

From individual dislocation motion to collective behaviour

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The dynamical behaviour of dislocations under load is analysed in terms of a balance between mutual interactions and lattice friction, defining a screening distance which is compared to dislocation separation. Large friction stresses or low dislocation densities obviously result in individual dislocation motion; a few examples taken from TEM *in situ* experiments illustrate how mechanisms recorded at the dislocation scale may help in understanding the macroscopic mechanical behaviour of such materials.

The pathologic case of strength anomalies is then analysed: the effect of lattice friction is overwhelmed by a strong strain localisation arising from a very low value of the strain rate sensitivity. The resulting collective and intermittent plastic flow makes difficult any direct analysis of dislocation mechanisms within avalanches, whereas observations made in lower density regions may not be representative of the mechanisms responsible for the strength anomaly. Beyond such transient regimes, the screening distance tends to infinity as the lattice friction vanishes. An obstacle-free and fully collective dislocation motion appears (domino effect), characterised by scale-free avalanche size distributions, in which avalanches of any sizes can occur. Such behaviour is reminiscent of the well known self-organised criticality (SOC), making questionable any micro-macro homogenization procedure based on a supposed representative elementary volume.

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1. Introduction

Plastic deformation of crystals results in most cases from motion of dislocations under stress. Individual dislocation motion has been studied both theoretically and experimentally for many years. Transmission electron microscopy (TEM) *in situ* straining experiments, first developed in Japan and Europe in the seventies, provided significant advances in this field. However, inferring macroscopic mechanical properties of materials from individual dislocation behaviour, traditionally performed using Orowan's equation, is a difficult task for at least two reasons: (i) the dislocation density is not a constant, and may depend on stress and temperature; (ii) the dynamical behaviour of dislocation groups may significantly differ from that of single dislocations. These two problems are not totally solved to-date. The former one is usually treated theoretically using evolution equations of the dislocation density [1–5]. The present paper will only focus on the latter.

Recent experiments performed on ice crystals [6] at temperatures relatively close to the melting point revealed that the strain response to a constant load consists of a series of dislocation avalanches. In this case, owing to their mutual elastic coupling, dislocations do not move independently from one another, and the motion of one of them may trigger the motion of many other ones (domino effect). By contrast, *in situ* experiments on *bcc* metals at low temperatures, or on semiconductors at intermediate temperatures, showed smooth motion of individual dislocations. We shall discuss here the transition between these two types of dynamical behaviour, and illustrate each of them with some examples.

2. Peierls screening of elastic interactions

Dislocations are extended defects associated with long-range elastic fields that decrease as the reciprocal distance

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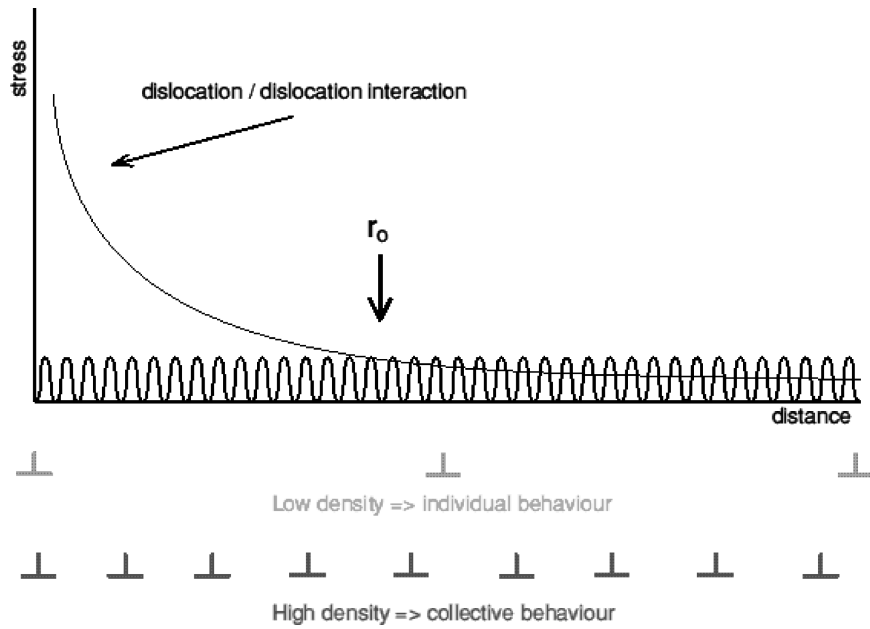


