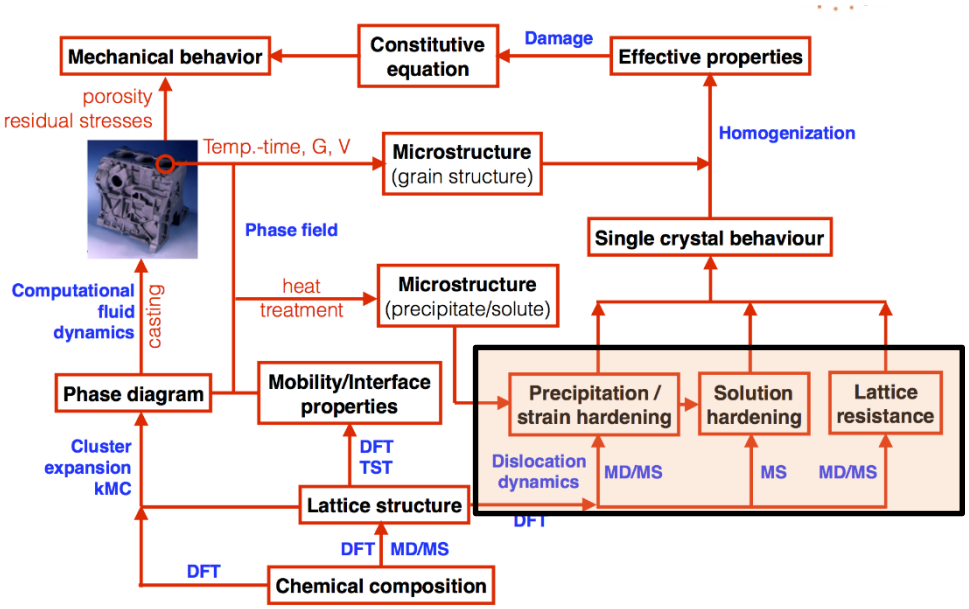
MOTIVATION

1 – VIRMETAL PROJECT

- Development a bottom- up multiscale strategy to design, process and test advances metallic alloys
- Six main tasks involved this project
  - **Connect atomistic-microscales**
  - Bridging microscale-macroscale
  - Multiscale modeling of plastic deformation and fracture
  - Computational thermodynamics and kinetics
  - Multiscale modeling of casting and solidification
  - Experimental validation

- Focused on **Al-Cu** and Mg-Al-Zn

- ***Objective :*** Provide information from classical atomistic approaches (MD, MC, NEB) to larger scale simulations.



MOTIVATION

2 – ATOMISTIC SIMULATION AND MODELING OF Al-Cu ALLOYS

- Investigate the **interaction of different type of dislocations with precipitates**.
  - Overcome mechanisms
  - Critical resolved shear stress
  - Activation energies
  - Thermodynamic study

- Quantify how **solid solution affects** to the motion of dislocation

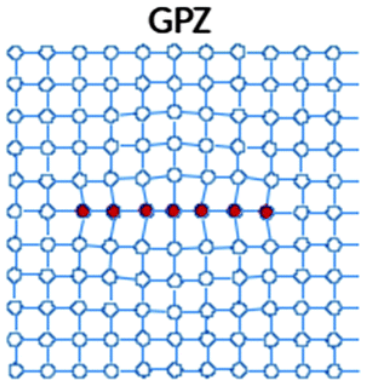
- Compute the **activation energies for other mechanisms** of overcoming obstacles. i.e. Cross Slip in screw dislocations

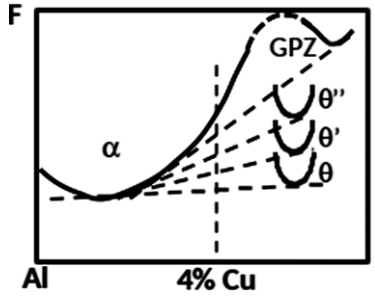
- **Development of models** to use in higher length scales i.e. Discrete Dislocation Dynamics

