A QUANTITATIVE MULTISCALE APPROACH FOR THE CLIMB OF JOGGED DISLOCATIONS

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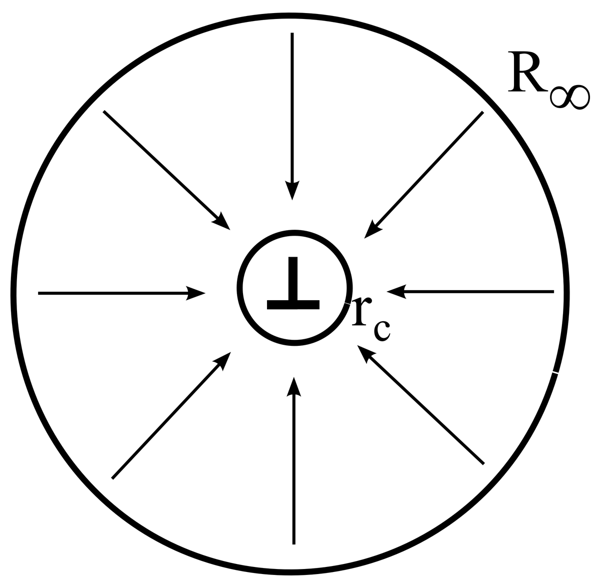
INTRODUCTION

Mesoscopic approaches to dislocation climb such as dislocation dynamics [1, 2] or crystal plasticity approaches [3] are based on several assumptions:

(i) Elastic interactions between dislocations and vacancies are neglected.
(ii) Transient regime is neglected.
(iii) **The dislocation is assumed to act as a perfect source/sink of vacancies (local equilibrium assumption).**
(iv) **Diffusion is considered to take place in a hollow cylinder.**



Solving the diffusion equation in cylindrical coordinate and integrating the flux arriving at r_c, we obtain the dislocation climb rate [1]:

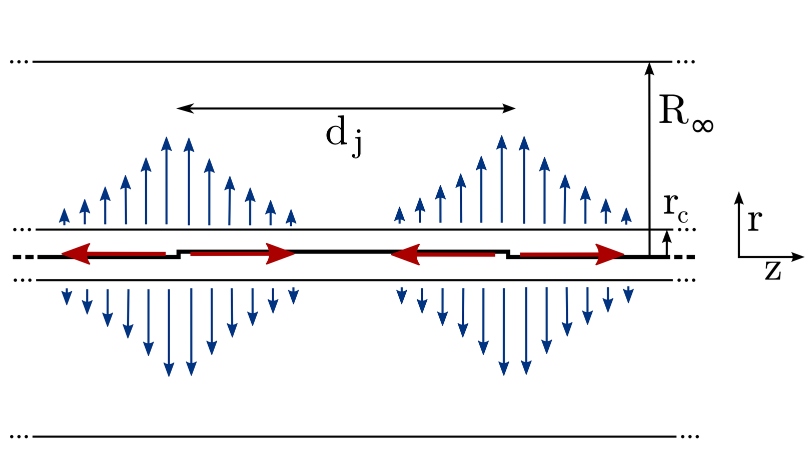
$$v_1 = \frac{2\pi c_0 D_v}{b \ln(R_\infty/r_c)}\left(\frac{c_\infty}{c_0} - e^{\frac{\sigma^a \Omega}{kT}}\right)$$

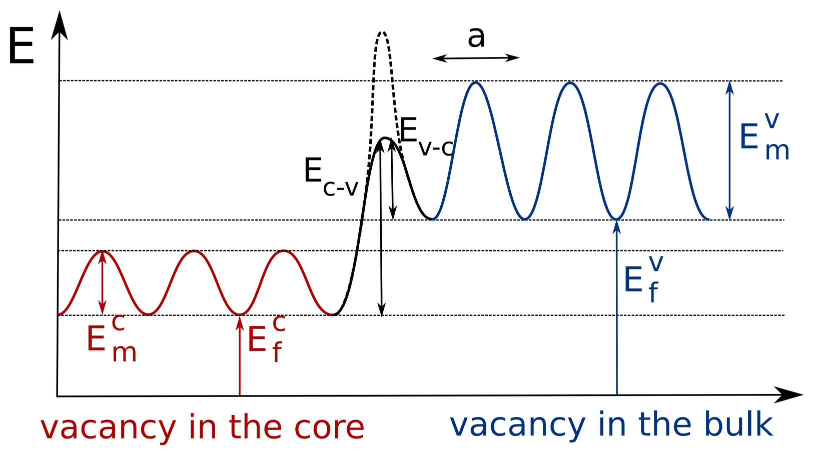
Objective: Discuss theoretically assumptions (iii) and (iv)

ANALYTICAL SOLUTION FOR A JOGGED DISLOCATION

1. Assumptions:

- Jogs separated by d_j are at local equilibrium with vacancies.
- Different formation energies and diffusion coefficients in the dislocation core and in the bulk.
- Energy barriers between the core and the bulk.