Figure 1 Schematic variations versus the distance r of the elastic field (scaling as $1/r$) of a dislocation located at the origin, compared with the Peierls friction (sinusoidal curve). The screening distance r_0 is defined as the distance at which both potentials are of the same order. Collective behaviour is favoured when r_0 becomes larger than the average dislocation separation. This may be obtained by either a decrease of the Peierls potential or an increase of the dislocation density.

$1/r$ from the dislocation core:

$$\sigma = \mu b / 2\pi r \quad (1)$$

Without any other obstacle opposing dislocation motion, a dislocation group would behave in a collective way: any perturbation in the position of one of these dislocations would result in a quasi-instantaneous rearrangement of the whole dislocation assembly. By contrast, obstacles to dislocation motion, and particularly lattice friction, are expected to hinder such a global rearrangement of dislocation positions. A screening length r_0 can be defined (Fig. 1) as the distance above which the elastic field of a dislocation becomes smaller than the lattice friction σ_p :

$$r_0 = \mu b / 2\pi \sigma_p \quad (2)$$

This means that dislocations separated by a distance larger than about $2r_0$ would experience a mutual interaction smaller than the lattice friction. Large lattice friction amplitudes, resulting in small screening distances, favour individual dislocation behaviour. This is obviously the case for *bcc* metals at low temperatures, or semiconductors at intermediate temperatures. By contrast, reduced lattice friction (e.g. *fcc* metals, or *bcc* at high temperatures) results in long-range coupling, and hence in collective dislocation behaviour.

The transition between these two regimes can be defined as the conditions for which this screening distance r_0 becomes comparable to the average dislocation separation

ration $\rho^{-1/2}$, giving

$$\rho = (2\pi \sigma_p / \mu b)^2 \quad (3)$$

Taking the example of Niobium at low temperatures, with a shear modulus of 40 GPa, and a typical lattice friction of 200 MPa, the dislocation density necessary for collective behaviour to appear would be of about 10^{16} m^{-2} , which is far above the usual densities in standard straining conditions. This is in perfect agreement with TEM *in situ* observations (Fig. 2) showing independent glide of non-correlated screw dislocations [7].

This situation is worth comparing with the case of aged FeCr alloys: a shear modulus of about 75 GPa and a friction stress of the order of 500 MPa give a dislocation density at the transition of the same order of magnitude (10^{16} m^{-2}) as for niobium. However, ageing causes a spinodal decomposition into Fe-rich and Cr-rich phases, resulting in a strong precipitation hardening [8]: shearing of the hardened structure by dislocations results in local softening and a strong subsequent slip localization (Fig. 3). Under similar loading conditions as for niobium, the local dislocation density in slip bands is significantly larger, by a factor $1/f_v$, where f_v is the slip band volume fraction. This density may increase by several orders of magnitude, becoming of the order of (or slightly larger than) the cutoff value, which results in obvious (but short-ranged) correlations between dislocation movements, as observed during *in situ* experiments.

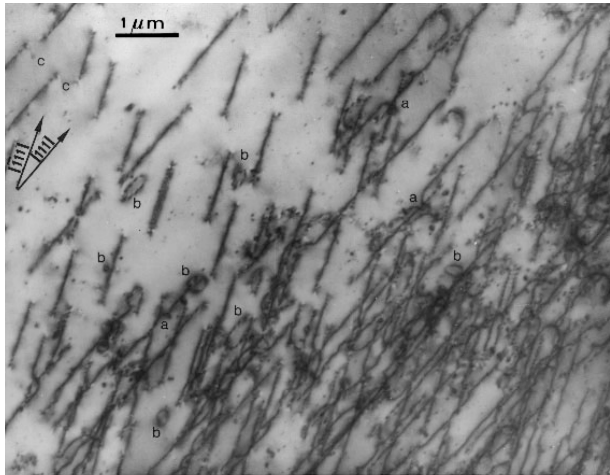


Figure 2 Niobium single crystal during *in situ* straining at 100 K. Due to the large Peierls potential, straight screw dislocations are observed to glide smoothly and independently of each other. (After [7]).

