

MAE 212: Spring 2001
Lecture 13
YIELDING OF SINGLE CRYSTALS
& POLYCRYSTALS
AND STRENGTHENING MECHANISMS
N. Zabaras

Significant portion of this lecture was developed using the information given in Chapters 9 and 10 of *Engineering Materials I* by Ashby and Jones (on reserve in the Engr. Library).

Introduction

In lecture 12 we already associated yielding with the motion of dislocations on particular slip planes and in particular slip directions. The slip planes are usually close-packed planes and the slip directions close-packed directions. We computed that the force on a dislocation due to an applied shear stress τ_R (resolved shear stress) is given as

$$f = \tau_R b \quad (1)$$

The existence of a critical shear stress τ_c (shear yield stress of the single crystal) at which the dislocation starts to move can be explained easily. Based on equation (1), we postulate that when f reaches a critical value f_c needed to overcome the natural barriers to dislocation motion in the crystal, then slip begins, i.e. slip begins when:

$$\begin{aligned} f &\geq f_c \quad \text{or} \\ \tau_R b &\geq f_c \quad \text{or} \\ \tau_R &\geq \frac{f_c}{b} \equiv \tau_c \end{aligned} \quad (2)$$

where the critical shear stress τ_c was defined as follows:

$$\tau_c \equiv \frac{f_c}{b} \quad (3)$$

Thus when $\tau_R > \tau_c$ plastic deformation starts (in practice τ_c can be as low as 1 MPa):

$$\text{Initiation of Plastic Deformation : } \tau_R = \tau_c \quad (4)$$

From Eq. (3) we can conclude that the crystal can be hardened (increase τ_c) by increasing the strength and barriers to dislocation motion. These microscopic sources of the critical

stress τ_c will be examined later in this lecture.

We will next examine how to compute τ_R from the macroscopic applied stresses. For example, we need to compute the relation between an applied tensile stress σ and τ_R in a uniaxial tensile experiment.

Relation of σ and τ_R in a uniaxial tensile test

Let us consider the uniaxial tensile test as shown in Fig. 1. We concentrate on slip on a particular slip system (slip plane and slip direction).

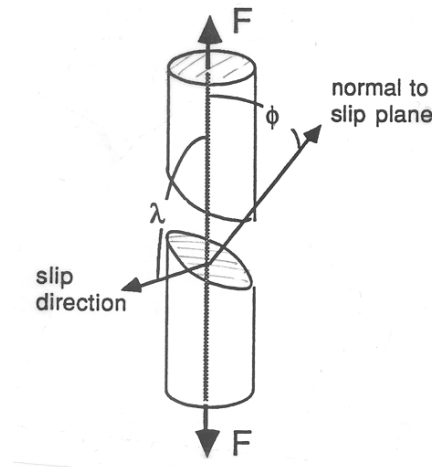


Figure 1: A uniaxial tensile test. Slip is considered in the particular slip system shown. The slip system is defined by the slip plane normal and the slip direction.

Relating to this tensile test let us define:

ϕ = angle between the loading axis and the slip plane normal

λ = angle between the loading axis and the slip direction

Note that the slip plane normal and the slip direction are generally not coplanar, i.e.

$$\phi + \lambda \neq 90^\circ \quad (5)$$

The force resolved in the slip direction is $F_s = F \cos \lambda$. Let A_o be the cross-section area of the specimen and A the cross-section area of the specimen in the slip plane:

$$A = \frac{A_o}{\cos \phi} \quad (6)$$

We can thus compute τ_R as follows:

$$\tau_R = \frac{F_s}{A} = \frac{F \cos \lambda}{\frac{A_o}{\cos \phi}} = \frac{F}{A_o} \cos \lambda \cos \phi = \sigma \cos \lambda \cos \phi \quad (7)$$

where σ is the tensile stress. We introduce the Schmid factor M as follows:

$$M = \cos\lambda \cos\phi \quad (8)$$

To find M we need to know the slip system and the orientation of the slip system with respect to the tensile axis.

