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Multiscale Modeling of Plastic Deformation

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Dislocation patterning and recovery under single slip: modelling micromechanisms from observations

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ABSTRACT

The paper is focused on the formation and on the role of prismatic loops during deformation. The analysis is restricted to non-diffusive processes in fcc-related crystals. Double cross-slip and cross-slip dipolar annihilation yield strings of loops such that one loop extremity is aligned in the screw direction with the extremity of its nearest neighbour. Reactions between prismatic loops and mobile dislocations are at the origin of a number of microstructural reactions including recovery, dislocation entanglements and patterning in single slip, and dislocation multiplication. There is indication that loops may nucleate twins.

INTRODUCTION

Dislocation dipoles and prismatic loops are very common debris encountered in crystals deformed *in single slip* at low temperature. They may appear as isolated features but they are also often incorporated in dislocation entanglements. The shape, dimensions and even the nature of prismatic loops depend on experimental constraints such as applied stresses in the primary and cross-slip planes and temperature. But they also depend on various crystal parameters such as crystal structure, which defines Burgers vectors and their dissociation reactions, stacking fault energy, elastic constants, dislocation mobility. Prismatic loops or loop derivatives containing stacking faults may vary considerably in nature (e.g. faulted dipoles and stacking fault tetrahedra).

In view of the abundant literature on loops, we restrict ourselves to two main topics:

- diffusion-free loop formation under single slip with the exception of mechanisms involving the by-passing of local obstacles.
- the role of loops during deformation. It will be shown in particular that in addition to some "passive" elastic interactions with mobile dislocations responsible for entanglements, loops are potential sources for dislocations and twins.

LOOP FORMATION

A prismatic loop generated by glide assumes the shape of a parallelogram including two elongated sides parallel to the slip plane, referred to as *loop edges* or *edges* in the following, and two *jogs* in the cross-slip plane. A prismatic loop is glissile on the prism surface defined by the loop line and its Burgers vector. The configuration of minimum energy is attained when the elongated segments are in edge orientation.

Loop formation under single slip requires that the participating dislocations cross-slip which, under the above assumptions, is the only way to engender a jog. This constraint was recognized long ago by Johnston and Gilman [1] who proposed the first cross-slip manoeuvre for loop formation. Concepts were however uncertain at that time as illustrated by comments from Fourie and Wilsdorf [2] :"While it may be too early to make definite statements […] the principal reason for rejecting the [Johnston and Gilman] theory is that it leaves a number of points unexplained. […] For instance, one fails to see what could cause screw dislocations to crossglide in such a spectacular fashion in the absence of any other detectable obstacles. […] The prismatic dislocation which represents a missing piece of atomic plane, and the other prismatic dislocation representing the corresponding portion of atomic plane would attract each other and, when moving together, annihilate. The theory also does not explain how dislocation tangles are produced, found even in pure single crystals strained only a few percent. […] Finally, and most important, one may raise the question why no such tangles nor isolated loops are formed […] in aluminium […] strained [in situ]." A time of incertitude, indeed after considering the work of Fujita on Al a few years later [3-5].

Loop formation by double cross-slip of a single dislocation

Figure 1(*a*) shows the starting step of the Johnston-Gilman process, i.e. double cross-slip of branch G followed by loop nucleation at jog J_0. From inspection of Figure 1(*b*) [6], it can be seen that in order to close the prismatic loop, the right-hand side dislocation branch (D) must undergo double cross-slip producing two jogs, J_1 and J_1', aligned in the screw direction. A property missed in [1] and in many subsequent papers. A portion J_2' of jog J_1' serves to close the loop (Figure 1(*c*)). Its remaining part, J_2", together with the companion jog, J_1, are free to slide in the cross-slip plane; they may serve as nuclei for subsequent loops (Figure 1(*d*)).

