Multiscale science of *dislocations*

Mark A. Peletier

January 14, 2019

Metals bend. If you bend them far enough, then they don't bend back when you release them—they remain bent. This permanent deformation is called *plastic deformation*, and surprisingly enough it still is very poorly understood.

What *is* known is this: plastic deformation in metals is caused by the concerted movement of many microscopic, curve-like defects in the crystal lattice, called *dislocations*. The figure below shows an artist's impression of a dislocation.

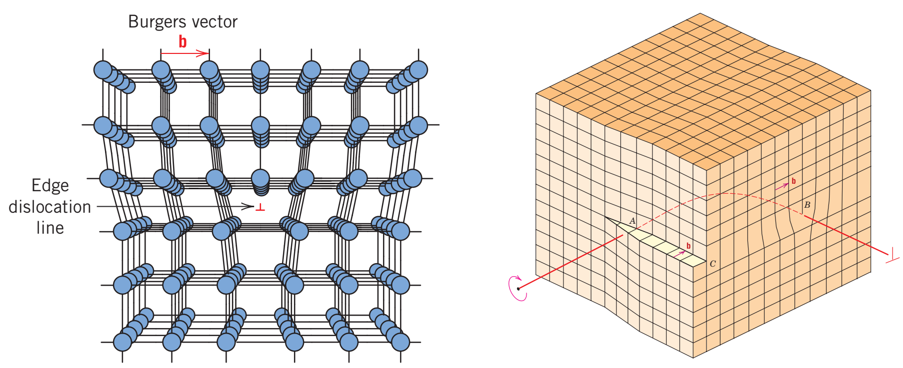

Figure 1: Left: a defect in the lattice. Right: zooming out, one sees that the defect is the boundary of an area that has slipped. (From Callister [Cal07])

In real metals, there is a very large number of such curves, criss-crossing the material, as in the figure below.

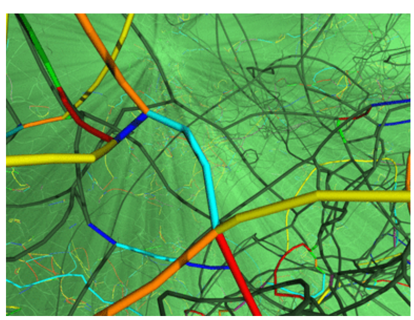

Figure 2: Another artist's impression, this time of the network of dislocation curves. The atoms are not shown, only the defect lines themselves are shown. (From `paradis.stanford.edu`)

It also is known that the permanent deformation that we mentioned above is the result of *movement* of these defects; therefore, in order to understand the behaviour of the metal, one has to understand how these curves move around, in response to external loading.

This is a very hard problem, and science is nowhere near to solving it yet. In the meantime we study much simpler problems, in the hope of developing understanding and tools that will eventually allow us to address the big problems.

These simpler problems are typically systems of particles, each representing a single defect, as a point on a line or a point in the plane. In the simplest case, such systems would evolve according to a system of ordinary differential equations of the form

$$\dot{x}_i = -\sum_{j=1}^{n} V'(x_i - x_j) + f, \qquad i = 1, \dots n. \tag{1}$$

Here $x_i(t)$ is the position of defect i, represented as a point on the real line; the right-hand side can be interpreted as the sum of forces generated by each of the other defects (the sum), and the external load (f).

Sometimes a deterministic model such as this is not the right choice, and we study stochastic models instead, of the form

$$dX_i = -\sum_{j=1}^{n} V'(X_i - X_j)dt + f\,dt + \varepsilon dW_i, \qquad i = 1, \dots n. \tag{2}$$

Here W_i are i.i.d. Wiener processes.

There are many, many open questions about these equations, and about their limits as the number n of particles tends to infinity. For instance,

1. What are the stationary points for the deterministic system (1)? How do they depend on the interaction potential V and on the external load f?
2. Are there stationary points for the stochastic problem (2)? How does the behaviour depend on the external load?
3. Are there regular structures, for instance equispaced configurations, that are stable?
4. What happens as the number n of dislocations tends to infinity? What is the right way to consider that limit?
5. What is the influence of the noise parameter ε?
6. How do we introduce defects of different signs ('Burgers vectors' in the literature) that can (partially or completely) cancel each other? What effect does that have?
7. How do defects interact with obstacles, such as grain boundaries? How can one describe this in the limit $n \to \infty$?

In a Bachelor or Master project, we will discuss these possible questions, and together make a choice that suits both of us.

References

[Cal07] W. D. Callister. *Materials Science and Engineering, An Introduction*. John Wiley & Sons, 2007.

[vM15] P. J. P. van Meurs. *Discrete-to-Continuum Limits of Interacting Dislocations*. PhD thesis, Technische Universiteit Eindhoven, 2015. Available as `https://research.tue.nl/en/publications/discrete-to-continuum-limits-of-interacting-dislocations`.