Analysis of a PDE to model Dislocation Motion

Luca Bollini

Contents

1 Introduction **2**
1.1 Sketch 2
1.2 Geometry 2
1.3 Discovery 3
1.4 Motion 4

1 Introduction

1.1 Sketch

In February 2023, renowned strength sports athlete Vispy Kharadi broke the world record for most iron rods bent over the head in one minute, achieving an impressive total of 24. You can watch an overly dramatic video of this feat here: Most Iron Bars Bent. While one might first wonder what would possess a person to take on such a challenge, or if bending metal rods over your head is medically advisable (it's not), as mathematicians, we ask a different question: "How do metals bend?". A physicist might quickly produce an answer such as: "Well, the man's head is exerting a shear stress force on the rod, causing defects in the crystalline structure of the metal, called *dislocations*, to move. This results in the atoms rearranging themselves into the shape of a bent iron rod.". We will go one step further. In this project, we formally introduce a model for the movement of a line dislocation, analysing the existence of solutions to the following linearised PDE. We then finish with a discussion about extending this model to include regions of different materials, simulating an alloy or a composite. Before we embark, let's give a summary of what dislocations are, and how they were discovered.

1.2 Geometry

Throughout this chapter, there will be numerous references to "Introduction to Dislocations" by Hull and Bacon [7], which can be regarded as the definitive source of background information regarding this topic. Their precise formulation of crystallographic defects' geometric structure and rich exploration of observational techniques are a fantastic way to immerse yourself in this theory.

Dislocations are the linear defects in crystalline structures responsible for plastic deformation. All crystalline materials can have these defects, but it is in metals that most of the interesting behaviour occurs; other materials such as coal and ceramics either have too few dislocations, or crack more easily than they are able to deform plastically. There are two types of dislocation: *edge* and *screw*. Let's outline how they look on the atomic level.

Imagine a simple cubic structure of atoms, as in figure (??), where we think of the vertical and horizontal lines as bonds between atoms, while the atoms themselves are placed at each intersection. Let's assume we may model the bonds as flexible springs between adjacent atoms, thus avoiding the complexity of how bonding works in real solids. What follows is a sequence of operations to describe how a dislocation can be formed from a

perfect crystal:

1. Break all the bonds intersecting the half-plane defined by $ABCD$. CD is the *leading-edge*, where our dislocation is to be positioned, and the half-plane extends upwards in the direction of $\overrightarrow{CB}$.

2. For an edge dislocation, insert a half-plane of atoms where the bonds have just been broken. This is shown in figure (??)[1].

   For a screw dislocation, shift all the atoms on one side of $ABCD$ by one bond length in the direction $\overrightarrow{AB}$. This can result in one of two chiral structures depending on which direction the shift is in; a shift by $+\overrightarrow{AB}$ is the mirror image of a shift by $-\overrightarrow{AB}$. The "left-handed" version is illustrated in figure (??).

Note that both types of dislocation distort the bonds close to the leading-edge CD, and that this distortion decreases with distance. This will be relevant in section (??)when discussing line tension.

Furthermore, we can see how these structures allow for the easy rearrangement of atomic bonds under shear. Figure (??)shows the cross section of a perfect crystal on the left, and an edge dislocation on the right. If we apply a shear force to the perfect crystal, we will need to break every bond along EF before shifting the top layer one to the left and reforming the bonds. Such an action requires immense force, much more than is observed in practice. In contrast, applying the same to the crystal with an edge dislocation is relatively easy. We can just break and reform bonds one at a time to "fill the gap" caused by the dislocation. This requires several orders of magnitude less force. In fact, this phenomenon is exactly how dislocations were discovered.

1.3 Discovery

Modern dislocation theory first appeared in the 1930s following calculations to determine the theoretical critical stress of materials. By *critical stress*, we mean the maximum stress a material can withstand before deforming plastically. As laid out by Hull and Bacon [7, § 1.4], this was done in 1926 by Frenkel, who showed the shearing force required to move one row of atoms across another is given by the equation

$$\tau = \frac{Gb}{2\pi a} \sin \frac{2\pi x}{b}$$

where b is the spacing of atoms in the direction of shear, a is the spacing between rows of atoms, x is the displacement of the two rows from the stable position, and G is the elastic modulus, or elastic shear stiffness, of

[1] (reference diagram style as being similar to [7, § 1.4])

the material. Figure (??)illustrates this setup. Realistic calculations for the maximum shearing force yield theoretical critical stresses around $\tau_{th} \approx \frac{G}{30}$. This is strikingly different from observational data, which indicates that critical stresses are generally between $10^{-8}G$ and $10^{-4}G$.

