technische universiteit eindhoven

Upscaling Walls of Dislocations in Finite Domains

P. van Meurs[†‡], A. Muntean[†], M. A. Peletier[†]

Understanding plasticity

The main challenge in many complex systems is to understand the collective behavior of interacting particles on the micro-scale. We examine dislocation networks (Figure 1), from which plastic deformation of metals arises as the emergent property.

Main challenge: Metals contain a large amount of dislocations, and every dislocation interacts with all the others. No general theory exists to rigorously upscale the number of dislocations for non-local dislocation interactions, which are moreover singular at 0 (Figure 2).

Microscopic model

We choose a specific configuration for the edge dislocations as motivated by [2] (Figure 1). Because of the imposed periodicity in the vertical direction, the only unknowns are the horizontal positions (denoted by $\tilde{x}_i$) of all n vertical walls of dislocations.

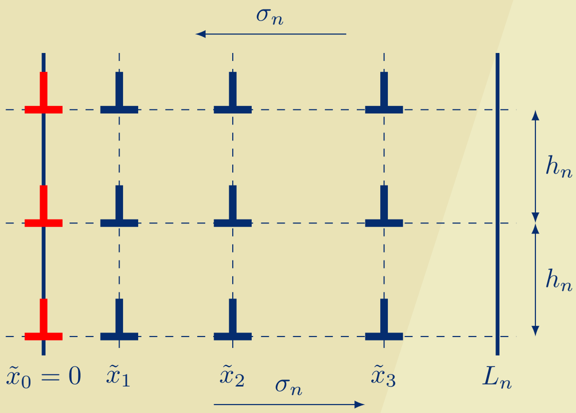

Figure 1. Configuration of dislocations for $n = 3$.

Any two of such walls repel each other. The corresponding potential is illustrated in Figure 2. The left boundary is modeled by a fixed wall of dislocations at $\tilde{x}_0 = 0$.

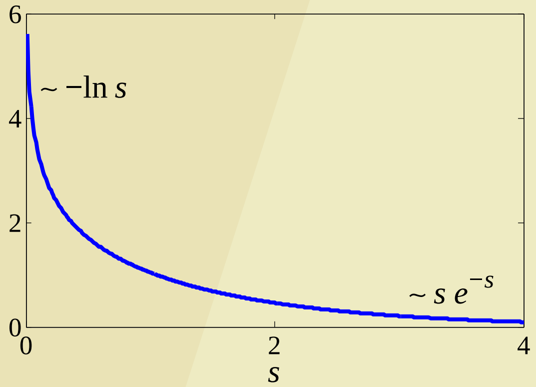

Figure 2. Interaction potential $V(s)$ with two-scale repulsion.

A proper length scale for the pile-up length (i.e. $\tilde{x}_n$) is given by $d_n := \min\{\ell_n, L_n\}$, where ℓ_n is obtained by balancing the interactions with the applied stress (see [1]). After scaling $x := \tilde{x}/d_n$, we can describe the energy landscape by

$$E_n(x_1, \dots, x_n) = A_n(\alpha_n) \sum_{k=1}^{n} \sum_{j=0}^{n-k} V\big(n\alpha_n(x_{j+k} - x_j)\big) + B(L_n/\ell_n)\frac{1}{n}\sum_{i=1}^{n} x_i + \chi_{\{x_n \le L_n/d_n\}},$$

where $\alpha_n := d_n/(nh_n)$ is asymptotically equal to the *aspect ratio* of the horizontal and vertical distance between dislocations (Figure 1), and where $\chi_{\{P\}}$ is 0 if P is satisfied, and ∞ otherwise. A minimizer of E_n corresponds to a stable configuration of the walls.

Results

We have proven [3] that

$$E_n \xrightarrow{\Gamma} E := E_{\mathrm{i}} + E_{\mathrm{F}} + E_{\mathrm{L}}$$

in $\mathcal{P}([0,\infty)$ with respect to narrow convergence, where

- the interaction term E_{i} has the same structure as in [1];
- the force term $E_{\mathrm{F}}(\mu)$ equals the first moment of μ when $L_n \gg \ell_n$. If $L_n \ll \ell_n$, we have $E_{\mathrm{F}}(\mu) = 0$;
- the finiteness of the domain is represented by $E_{\mathrm{L}}(\mu) = \chi_{\{\operatorname{supp}\mu \subset [0,1]\}}$ when $L_n \ll \ell_n$. If $L_n \gg \ell_n$, we have $E_{\mathrm{L}}(\mu) = 0$.

If $L_n \sim \ell_n$, both E_{F} and E_{L} do not vanish. The prefactor in E_{F} describes the transition between $L_n \ll \ell_n$ and $L_n \gg \ell_n$. It is in this transition region that d_n (the pile-up length scale) changes from L_n to ℓ_n.

Future plans

How to upscale dislocation *dynamics*? That is, pass to the continuum limit $n \to \infty$ in

$$\frac{d\mathbf{x}}{dt}(t) = -\nabla E_n\big(\mathbf{x}(t)\big).$$

References

[1] M.G.D. Geers, R.H.J. Peerlings, M.A. Peletier, and L. Scardia. Asymptotic behaviour of a pile-up of infinite walls of edge dislocations. Submitted.

[2] A. Roy, R.H.J. Peerlings, M.G.D. Geers, and Y. Kasyanyuk. Continuum modeling of dislocation interactions: Why discreteness matters? *Materials Science and Engineering*, 486:653 – 661, 2008.

[3] P. van Meurs, A. Muntean, and M.A. Peletier. Upscaling of dislocation walls in finite domains. In preparation.

[†] Centre for Analysis, Scientific computing and Applications (CASA), Department of Mathematics and Computer Science, Eindhoven University of Technology, The Netherlands
[‡] p.j.p.v.meurs@tue.nl