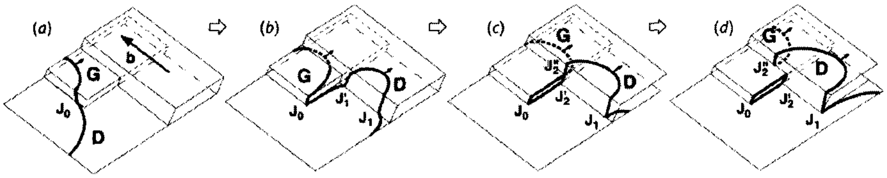

Figure 1. The generation of a prismatic loop by double cross-slip of a single mobile dislocation ([1], [6]). (*a*) The loop nucleation step at jog J_0 (the jogs are ascribed to glide on the cross-slip plane). (*b*) Branch D has double cross-slipped forming two jogs of equal height but with opposite signs (J_1, J_1'). (*c*) The jogs slide sideways and jog J_2' which is a portion of J_2', closes the loop. (*d*) The three jogs J_2', J_2" and J_1 are aligned in the screw direction.

By repetition of the same manoeuvre now starting from jogs J_2" and J_1, two prismatic loops of opposite signs will be formed. If the loop nucleated at J_0 is of vacancy type, then that at J_1 is also a vacancy loop while that at J_2" is interstitial in nature. Loops formed by G and D exhibit a stepped succession such that the upper edge of one given loop (e.g. J_0) is coplanar with the lower edge of the next loop (i.e. J_2") and such that the rear and front jogs of the loops nucleated at J_0 and J_2", respectively, are aligned in the screw direction.

In brief, a loop string formed by repeated double cross slip involving an *isolated* dislocation is comprised of loops of both signs located at various heights and linked one to the next by geometrical relationships on edges and jogs.

Finally, it is interesting to note that when the free-flight distance on the cross-slip plane projected on the normal to the slip plane is too large, the dipoles engendered subsequently are not stable under stress thus precluding further addition of loops to the string.

When cross-slip becomes frequent

An interesting implication of the above mechanism is when the frequency of cross-slip is high. This is illustrated in Figure 2 for an initially near-screw dislocation portion with moderate mobility. In this case, the above geometrical relationships hold in part. The correspondence between segments generated by the same double cross-slip event is, however, hidden by the fact that the loops are highly stepped. Two examples of the orientation relationship between jogs are indicated by the double-headed arrows labelled V. By contrast, arrow W shows one situation where the extremities of two consecutive loops on the left-hand side do not correspond with a loop extremity on the right-hand side.

The debris resulting from the operation of frequent double cross-slip consist of a high density of irregular loops elongated in the edge direction. Cai *et al.* [7] had reached similar configurations by kinetic Monte Carlo modelling of dislocation motion in bcc metals.

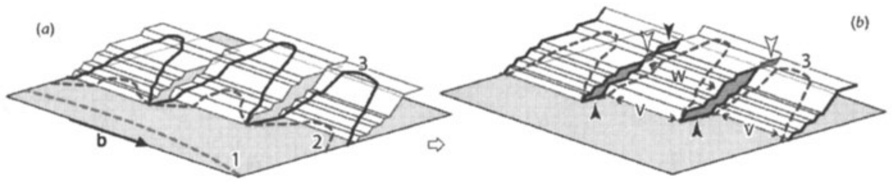

Figure 2. Genesis of prismatic loops by frequent double cross-slip (previous steps are indicated by dotted lines). (*a*) Various stages (1-3) of the evolution of an initially near-screw dislocation. (*b*) The lateral, mixed segments of the double cross-slipped portions (3) expand sideways to merge forming strings of prismatic loops. The loops indicated by black arrowheads and by white arrowheads differ in nature (i.e. vacancy and interstitial).