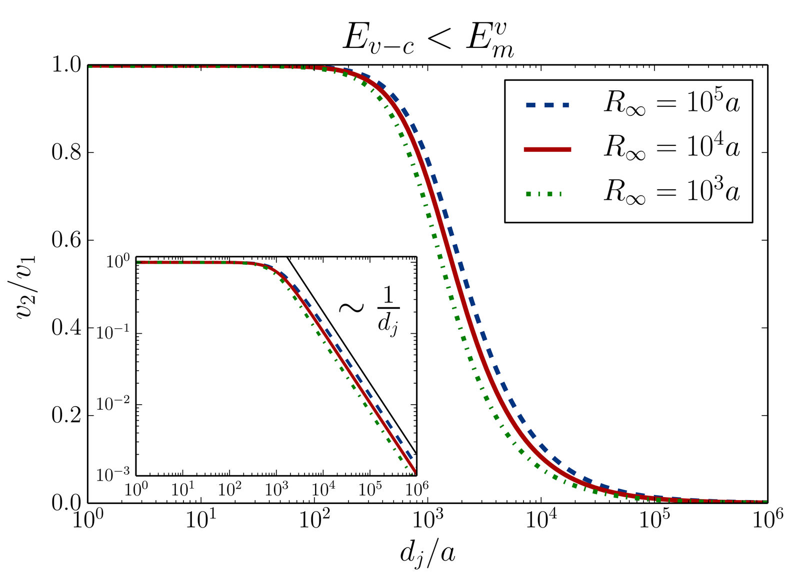
2. Stationary diffusion equations in the bulk and in the core:

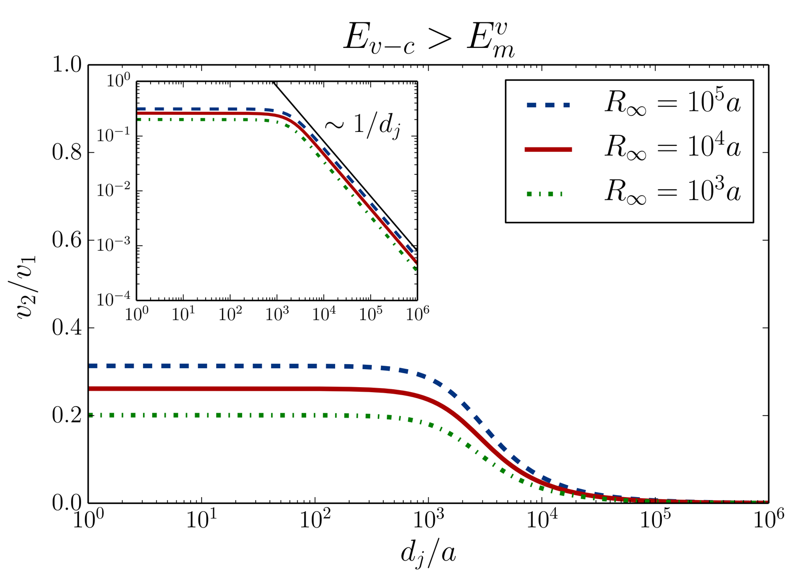
$$\frac{\partial^2 c_v}{\partial r^2} + \frac{1}{r}\frac{\partial c_v}{\partial r} + \frac{\partial^2 c_v}{\partial z^2} = 0 \quad (1)$$

$$D_c \frac{\partial^2 c_c}{\partial z^2} + \frac{2D_v}{r_c}\left.\frac{\partial c_v}{\partial r}\right|_{r=r_c} = 0 \quad (2)$$