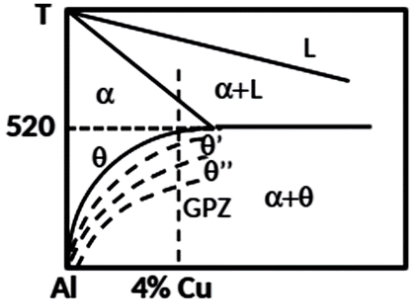
MOTIVATION

3 – Al-4%Cu ALLOY PRECIPITATION SEQUENCE

- Al4%Cu alloys presents a well-stablished sequence of precipitation
- Solid Solution → **Guinier-Preston zones** → θ'' → θ' → θ
- Depending on the heat treatment, different precipitation will appear.
- Naturally aged Al-4%Cu (504 h at room temperature) alloy contains in **mostly Guinier-Preston zones (GP).**
- GP zones features:
  - Aggregates of Cu atoms
  - Mono layer disk shaped precipitates
  - {100} family of planes
  - Totally coherent precipitates
  - From 2-10 nm of diameter.





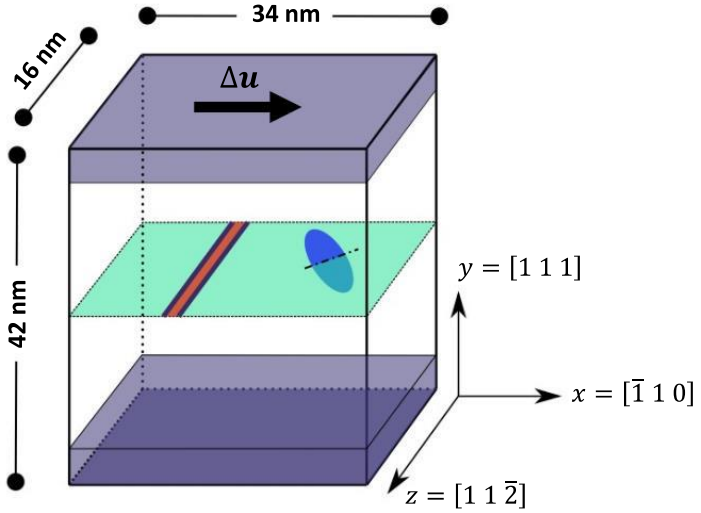


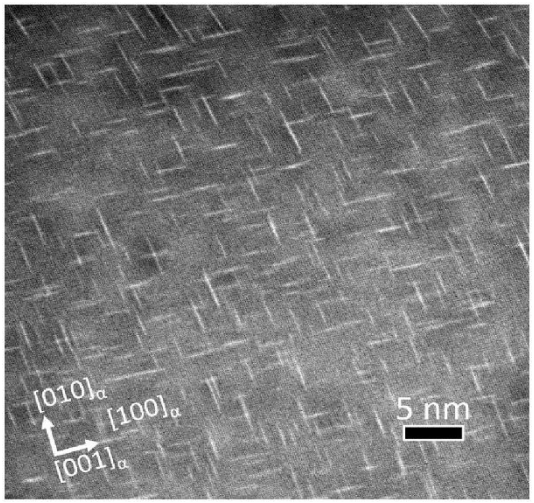
Images from: Phys.Chem.Chem.Phys. 17, (2015), pp 27249--27257

ATOMISTIC SIMULATIONS OF DISLOCATION GUINIER-PRESTON ZONES INTERACTION

1 – ATOMISTIC SETUP

- The system contains around **1.38 million** of atoms
- Inserted an **edge dislocation** with Volterra's displacement field.
- GP zones show **2 different interaction angles as a function of Burgers vector** of a dislocation in its slip plane: 60 degrees, 0 degrees
- Inserted **GP zone in the (100) plane**, which represent a 60 degree obstacle for the dislocation in the slip plane.
- The atomic setup try to **mimic** as close as possible the microstructure of **Al-4%Cu alloy** naturally aged.