Loop strings formed by cross-slip dipolar annihilation

Figure 3 illustrates two equivalent processes yielding loop strings. Significant differences with strings generated by double cross-slip should be noted. Consider two dislocations gliding in parallel planes that approach one another (Figure 3(*a*)-(*c*)). For clarity, Figure 3(*a*) represents what the final configuration would have looked like could cross-slip annihilation be suppressed. The dipole meandering aspect then reflects differences in velocities during the approach. In Figure 3 *b*) the dipole parts in near-screw orientation (circled) are annihilated (in practice, cross-slip annihilation occurs sequentially as the two branches merge zipping the dipole). Energy minimization occurs by reorientation of the loops in their glide prism towards the edge orientation (Figure 3(*c*)). Figure 3(*d*)-(*f*) reproduces the mechanism proposed in [8] for the formation of a string of loops from a single-jogged dislocation. This mechanism is totally equivalent to that sketched in Figure 3(*a*)-(*c*). In both manoeuvres, because of the operation of cross-slip, the extremities of consecutive loops are aligned in the screw direction. In addition, it is seen that all loops of a string have all the same height, that they are all of the same type and that they are all located at the same height along the normal to the slip plane.

Again, string formation ceases if one of the dipole branches cross-slips in such a way that the dipole height is increased, causing its instability.

It should be mentioned that Figure 17 of [3] (from which the starting configuration of Figure 3(*a*) is inspired) deals with two mutually intersecting dislocations previously jogged by double cross-slip. It is in addition noted that the configuration in Figure 17(*c*) of [3] requires climb in order for the loop extremities to lose their orientation relationship along the screw direction.

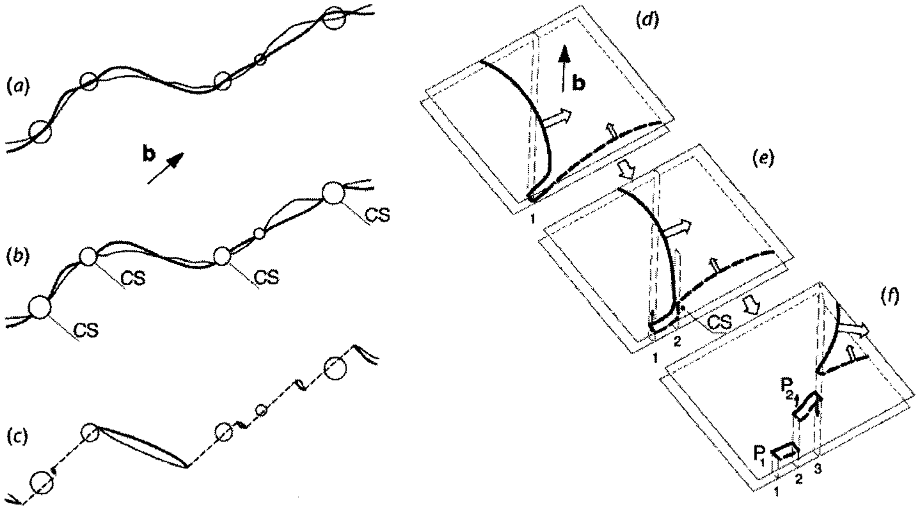

Figure 3. The formation of loops by cross-slip annihilation. (*a*) A possible dipolar configuration in the absence of cross-slip (from [3]); circled are the portions in near-screw orientation. (*b*) Truncation of the dipole into prismatic loops by cross-slip annihilation (CS). (*c*) After the loops have evolved toward their equilibrium configuration by glide, the fully relaxed configuration is a string of near-edge loops (the extremities of consecutive loops are connected by dotted lines). (*d*) The two branches of a dislocation containing a jog at (1) form an elongated hairpin under stress. The hairpin mean orientation is determined by the difference in velocities (arrows) between the branches. (*e*) A slight misorientation at (2) favours local cross-slip annihilation. (*f*) A loop string generated by repetition of the process (from [8]).