The mystery behind such contrast was solved in 1934, when three scientists, Orowan, Talyor and Polyani, independently theorised the presence of dislocations and reasoned that they could account for the difference between prediction and experiment. Their work induced an explosion of research into dislocations throughout the 1940s and into the early 1950s, which is when the famous Peach-Koehler equation [8] was first presented. We will make use of this in section (??). It wasn't until 1956 that direct observation of dislocation movement was made by electron microscopy.

1.4 Motion

Central to dislocation motion is the concept of the *Burgers circuit* and *Burgers vector*. *"A* Burgers circuit *in a crystal containing dislocations is an atom-to-atom path which forms a closed loop"* [7, § 1.4]. Crucially, if the same path is made in a crystal containing no dislocation, and the path does not close, then the circuit must contain at least one dislocation. You can see this in figure (??), where (a) shows a Burgers circuit encapsulating an edge dislocation, while (b) shows the same path superimposed onto a dislocation-free crystal. The vector required to close the loop is labelled as the *Burgers vector*. Furthermore, we can see from figure (??)that the Burgers vector of any edge dislocation is perpendicular to its dislocation line (the line is going into the page). For screw dislocations, the Burgers vector is parallel to the dislocation line, illustrated in figure (??).

In this project, we shall be modelling the movement of an arbitrary dislocation (either edge or screw) under conservative motion, called *glide*. Dislocations capable of glide are called *glissile*, and the resulting process is known as *slip*; two planes of atoms slide over one another, while the only moving part is the dislocation itself. Think of this like using a squeegee to remove an air bubble trapped in a sticker. The dislocation is the air bubble and the squeegee is the shear force inducing slip. The sticker creeps forward as the air bubble moves, which you can imagine as the planes of atoms sliding over each other while the dislocation leads the way.

In figure (??), we can see that regions of crystal either side of the so-called *slip plane* remain undisturbed, and that the Burgers vector is depicted as being parallel to the direction of motion. This is because neighbouring atoms across the slip plane move relative to each other by precisely the Burgers vector. You can find many detailed diagrams of this in Hull and Bacon's book. It is for this reason that the Burgers vector is so important in dislocation motion.

Finally, we'll discuss slip planes in more depth. For edge dislocations,

note the Burgers vector and dislocation line are enough to uniquely specify the slip plane, while for screw dislocations this is not the case. We will always impose, however, that motion is confined to a single slip plane and further use that the Burgers vector lies in this plane.

We now aim to formally write down a model for the motion of a dislocation undergoing slip, then prove existence and uniqueness results for the derived equation.

Some citations: [5], [1], [6], [2], [7], [8], [4], [3].

References

[1] Aluminum in Space: Pushing the Limits of Aerospace Technology, 2024. URL https://elkamehr.com/en/aluminum-in-space-pushing-the-limits-of-aerospace-technology/. Accessed on 27th January 2025.

[2] P. M. Anderson, J. P. Hirth, and J. Lothe. *Theory of dislocations*. Cambridge University Press, 2017.

[3] Á. Bényi and T. Oh. The sobolev inequality on the torus revisited. *Publicationes Mathematicae Debrecen*, 83(3):359, 2013.

[4] J. Colliander, M. Keel, G. Staffilani, H. Takaoka, and T. Tao. Sharp Global Well-Posedness for KdV and Modified KdV on **R** and **T**. *Journal of the American Mathematical Society*, 16(3):705–749, 2003.

[5] L. C. Evans. *Partial differential equations*, volume 19. American Mathematical Society, 2 edition, 2022.

[6] T. Hudson, F. Rindler, and J. Rydell. A quantitative model for the frank-read dislocation source based on pinned mean curvature flow. 2024. https://arxiv.org/abs/2409.20294.

[7] D. Hull and D. J. Bacon. *Introduction to dislocations*, volume 37. 5 edition, 2011.

[8] M. Peach and J. Koehler. The forces exerted on dislocations and the stress fields produced by them. *Physical Review*, 80(3):436, 1950.