Note that M is zero when either ϕ or λ are 90° and maximum when both ϕ and λ are 45° . In this last case we can compute:

$$\tau_{R\max} = \sigma \cos 45^\circ \cos 45^\circ = \frac{\sigma}{2} \quad (9)$$

Yielding for single crystals: Schmid Law

Combining equations Eqs. (4), (7) and (8), we can now restate that metal flows (yields) when the resolved shear stress acting on the slip plane and along the direction of slip reaches a critical value

$$\text{Schmid law : } \tau_c = Y \cos\lambda \cos\phi \equiv YM \quad (10)$$

The critically resolved shear stress τ_c is a material property. We use here Y to denote the value of σ at which τ_R reaches the critical value τ_c . Note however that since we are talking about a single crystal only, Y as used here is not the yield stress of a polycrystalline material. Also note that as ϕ and λ change, Y changes.

For a given single crystal and a given tensile axis one can compute the Schmid factors for each slip system. Using $\tau_R = M\sigma$, the slip system with the maximum Schmid factor M will be the active slip system as it will first reach a level of the resolved shear stress such that $\tau_R = \tau_c$.

Example 1

Consider tension in the direction $[100]$ (direction of the tensile stress) as shown in Fig. 2 and the particular slip system $(111)[10\bar{1}]$. You can verify (by taking the dot product) that indeed the direction $[10\bar{1}]$ lies on the slip plane (111) .¹

For the particular slip system $(111)[10\bar{1}]$, we can compute:

$$\begin{aligned} \cos\phi &= \frac{[100] \cdot [111]}{\|[100]\| \|[111]\|} = \frac{1 \times 1 + 0 + 0}{\sqrt{1^2 + 0^2 + 0^2} \sqrt{1^2 + 1^2 + 1^2}} = \frac{1}{\sqrt{3}} \\ \cos\lambda &= \frac{[100] \cdot [10\bar{1}]}{\|[100]\| \|[10\bar{1}]\|} = \frac{1 \times 1 + 0 + 0 \times (-1)}{\sqrt{1^2 + 0^2 + 0^2} \sqrt{1^2 + 0^2 + (-1)^2}} = \frac{1}{\sqrt{2}} \end{aligned} \quad (11)$$

¹For a cubic structure, a simple way to determine whether a plane contains a certain direction is to do a dot product between the indices of the plane and the direction i.e. the (111) plane contains both the $[10\bar{1}]$ and $[\bar{1}10]$ directions since $[111] \cdot [10\bar{1}] = 0$ and $[111] \cdot [\bar{1}10] = 0$.

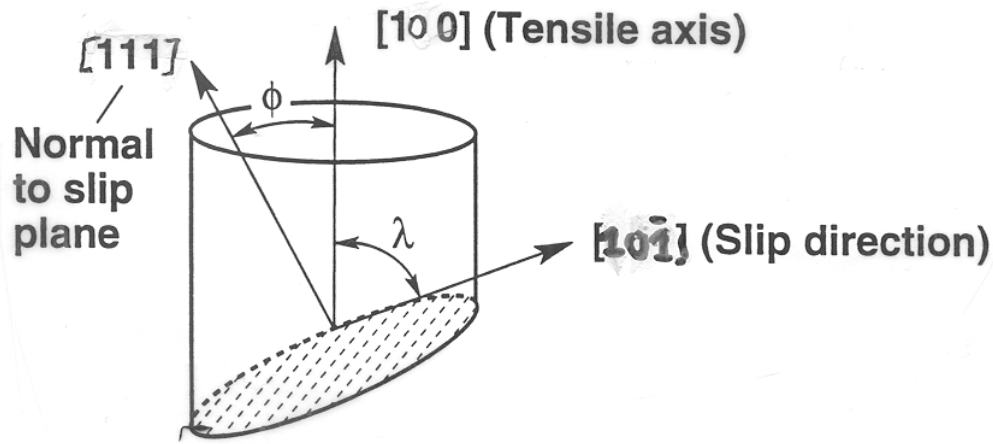


Figure 2: A particular slip system and the tensile axis in the direction [100].