Experimental observations of loop strings

The first evidence of a loop string was found in Ni_3Al [9] and an interpretation given in terms of the cross-slip annihilation of dislocations with <011> total Burgers vector (actually, twice as long as in fcc crystals, and dissociated into two 1/2<011> partials separated by an antiphase boundary). String properties were subsequently analyzed more extensively on the simpler case of undissociated dislocations with 1/2<110] Burgers vector in TiAl (the <hkl] notation stands for the fact that since the structure is tetragonal, the projection of a direction along the **c**-axis is not equivalent to and has to be distinguished from the other two projections). The microstructure in samples deformed at room temperature in single slip along <110]{111} contains prismatic loops and loop strings in large quantities (Figure 4). By means of standard and simple contrast transmission electron microscope experiments, it has been shown [10] that the loops of a given string are essentially of the same type thus supporting loop string formation by cross-slip annihilation (Figure 3).

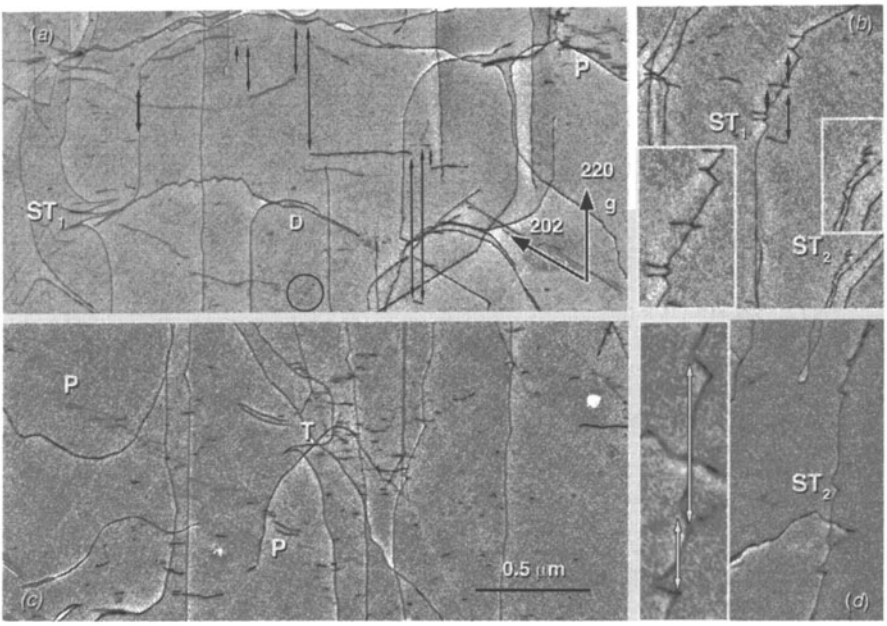

Figure 4. Examples of loop arrangements in TiAl deformed at room temperature in single slip (foil sectioned parallel to the slip plane). The fact that the [110] screw dislocation orientation is favoured is typical of TiAl. (*a*) The orientation relationship between loop extremities is embodied by double-headed arrows (single-headed when separation is too short). Another string made of very small loops is circled at the bottom. (*b*) Two different sawtooth configurations (ST) (zones of interest are enlarged in boxes). (*c*) Sample area containing a large loop density. In the dense part (T) loop strings are thought to have disappeared. The feature between letters P is comprised of two strings. (*d*) Another sawtooth configuration resulting from the intersection of a loop string by a mobile dislocation.

In principle, loop strings should be formed in a number of crystals because the only pre-requisite for these debris is the occurrence of cross-slip. We have accordingly re-visited deformation microstructures in model metals supposed to provide simple situations. We have explored Al and Cu single crystals deformed to 2% of permanent strain in single slip at liquid nitrogen. As already reported in the literature, debris distribution is very heterogeneous including entanglements in places. As to loop strings though, preliminary observations were somewhat disappointing. There are strings indeed, but in insignificant proportions. They are generally hard to distinguish within an overwhelming population of loops seemingly distributed at random.