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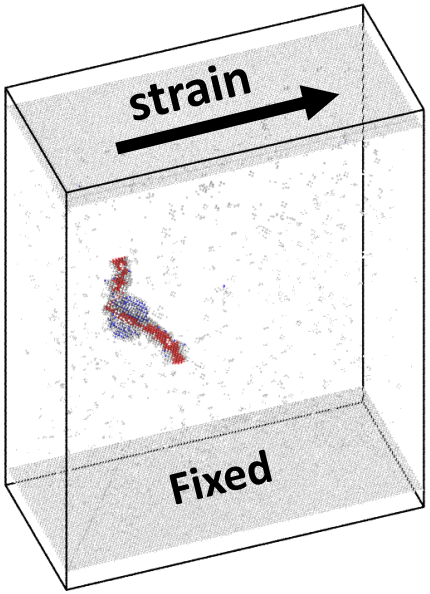
ATOMISTIC SIMULATIONS OF DISLOCATION GUINIER-PRESTON ZONES INTERACTION

2 – SIMULATIONS METHODOLOGY

- **Activation enthalpy (ΔH) and activation Gibbs free energy (ΔG)** of interaction between dislocation and GP60 zones a have been study by means of **two different classical atomistic approaches:**
  - Classical **Molecular Dynamics** simulations (MD) have been devoted to **obtain the rate of the dislocation to overcome GP zone** . Using transition state theory (TST) obtain the activation Gibbs free energy.

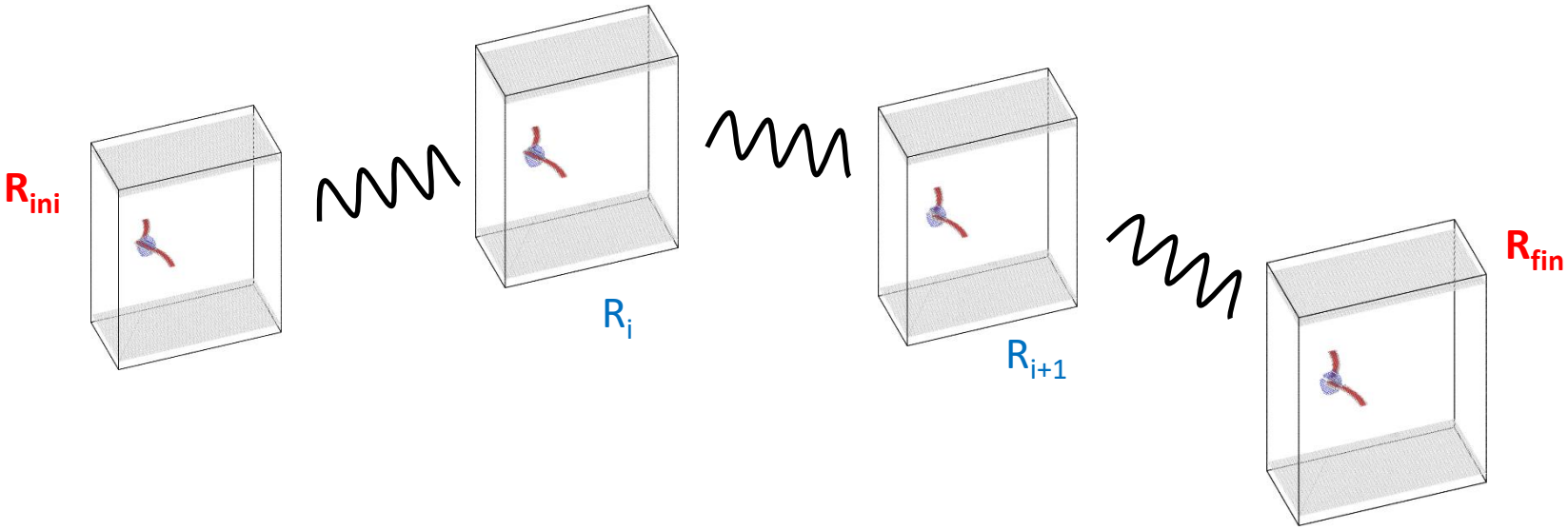


- **NVT ensemble with Langevin thermostat** and constant strain applied in the upper boundary.
- With a timestep of **2 fs** wait until the dislocation overcome the GP zone.
- A range of **temperatures from 400-600 K** in steps of 50K and **from 140 to 170 MPa** in steps of 10 Mpa.
- **8 independent MD simulations** for each couple of stress and temperature.