3. We solve Eqs. (1-2) with $\xi = D_v \tau_{v-c}/a$. The climb rate is obtained by integrating the incoming flux:

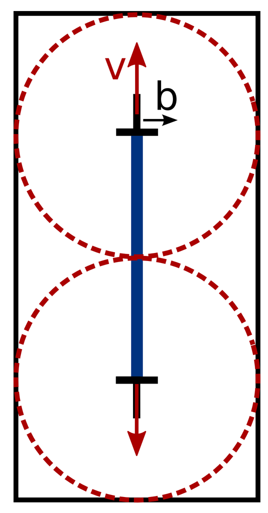
$$v_2 = \frac{\frac{2\pi D_v c_v^0}{b}\left(\frac{c_\infty}{c_0} - e^{\frac{\sigma^a\Omega}{kT}}\right)}{\ln\left(\frac{R_\infty}{r_c}\right) + \frac{\xi}{r_c}\left[1 + 4\sum_{k=1}^{+\infty}\frac{\xi - H_k(r_c)}{\xi + 2\alpha_k^2(\xi - H_k(r_c))}\right]} \quad (3)$$





UPSCALING TO A CONTINUOUS PHASE FIELD MODEL [4]

1. Free energy $\mathcal{F} = \int dr\{f_{ch} + f_{core} + f_{el}\}$ with:



$$f_{ch}(c) = \frac{kT}{2\Omega c_0}(c - c_0)^2$$

$$f_{core}(\phi) = A\phi^2(1-\phi)^2 + \frac{B}{2}|\boldsymbol{n} \wedge \boldsymbol{\nabla}\phi|^2$$

$$f_{el}(\phi, \boldsymbol{\epsilon}) = \frac{1}{2}(\boldsymbol{\epsilon} - \boldsymbol{\epsilon_0}(\phi)) : \boldsymbol{C} : (\boldsymbol{\epsilon} - \boldsymbol{\epsilon_0}(\phi)) - \boldsymbol{\sigma^a} : \boldsymbol{\epsilon}$$

2. Dynamic equations obtained after writing a Cahn-Hilliard dynamics on the total vacancy population $\psi = c + c^*\phi$:

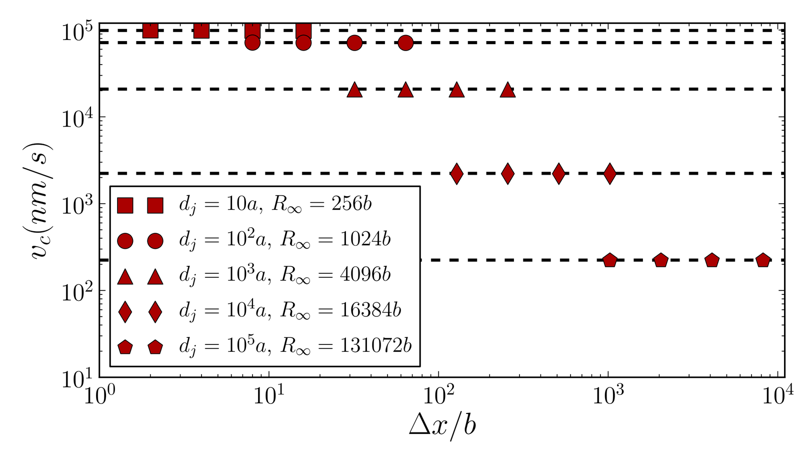
$$\dot{c} = \nabla \cdot M \nabla \frac{\delta F}{\delta c} + L c^*\left(\frac{\delta F}{\delta \phi} - c^*\frac{\delta F}{\delta c}\right) \quad (4)$$

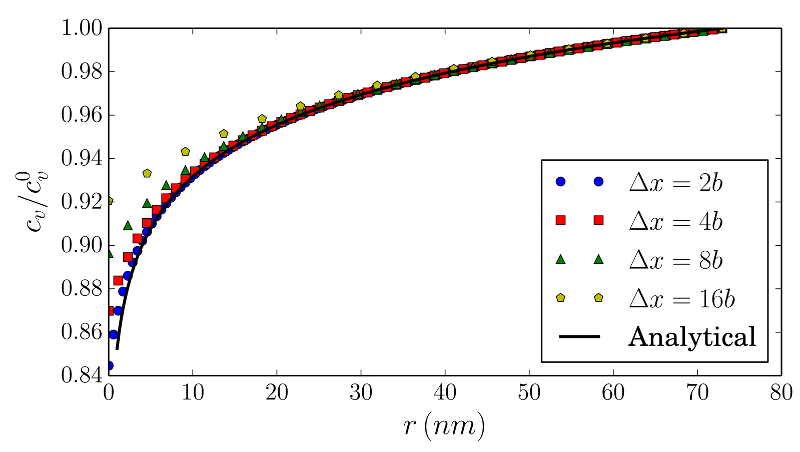
$$\dot{\phi} = -L\left(\frac{\delta F}{\delta \phi} - c^*\frac{\delta F}{\delta c}\right) \quad (5)$$