Thus $M = \cos\phi \cos\lambda = \frac{1}{\sqrt{6}}$.

Example 2

If for the particular crystal of Example 1, $\tau_c = 5$ MPa, find the tensile stress σ that causes slip (plastic deformation) on the (111)[10 $\bar{1}$] slip system?

From $\tau_c = M\sigma$ we conclude: $\sigma = \frac{5 \text{ MPa}}{\frac{1}{\sqrt{6}}} = 5\sqrt{6}$ MPa.

Example 3

You are designing a turbine engine part made of an FCC single crystal. By using the Schmid law, determine the τ_c necessary for the part to have a uniaxial yield strength of 200 MPa in the [331] crystallographic direction?

Slip Systems	(111)	(111)			(111)			(111)			(111)		
		[$\bar{1}$ 10]	[0 $\bar{1}$ 1]	[10 $\bar{1}$]	[110]	[0 $\bar{1}$ 1]	[101]	[110]	[011]	[10 $\bar{1}$]	[$\bar{1}$ 10]	[011]	[101]
Tensile	$\cos\phi$	$\frac{7}{\sqrt{57}}$	$\frac{7}{\sqrt{57}}$	$\frac{7}{\sqrt{57}}$	$\frac{1}{\sqrt{57}}$	$\frac{1}{\sqrt{57}}$	$\frac{1}{\sqrt{57}}$	$\frac{1}{\sqrt{57}}$	$\frac{1}{\sqrt{57}}$	$\frac{1}{\sqrt{57}}$	$\frac{-5}{\sqrt{57}}$	$\frac{-5}{\sqrt{57}}$	$\frac{-5}{\sqrt{57}}$
Axis	$\cos\lambda$	0	$\frac{-2}{\sqrt{38}}$	$\frac{\sqrt{38}}{2}$	$\frac{6}{\sqrt{38}}$	$\frac{2}{\sqrt{38}}$	$\frac{\sqrt{38}}{4}$	$\frac{\sqrt{38}}{6}$	$\frac{\sqrt{38}}{4}$	$\frac{\sqrt{38}}{2}$	0	$\frac{4}{\sqrt{38}}$	$\frac{\sqrt{38}}{4}$
[331]	M	0	$\frac{-14}{19\sqrt{6}}$	$\frac{14}{19\sqrt{6}}$	$\frac{6}{19\sqrt{6}}$	$\frac{2}{19\sqrt{6}}$	$\frac{4}{19\sqrt{6}}$	$\frac{6}{19\sqrt{6}}$	$\frac{4}{19\sqrt{6}}$	$\frac{2}{19\sqrt{6}}$	0	$\frac{-20}{19\sqrt{6}}$	$\frac{-20}{19\sqrt{6}}$

The maximum Schmid factor is thus $\frac{20}{19\sqrt{6}}$.

So: $\tau_c = MY = \frac{20}{19\sqrt{6}} \times 200 = 86$ MPa

Strengthening methods

A crystal yields when the force $\tau_R b$ (per unit length) exceeds f_c , the resistance (a force per unit length) opposing the motion of a dislocation. This defines the dislocation yield strength

$$\tau_c = \frac{f_c}{b} \quad (12)$$

Most crystals have a certain intrinsic strength f_i , caused by the bonds between the atoms which have to be broken and reformed as the dislocation moves. Covalent bonding, particularly, gives a very large intrinsic lattice resistance, f_i per unit length of dislocation. It is this resistance for example that causes the enormous strength and hardness of diamond. But pure metals are soft: they have a very low lattice resistance. Then it is useful to increase f_i by solid solution strengthening, by precipitate or dispersion strengthening, or by work-hardening, or by any combination of the three. Remember, however, that there is an upper limit to the yield strength: it can never exceed the ideal strength examined in lecture 12. In practice, only a few materials have strengths that even approach it. Accounting for all possible mechanisms of hardening, we can approximate that:

$$\tau_c = \frac{f_i}{b} + \frac{f_{ss}}{b} + \frac{f_0}{b} + \frac{f_{wh}}{b} \quad (13)$$

where

- f_i - - - - > intrinsic lattice resistance
- f_{ss} - - - - > solid solution strengthening
- f_0 - - - - > precipitation hardening
- f_{wh} - - - - > work hardening

We next examine in some detail each of the above strengthening mechanisms.