ATOMISTIC SIMULATIONS OF DISLOCATION GUINIER-PRESTON ZONES INTERACTION

2 – SIMULATIONS METHODOLOGY

- **Activation enthalpy (ΔH) and activation Gibbs free energy (ΔG)** of interaction between dislocation and GP60 zones a have been study by means of **two different classical atomistic approaches**:
    - The **nudged elastic band method (NEB)** has been utilized to compute the **activation enthalpy** as a function of the applied strain with 16 replicas.



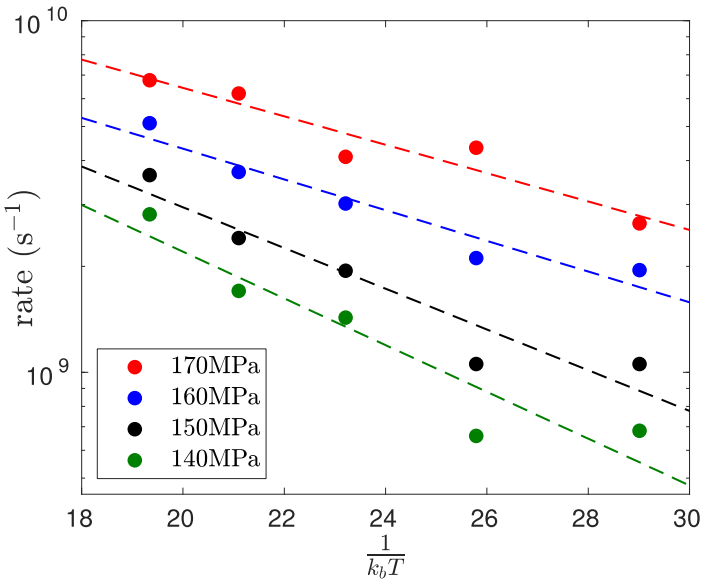
ATOMISTIC SIMULATIONS OF DISLOCATION GUINIER-PRESTON ZONES INTERACTION

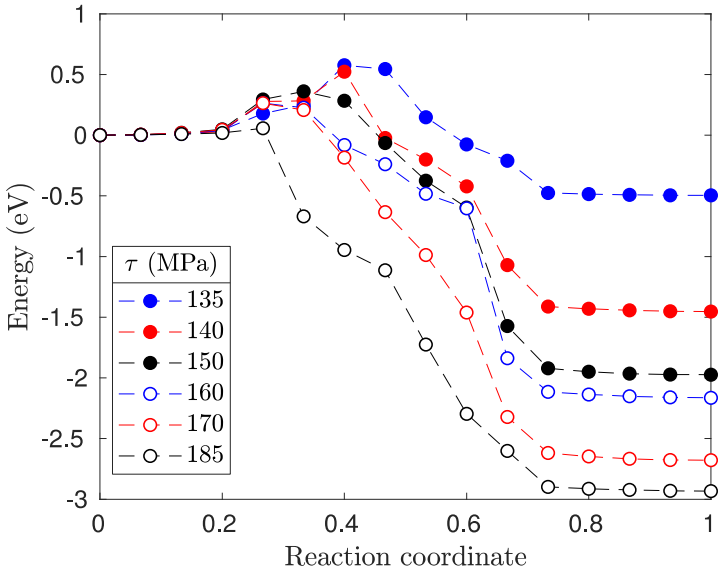
3 – RESULTS

- Molecular dynamics simulations have provide the average rate for the dislocation to overcome the GP zone.

$$\frac{N}{\sum_1^N t_{MD}} = \bar{\Gamma} = v_0 exp\left(\frac{-\Delta G(\tau)}{k_b T}\right) \rightarrow v_0 = 4 - 5x10^{10}\ \frac{1}{s}$$

- Nudged Elastic band simulations gave the activation enthalpy profile as a function of the shear stress applied.