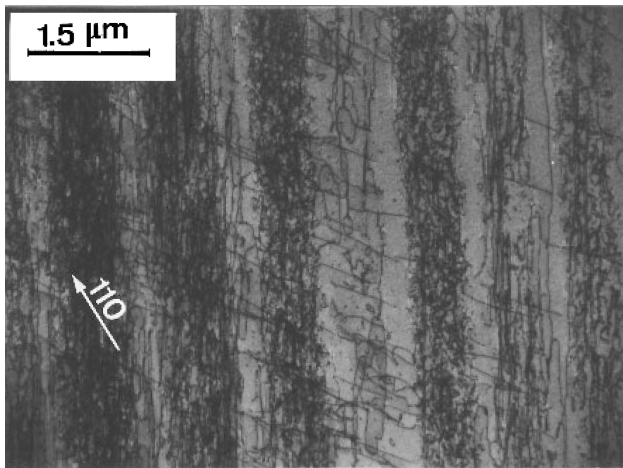


Figure 3 Fe 35 at% Cr alloy aged 505 h at 500°C, and deformed at room temperature, showing strong strain localization. Jerky motion of dislocations was observed in this case, suggesting that, owing to strain localization, the dislocation separation in the band was of the order of the screening distance r_0 .

The following paragraphs illustrate the counteracting roles of lattice friction and of dislocation density and strain localisation on three typical examples.

3. Examples of individual dislocation motion

As mentioned above, smooth individual dislocation motion, associated with lattice friction, allows an easier observation of dislocation behaviour using TEM *in situ* experiments. Typical results were obtained in semiconductors, and *bcc* metals and alloys at low temperatures. In addition, owing to the uncorrelated dislocation motion, the macroscopic plastic behaviour can be reasonably inferred from individual dislocation mechanisms, using Orowan's equation. Specific multiplication processes involved in the

achievement of a steady-state mobile dislocation density can also be identified.

As an example, early TEM *in situ* experiments performed in Japan in the seventies allowed dynamical observations of single-pole dislocation sources in Fe [9] and in Mo [10]. In the same way, the first real-time recording of the operation of a double-ended Frank–Read source was performed in silicon using a similar technique [11], as shown in Fig. 4. Other types of (less classical) sources were evidenced by this technique. The “Amenophis Scolopendra” for instance [12], discovered in pearlitic steels [13], is based on non-planar Orowan by-passing of elongated cementite islands: owing to continuous cross-slip of screw dislocations in the *bcc* structure the two dislocation arms cross over and turn backwards to reinitialize the process, instead of annihilating after by-passing the obstacle, generating two fresh dislocation arms at each operation.

Such individual behaviour allows direct measurements of dislocation mobility, without significant perturbations from long-range elastic interactions. For instance, the dependence of dislocation velocity on the free dislocation length L was shown for the first time in silicon under these conditions [14]. This is also the case in germanium, as illustrated in Fig. 5 [15]. As predicted by Hirth and Lothe [16], the velocity of short and long dislocations is shown to be quite different. The velocity of short dislocations is controlled by kink pair (kp) nucleation, which is in turn proportional to the number of possible nucleation sites, i.e., to the dislocation length. They assume that the behaviour of long dislocations (i.e., longer than the kink mean free path X) is different in that a single kp nucleation only moves forward a dislocation length equal to twice the kink mean free path: the dislocation velocity becomes independent of the dislocation length. Under this kink collision assumption, a fit of the velocity vs length curves of Fig. 5 [15] allowed a determination of kink-formation and migration energies. The corresponding velocity expressions may be used in Orowan's equation, together with the mobile dislocation density, to obtain the constitutive equation of the bulk crystal.

4. The intermediate (and pathological) case of strength anomalies

A number of materials (essentially intermetallic alloys) exhibit a counterintuitive stress-temperature behaviour: flow stress exhibits a positive temperature dependence in a finite temperature range. The mechanisms responsible for such behaviour usually involve thermally activated locking of mobile dislocations, which is most often associated with cross-slip of screw dislocations in a significant Peierls friction.