Solid solution hardening:

A good way of hardening a metal is simply to make it impure. A good example is the addition of zinc to copper to make the alloy called brass. The zinc atoms replace copper atoms to form a random substitutional solid solution. At room temperature Cu will dissolve up to 30% Zn in this way. The Zn atoms are bigger than the Cu atoms and squeezing them into the Cu structure generates stresses. These stresses ‘roughen’ the slip plane, making it harder for dislocations to move; they increase the resistance, and thereby increase the dislocation yield strength τ_c . If the contribution to f given by the solid solution is f_{ss} then τ_c is increased by $\frac{f_{ss}}{b}$. In a solid solution of concentration C , the spacing of dissolved atoms on the slip plane varies as $\frac{1}{\sqrt{C}}$ and the smaller the spacing, the ‘rougher’ is the slip plane. As a result, τ_c increases about parabolically (i.e. as \sqrt{C}) with solute concentration (Fig. 3). Many other metallic alloys, derive their strength in this way.

Precipitate and dispersion strengthening:

If an impurity (copper, say) is dissolved in a metal or ceramic (aluminum, for instance) at a higher temperature, and the alloy is cooled to room temperature, the impurity may precipitate as small particles. An alloy of Al containing 4% Cu (Duralumin), treated in this way, gives very small, closely spaced precipitates of the hard compound CuAl_2 . Optimum precipitates are obtained by a more elaborate heat treatment:

- the alloy is solution heat-treated (heated to dissolve the impurity),
- quenched (cooled fast to room temperature, usually by dropping it into oil or water) and finally
- tempered or aged for a controlled time and at a controlled temperature (to cause the precipitate to form).

These approaches distribute small, hard particles in the path of a moving dislocation. Figure 4 shows how they obstruct its motion. The stress has to push the dislocation between the obstacles. A very large stress is needed to bulge the dislocation between the obstacles, though once a large enough bulge is formed, it can easily expand further. The critical configuration is the semicircular one (Fig. 4c) here the force τbL on one segment is just balanced by the force $2T$ due to the line tension, acting on either side of the bulge. The dislocation escapes (and yielding occurs) when

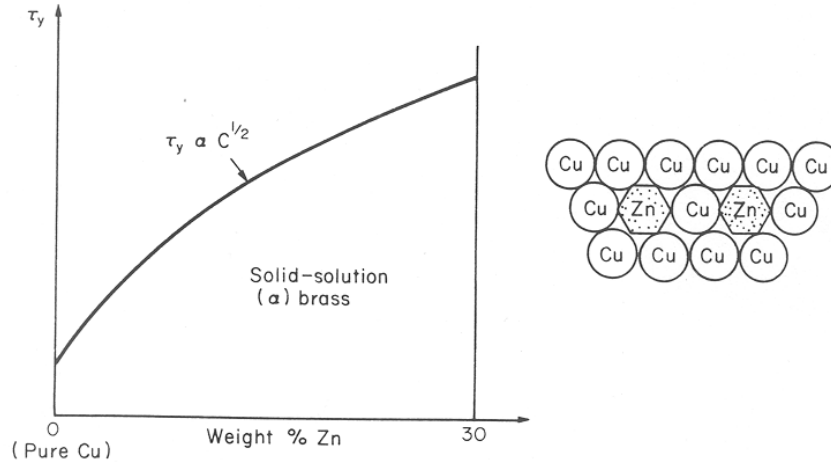


Figure 3: Solid solution hardening. The yield stress τ_y in shear for the crystal (same as τ_c) increases as \sqrt{C} .

$$\tau_c = \frac{2T}{bL} \quad (14)$$

Thus the obstacles exert a resistance of $f_0 = \frac{2T}{L}$ (see Eq. (13)). Obviously, the greatest hardening is produced by strong, closely spaced precipitates or dispersions (Fig. 4).