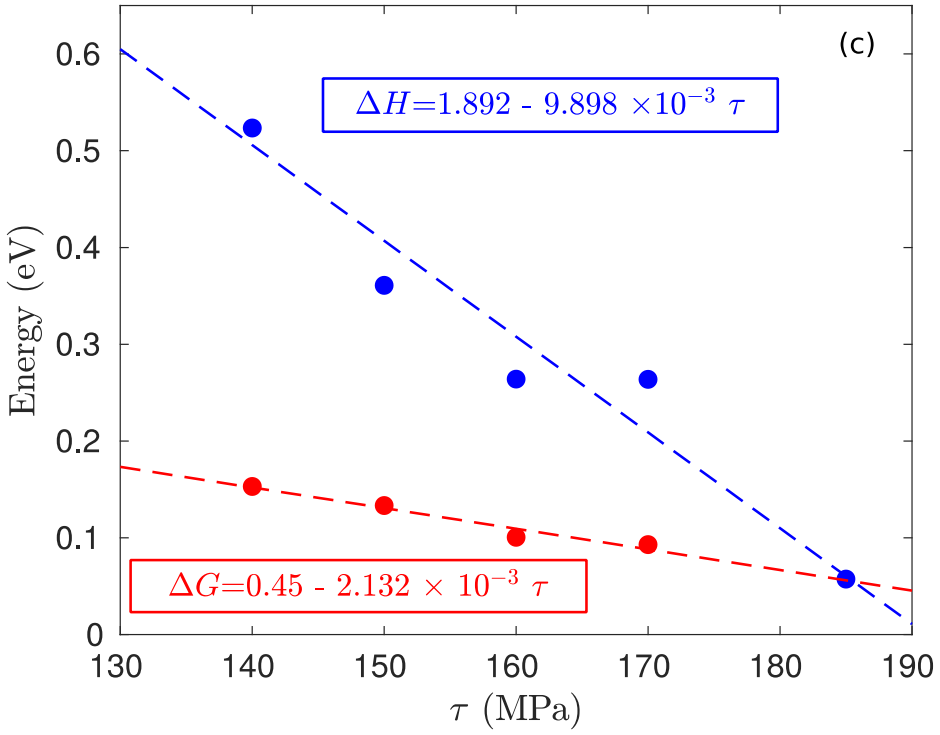




ATOMISTIC SIMULATIONS OF DISLOCATION GUINIER-PRESTON ZONES INTERACTION

3 – RESULTS:

- Comparing the thermodynamic results obtained with both NEB and MD simulations.



$$\Delta G = \Delta F - \tau V_a = \Delta F \left(1 - \frac{\tau}{\tau_a}\right)$$

$$-\frac{\partial \Delta G}{\partial \tau} = \frac{\Delta F}{\tau_a} = V_a$$

$$\boldsymbol{\Delta F = 0.45\ eV \quad V_a = 14 b^3}$$

$$\Delta H = A - B\tau$$

$$\Delta G = \Delta H(\tau) - T\Delta S$$

- **Difference** between both results should come from the **entropic factor** $\Delta S(T, \tau)$.

ATOMISTIC SIMULATIONS OF DISLOCATION GUINIER-PRESTON ZONES INTERACTION

3 – RESULTS:

- Up to the moment we have obtained
  - $\Delta \boldsymbol{G}$ as a **function of stress** applied, but does **not** depend on **temperature**.
  - $\Delta \boldsymbol{H}$ as a function of applied stress.
  - **Activation volume $\boldsymbol{V_a}$** is **constant** with respect to the stress.

$$-\frac{\partial \Delta G}{\partial \tau} = -\frac{\partial \Delta U}{\partial \tau} + V_a + T\frac{\partial \Delta S}{\partial \tau} \rightarrow \frac{\partial \Delta F}{\partial \tau} = 0 \rightarrow \frac{\partial \Delta U}{\partial \tau} = T\frac{\partial \Delta S}{\partial \tau}$$