Another interesting feature is that the anomaly is systematically associated with a very small value of the strain

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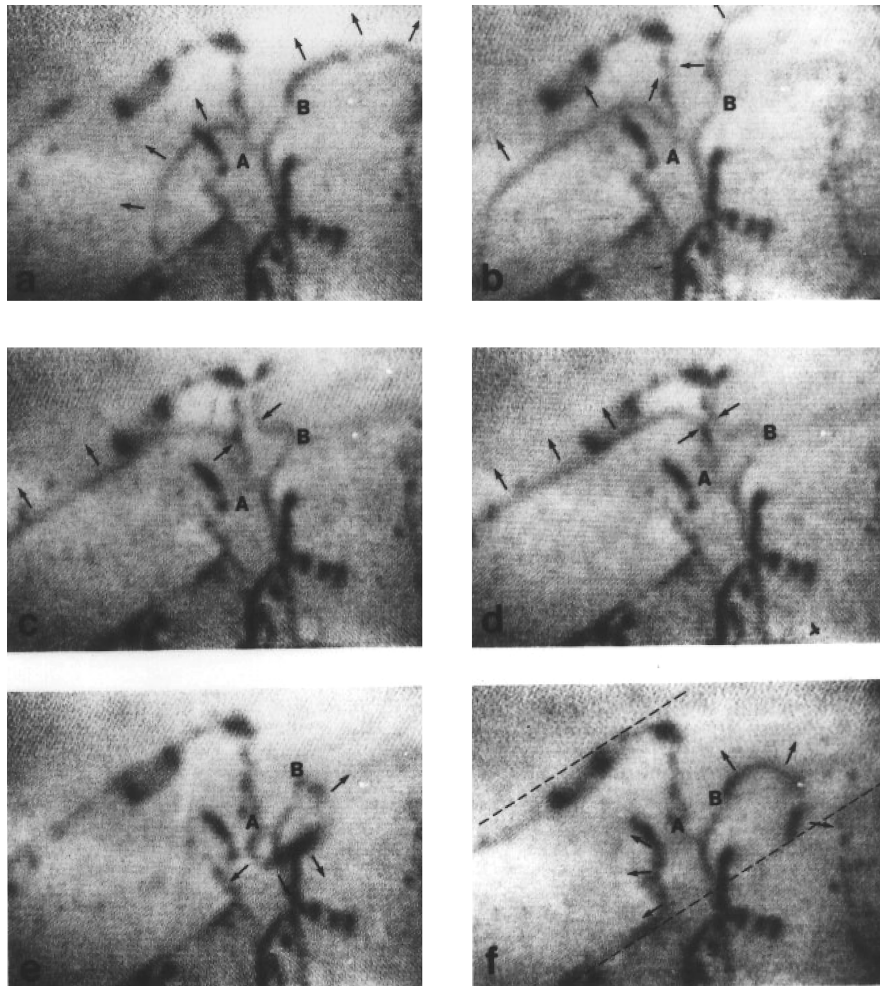


Figure 4 Operation of a Frank-Read source in Silicon strained *in situ* at 600°C, 270 MPa. The source pinning points are labelled A and B. The distance between A and B is of about 0.3 μm . The two arms rotating in opposite directions (arrows) meet and annihilate between (d) and (f). The dashed lines in (f) show the intersections of the slip plane with the thin foil surfaces. The height of each picture is about 1 μm .

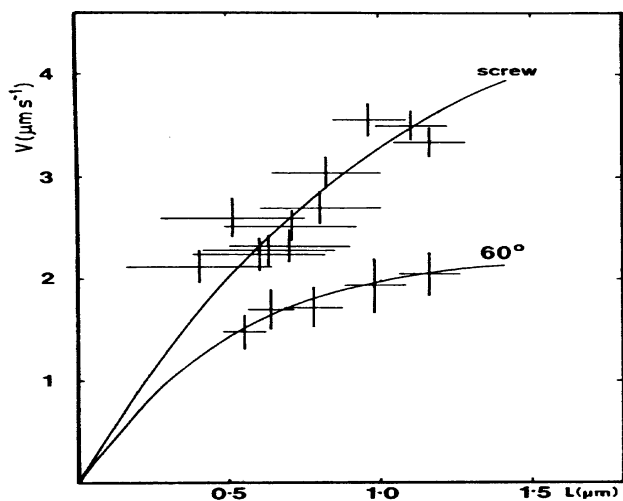


Figure 5 Example of *in situ* dislocation velocity measurements for a constant stress of 40 MPa at $T = 703 \text{ K}$. Velocities of screw and 60° dislocations increase with their free lengths L . The gradual velocity saturation for increasing L values allows a determination of both kink formation and migration energies. (After [13]).