Work-hardening:

When crystals yield, dislocations move through them. Most crystals have several slip planes, e.g. the FCC structure, which slips on $\{111\}$ planes has four, for example. Dislocations on these intersecting planes interact, and obstruct each other, and accumulate in the material.

The result is work-hardening: the steeply rising stress-strain curve after yield. Work-hardening can be a nuisance: if you want to roll thin sheet, work-hardening quickly raises the yield strength so much that you have to stop and **anneal** the metal (heat it up to remove the accumulated dislocations) before you can go on. But it is also useful: it is a potent strengthening method, which can be added to the other methods to produce strong materials.

The analysis of work-hardening is difficult. Its contribution to the total dislocation resistance is considerable and increases with strain (Fig. 5).

Polycrystalline Behavior Based on Single Crystals

Let us consider the progressive nature of yielding in a polycrystalline material (see Fig. 6).

The process of accounting for progressive yielding in each crystal is more complex than simple superposition. Total yielding for the polycrystal (obtained by averaging over the grains) does not occur at the dislocation yield τ_c because not all grains are oriented favorably (see Fig. 6). Slip begins in grains where there are slip planes as nearly parallel to τ_R as possible, e.g. grain (1). Slip later spreads to grains like (2) which are not so favorably oriented, and lastly to the worst oriented grains like (3). Yielding does not take place all at once and therefore there is no sharp polycrystalline yield point on the stress-strain curve (contrary to the simplifications introduced in earlier lectures!). The gross-yielding strength is higher, by a factor called **the Taylor factor**, which is calculated by averaging stress over all possible slip planes; it is close to 1.5 (see Fig. 6).

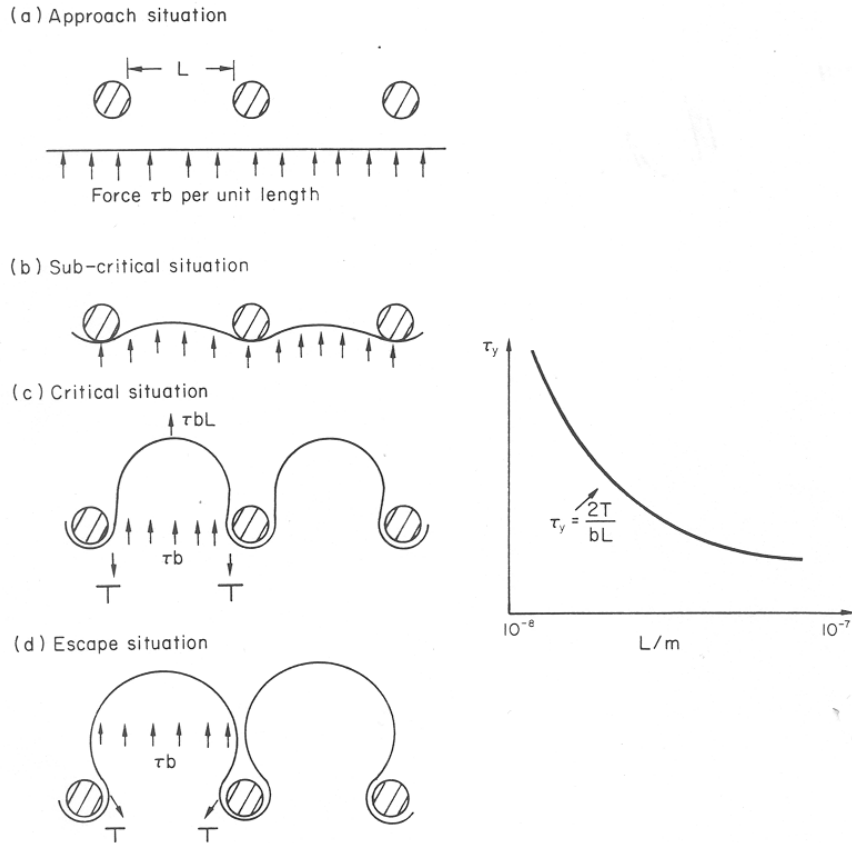


Figure 4: Dispersed precipitates help prevent the movement of dislocations.