- Variation of internal energy and variation of entropy should be parallel curves.

$$\Delta S = \frac{1}{T}(\Delta H - \Delta G) \rightarrow \boxed{\Delta \boldsymbol{S} = \frac{\boldsymbol{1}}{\boldsymbol{T}}[(\boldsymbol{A} - \Delta \boldsymbol{F}) - (\boldsymbol{B} - \boldsymbol{V_a})\boldsymbol{\tau}]}$$

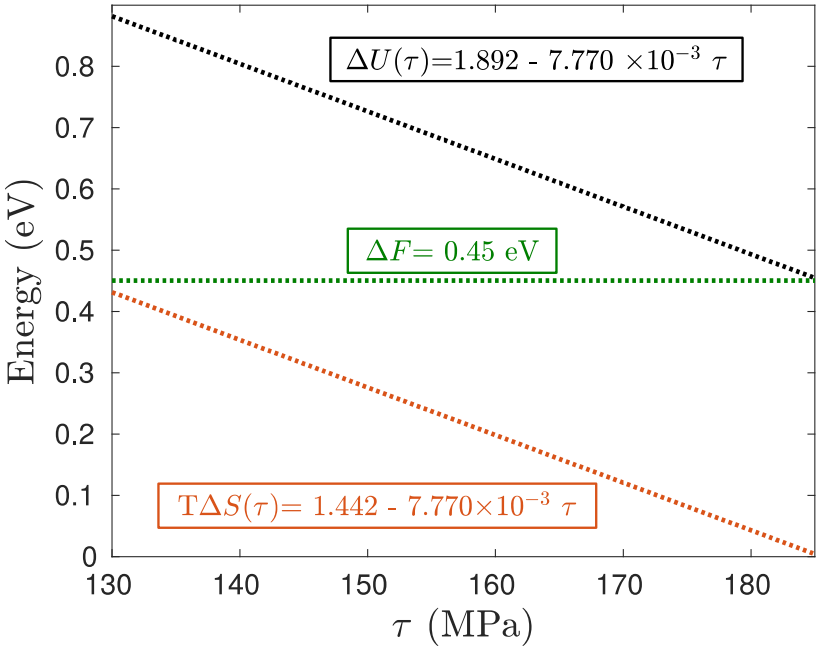
- Finally using the the definition of activation Gibbs free energy is obtained

$$\Delta G = \Delta U - T\Delta S - \tau V_a \rightarrow \boxed{\Delta \boldsymbol{U} = [\boldsymbol{A} - (\boldsymbol{B} - \boldsymbol{V_a})\boldsymbol{\tau}]}$$

ATOMISTIC SIMULATIONS OF DISLOCATION GUINIER-PRESTON ZONES INTERACTION

3 – RESULTS:

- **Entropic factor** is a **function of the temperature O(T^{-1}) and applied stress**
- Variation of **internal energy** depends just on the **stress**. Activation Helmholtz free energy is the distance between both thermodynamic functions.



$$\Delta U = [A - (B - V_a)\tau]$$

$$\Delta S = \frac{1}{T}[(A - \Delta F) - (B - V_a)\tau]$$

- HTST to hold the entropic factor:

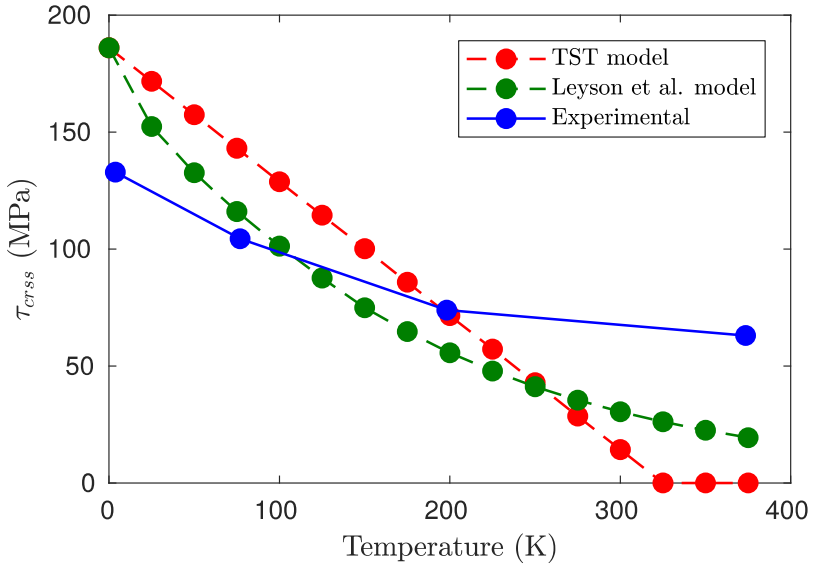
$$\Delta S = k_b log\left(\frac{\prod_i^{N-1} \nu_i^{min}}{\prod_i^{N-1} \nu_i^{saddle}}\right)$$

- In the case studied, dependence of temperature of ΔS(T^{-1}) suggest that HTST does not hold.

ATOMISTIC SIMULATIONS OF DISLOCATION GUINIER-PRESTON ZONES INTERACTION

3 – RESULTS:

- **Prediction of the thermal contribution of the flow stress** of Al-4%Cu naturally aged based on thermodynamic results and TST.



$$\tau_y = \tau_y^a + \tau_y^t$$

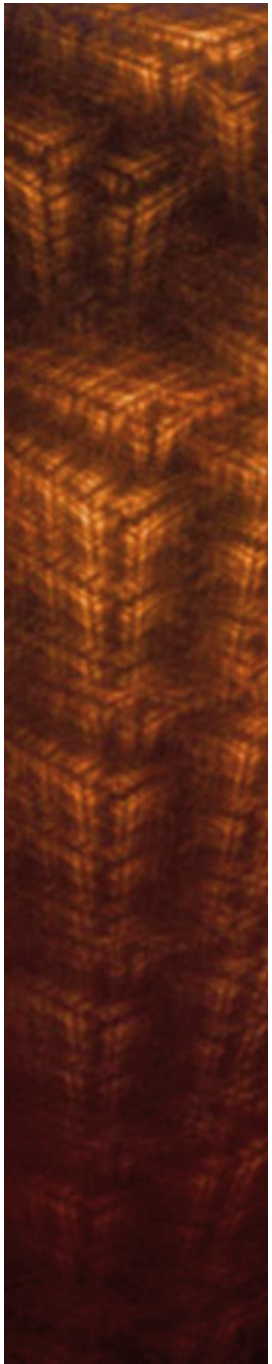
$$\tau_y^t = \tau_0 \left[1 - \frac{k_b T}{\Delta F} log\left(\frac{\dot{\gamma}_0}{\dot{\gamma}}\right)\right]$$

$$\tau_y^t = \begin{cases} \tau_0 \left[1 - \left(\frac{k_b T}{\Delta F} log\left(\frac{\dot{\gamma}_0}{\dot{\gamma}}\right)\right)^{\frac{2}{3}}\right] & \frac{\tau_y^t}{\tau_0} \geq 0.55 \\ \tau_0 exp\left[-\frac{1}{C}\frac{k_b T}{\Delta F} log\left(\frac{\dot{\gamma}_0}{\dot{\gamma}}\right)\right] & \frac{\tau_y^t}{\tau_0} < 0.55 \end{cases}$$

- The source of discrepancies might be:
  - Just GP60 zones and edge dislocation taken into account.
  - Athermal contribution of the flow stress.
  - Distribution of precipitates.

CONCLUSIONS

- Our simulations suggest that harmonic transition state theory does not hold to this phenomenon.
- A prediction of thermal contribution of the flow stress has been carried out, with the thermodynamic results obtained.
- Experiments proved more complex behavior than the one study here.



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THANK YOU FOR YOU ATTENTION