rate sensitivity $S = d\sigma/d \ln \dot{\epsilon}$. This particular feature directly results from a steady state for the mobile dislocation density, assuming that multiplication is balanced by irreversible dislocation locking (exhaustion), other mechanisms for the evolution of the dislocation density playing a negligible role [5]. As a consequence, stress anomalies appear as a property of the whole dislocation population rather than of individual dislocations.

Furthermore, if S had a large positive value, any attempt of strain-rate localisation would require an increase of stress, and would therefore be hindered. By contrast, in the present case, a very small value of S means that the strain rate may locally increase without any stress penalty, resulting in strong plastic bursts. Such strain instabilities and localisation are actually observed in these materials, for instance in TiAl [17, 18], in Ni_3Al [19–22], or in CuZn [23], if deformed in the anomaly domain. As in the case of FeCr alloys mentioned above, the associated local increase of mobile dislocation density may bring the system from a typical Peierls-type glide of indepen-

dent dislocations to a state of highly collective behaviour. Again, despite some recordings of slow individual dislocation glide in the vicinity of intense slip bands, the major part of plastic strain is currently observed to proceed from very fast dislocation avalanches during TEM *in situ* testing of these materials (e.g. [24]). The mean-field approach mentioned above [5], that predicts the occurrence of such strain bursts, cannot describe the details of the resulting dynamical dislocation behaviour. Further information on the mechanisms at the origin of stress anomalies are obviously to be found analysing such dynamical effects. Unfortunately, dislocation densities are so high, and propagation times so short, that such an analysis using TEM methods is almost hopeless. At the very most, the observation of slower dislocations in the vicinity of slip bands, if used very carefully, may give some hints on the actual behaviour within avalanches, and help in understanding the mechanisms responsible for the anomaly in each particular material. It should however be kept in mind that these slower dislocations gliding in the vicinity of an active slip band should be found close to the intermediate regime where dislocation separation is of the order of the screening length. This situation may result in short-ranged jerky dislocation motion as sometimes observed in various materials (exhibiting or not an anomalous behaviour), as for instance in Fig. 3 in the somewhat different case of FeCr alloys. This particular feature may significantly differ from the actual dislocation behaviour within avalanches.

In addition, the large velocities involved in avalanches are expected to alter the efficiency of the associated thermally activated mechanisms significantly, and in particular the one responsible for dislocation exhaustion.

A thorough understanding of mechanisms responsible for stress anomalies would therefore require an analysis of dynamical avalanche triggering, propagation and locking mechanisms. Owing to the complexity of the system, that consists of a large number of interacting objects, the use of statistical analysis methods similar to those detailed hereafter would probably be necessary.

5. Spatial coupling and collective effects

Acoustic emission (AE) signals recorded from ice single crystals demonstrate the intermittent character of deformation, i.e., of dislocation motion, under constant load [6]. Corresponding distributions of strain burst amplitudes clearly obey a power law (Fig. 6), with a critical exponent close to 2 in frequency distributions (equivalent to 1 in cumulative distributions). Such a scale invariance means that strain bursts do not exhibit any characteristic size: small avalanches are more frequent than big ones, but avalanches of any size can occur.