But we want to find the tensile yield strength Y ? A tensile stress σ creates a shear stress τ on the material that has a maximum value of $\tau = \frac{\sigma}{2}$ (think of a Mohr circle for a tensile test!).

Thus to calculate the tensile yield stress σ_y of a polycrystal, we need to combine the Taylor factor with the resolution factor to obtain:

$$\sigma_y = 3\tau_c \quad (15)$$

where σ_y here denotes the yield stress in tension of the bulk polycrystalline material (what we used to call Y in earlier lectures) and τ_c is the dislocation shear strength introduced earlier.

Note: In some books, the Taylor factor is defined as relating σ_y and τ_c (i.e. as the factor 3).

Relation between dislocation movement and plastic flow

Suppose we have a crystal in the shape of a cube, where the edge length is L . Under the application of an appropriate shear stress, a dislocation is 'somehow' produced on the left hand side of the crystal and is allowed to move all the way through the crystal (Fig. 7).

In moving a distance x , the dislocation has swept out $\frac{x}{L}$ of its slip plane and the resulting plastic shear strain γ_p is given as:

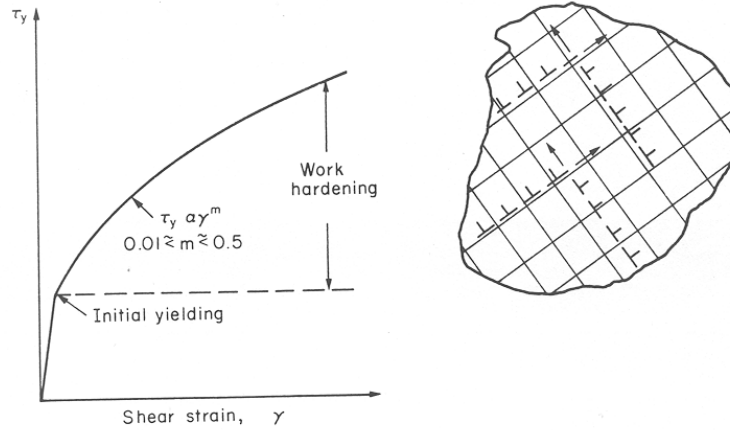


Figure 5: Collision of dislocations leads to work-hardening.

$$\gamma_p = \frac{x}{L} \frac{b}{L} \quad (16)$$

If instead of one-dislocation, we had N dislocations (see Fig. 8), all moving an average distance \bar{x} , the resulting shear strain would be:

$$\gamma_p = N \frac{\bar{x}}{L} \frac{b}{L} \quad (17)$$

The above equation can be re-written as follows:

$$\gamma_p = \frac{N}{L^3} b \bar{x} \quad (18)$$

But the dislocation density was defined in lecture 12 as $\rho = \frac{NL}{L^3}$. We thus can conclude that: The above equation can be re-written as follows:

$$\gamma_p = \rho b \bar{x} \quad (19)$$

If the shear strain γ_p occurs over a time t ,

$$\frac{\gamma_p}{t} = \rho b \frac{\bar{x}}{t} \quad (20)$$

or

$$\dot{\gamma}_p = \rho b \bar{v} \quad (21)$$

where $\dot{\gamma}_p$ is the **shear strain rate** and \bar{v} is the average dislocation velocity.

The above equation is a transport equation that occurs often in physics and engineering. It simply states that: ‘the strain rate is equal to the density of the defects producing strain (dislocations) times the strength of each defect (the amount of strain associated with each defect), times the average velocity of the defects.