3. An asymptotic analysis in the sharp interface limit gives:

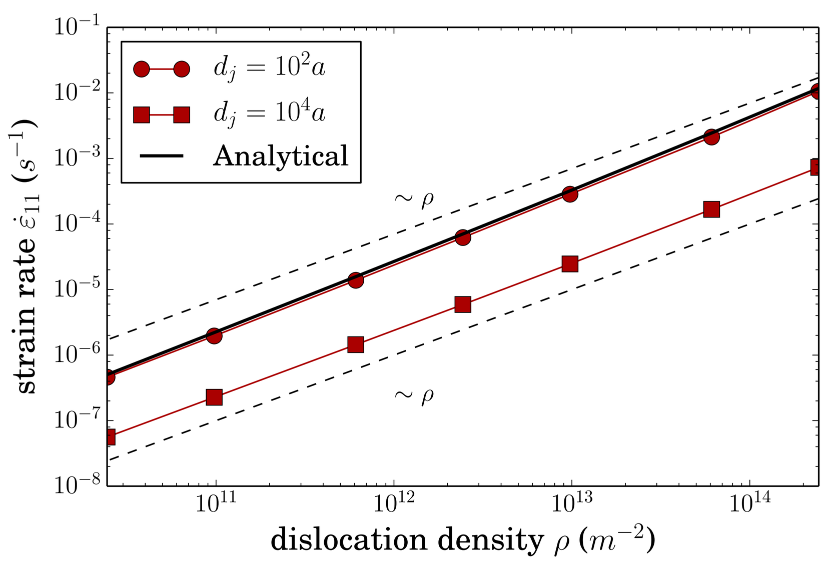
$$v_{\text{PFM}} = \frac{\frac{2\pi D_v c_0}{b}\left(\frac{c_\infty}{c_0} - \frac{\sigma^a\Omega}{kT} - 1\right)}{\ln\left(\frac{R_\infty}{r_c^{\text{eff}}}\right) + \Gamma/L} \quad (6)$$

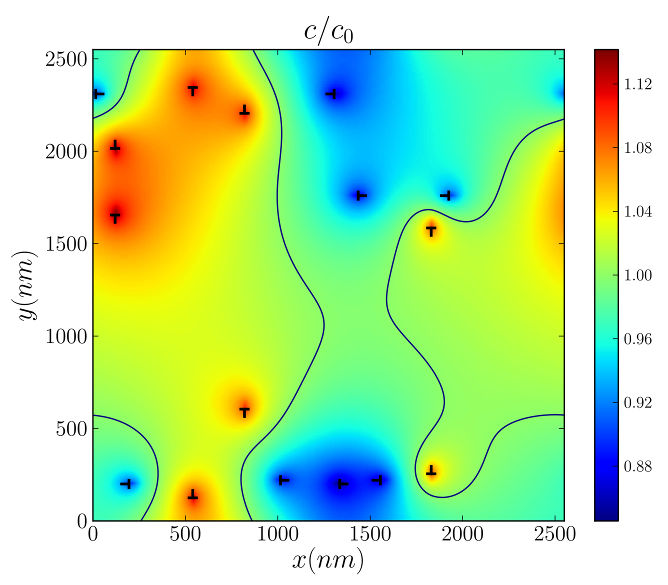
4. We then identify with Eq. (3) and choose the kinetic coefficient L to reproduce the climb behavior of a jogged dislocation.





5. Collective climb of dislocations:





CONCLUSION

- Thorough analytical solution for the climb of a jogged dislocation.
- Assumption (iii) is shown to be valid only for high jog concentrations.
- Brings insights on the activation energy of climb.
- Quantitative upscaling to a phase-field model enabling large scale simulations.
- Collective climb simulations show that the cylindrical assumption (iv) systematically overestimates the climb rate.

PERSPECTIVES

- Investigate the influence of elastic interactions between vacancies and dislocations.
- Choose L for a regime limited by jog nucleation (higher stresses).
- Couple with a phase-field model for dislocation glide.

REFERENCES

[1] D. Mordehai et al. Phi.Mag. 88, p.899, 2008
[2] S. Kelavarma et al. PRL 109, p.265504, 2012
[3] M. Geers et al. JMPS 70, p.136, 2014
[4] P.-A. Geslin, B. Appolaire, A. Finel. APL 104, p.011903, 2014