Such behaviour is reminiscent of the well known self-organised criticality (SOC) [25] already recognised to control phenomena as different as traffic jams, earthquakes or stock exchange rates. Fig. 6 also shows that

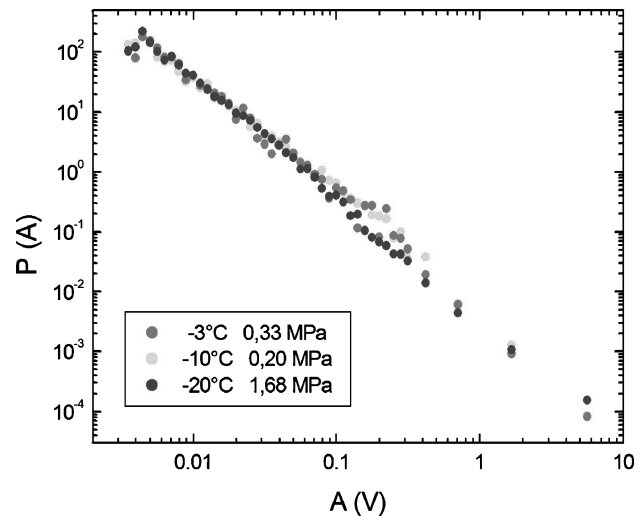


Figure 6 Distribution of dislocation avalanche sizes in ice single crystals at different temperatures and (macroscopic) stresses. (After [24]).

the strain burst size distribution is independent of temperature, at least in the elevated temperature range explored here (expressed in terms of T/T_m). These findings suggest (as expected) that the collective behaviour is driven by elastic interactions [26–28].

In polycrystalline ice, grain boundaries act as barriers to dislocation glide. The situation is therefore different from the single-crystal case in two respects: (i) in contrast with scale-free avalanches recorded in single crystals, the grain size introduces a characteristic length in the system, that results in a cutoff in large amplitude dislocation avalanches, and (ii) the distribution of avalanches smaller than the cutoff size still obeys a power law, but with a different exponent (0.35 instead of 1 in cumulative distributions).

This last point suggests that this grain-size effect is not a trivial one, that would have introduced a cutoff without changing the exponent value. The basic reason is that grain boundaries act as obstacles to dislocation motion, but not to internal stresses. Recent work based on Monte Carlo simulations [27] shows indeed that internal stresses generated by dislocation avalanches larger than the cutoff size may in turn nucleate new avalanches in neighbouring grains. Such a load redistribution is no more consistent with one of the main conditions for SOC, i.e., that the loading rate has to be negligible as compared to the relaxation rate. The system seems therefore to be pushed off the critical state. Despite the fact that the presence of grain boundaries result in a cutoff in avalanche sizes, the size distribution of small avalanches is controlled by long-range internal stresses extending over distances much larger than the grain size.

A fairly similar behaviour may be expected in the case of strength anomalies discussed in Section 4. The introduction of a (thermally activated) dislocation locking may

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modify the characteristics of their collective behaviour as compared with the obstacle-free motion of interacting dislocations: locking of one given dislocation will indeed affect the motion of a large number of other dislocations interacting with it, probably leading to particular strain bursts statistics.

As a consequence, these findings may invalidate classical micro-macro procedures based on a so-called “representative volume element”.

6. Summary and conclusions

Obstacles to dislocation motion, and more particularly lattice friction, introduce a screening length in long-range elastic interactions between dislocations, that govern their dynamical behaviour. In the case where this screening length is smaller than the dislocation separation, deformation proceeds through the individual motion of independent (i.e., non-correlated) dislocations. In this case, the global behaviour can be considered as the sum of the individual ones, and the non-correlated character of dislocation behaviour allows a mean-field treatment of the problem. Nevertheless, inferring macroscopic mechanical properties from individual dislocation motion still remains in this case a difficult task, as it requires the knowledge of evolution kinetics of dislocation densities.

An increase of the screening length defined above may arise either from a decrease of lattice friction or an increase of dislocation density (e.g., through strain localisation). In the extreme case where the screening distance tends to infinity, the plastic behaviour involves strong collective dynamical effects. The system is brought into a self-organised critical state in which dislocation avalanches of any sizes may occur. The intermediate case in which the avalanche size is limited by obstacles is not trivial. Stress fields associated with moving dislocation groups may extend to distances much larger than the avalanche cutoff distances, resulting in unexpected effects on the behaviour of smaller avalanches. The question on how obstacles to dislocation motion (grain boundaries, dislocation irreversible self-locking, sessile dislocations arrays or precipitates) may affect the behaviour of other dislocations is still open. These findings make both TEM *in situ* experiments and micro-macro homogenization procedures somewhat questionable in this case.

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