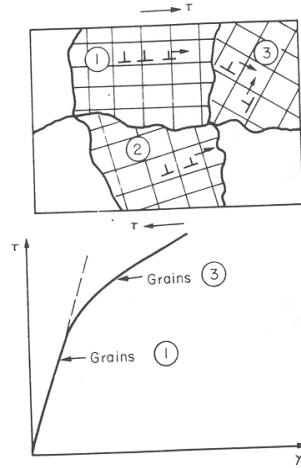


Figure 6: Yielding in a polycrystalline material. The shear stress τ for the polycrystal to yield is 1.5 times the critical yield stress τ_c for a single crystal.

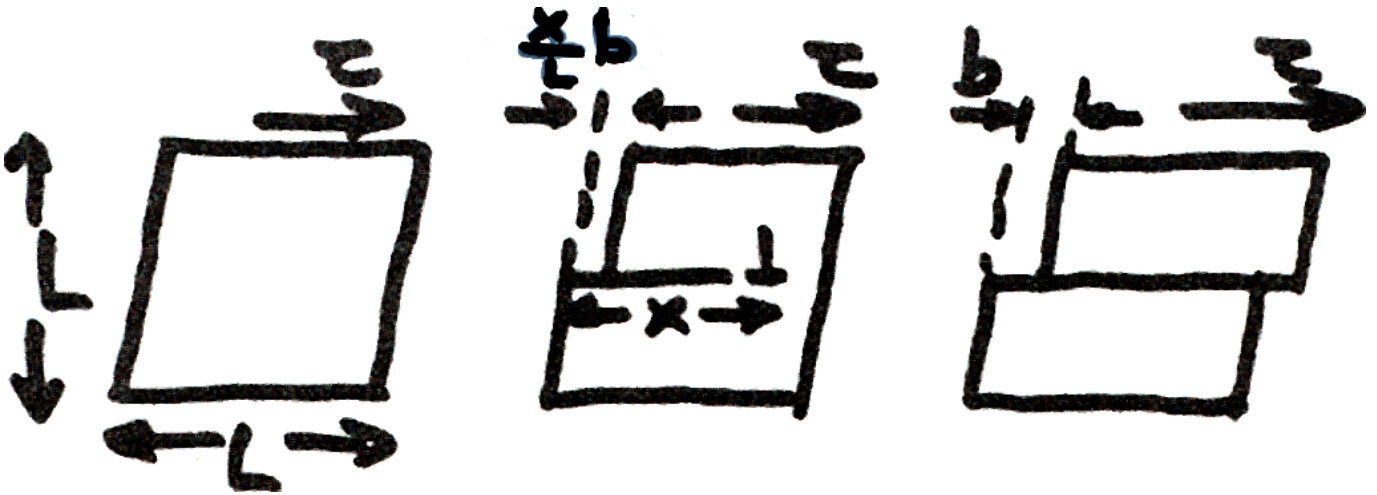


Figure 7: Motion of a dislocation. If the dislocation moves by a distance x , the displacement of the upper part of the block with respect to the lower is approximated with the following linear expression: $\frac{x}{L} b$ (Note that for $x = 0$ this relative displacement is zero and at $x = L$ it is b).

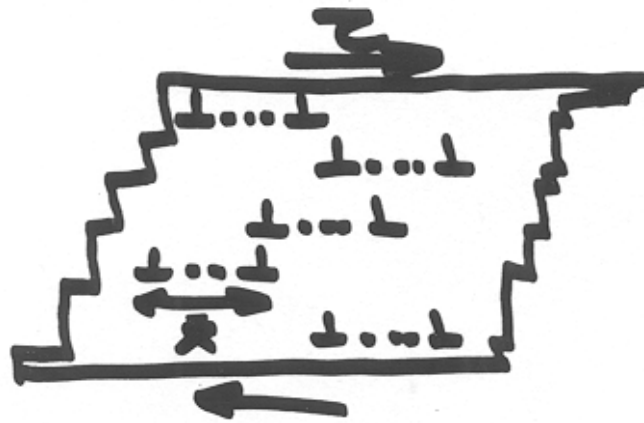


Figure 8: Motion of N dislocations.