- So far, the situation in Cu is the least favourable to string identification because loop visibility is obscured by the presence of the so-called faulted dipoles (see Figure 7).
- In consistency with flow stresses differing by two orders of magnitude, loop and dipole mean heights are generally larger in Al than in TiAl. Between tangles, the deformation

microstructure of Al is void of debris. In fact, tangles are comprised of several sub-tangles and what characterizes Al is that, in between these, loops are mostly very small (a few nm in weak-beam conditions), whereas the sub-tangles are dominated by loops of larger dimensions. So far, only very few strings made of very small loops have been found.

It has been independently suggested that prismatic loops would anneal out upon storage of Al at room temperature [3], but we do not have obtained supporting evidence for this so far. One explanation for the fact that loop strings are not generally observed could be that loops are relatively mobile in Cu and Al and that they are partly destroyed or shuffled up after being swept by a few mobile dislocations. Work is in progress to explore these properties in detail.

Frank loops and stacking fault tetrahedra

The formation of a stacking fault tetrahedron has been elucidated by Loretto *et al.* [11]. The mechanism, sketched in Figure 5, is based on the presence of a jog elongated in a <110> direction (**AD**) perpendicular to the Burgers vector (**CB**) of the mobile dislocation (Figure 5(*a*)). The dislocation is dissociated in the primary slip plane (α). The jog is thus of Lomer type and basically immobile (it is actually glissile in a cube plane). The upper branch cross-slips onto plane δ (where it dissociates) until it merges with the lower branch forming a fully glissile configuration after cross-slipping back to the primary slip plane. Cross-slip of the upper branch may be favoured by the constriction initially located at the upper jog extremity. There are two equivalent paths that may yield a Frank loop located on either one of the β or γ planes (Figure 5(*c*) and (*d*), respectively). The full tetrahedron results from dissociation of the edges of the Frank loop (not shown) in the corresponding cozonal planes. For a more complete discussion of stacking fault tetrahedra, see [12, 13].

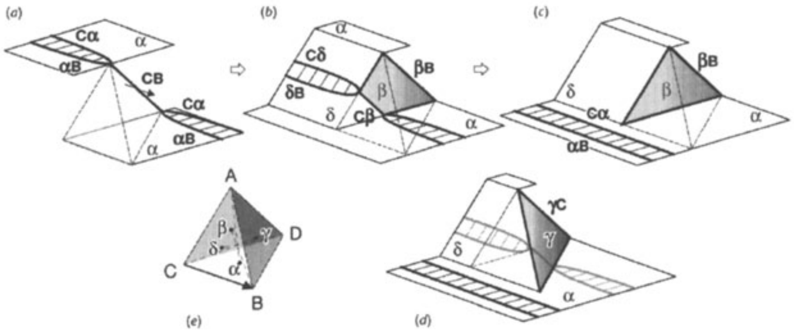

Figure 5. The formation of a stacking fault tetrahedron by glide (after [11]). (*a*) The required configuration includes a jog of Lomer type. (*b*) As the upper branch cross-slips in plane δ, the jog dissociates into a sessile **βB** Frank partial and a **Cβ** Shockley partial which is glissile in plane β. (*c*) The latter partial disappears as the left-hand side and right-hand side branches merge in the lower α plane. (*d*) A variant of the preceding process where the Frank loop forms on the other possible plane (γ). (*e*) The reference Thompson tetrahedron.

The manoeuvre is in fact rather restrictive for it requires that a Lomer-type jog be formed prior to the transformation and this, in turn, implies that the parent dislocation has been intersected by a succession of dislocations, all strictly coplanar, with Burgers vector **CB**, itself

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orthogonal to **AD**. It is noted that this process does not allow for stacking fault tetrahedron production under single slip conditions.

REACTIONS BETWEEN LOOPS AND BETWEEN LOOPS AND MOBILE DISLOCATIONS

Loops and loop strings are formed as soon as dipolar interaction takes place, probably from the early stages of deformation. They are subsequently approached, by-passed or intersected by mobile dislocations giving rise to a number of reactions.

Specific deformation debris

When the slip plane of the approaching dislocation intersects the jogs, the impacted jog is cut into two shorter ones and the loop turns out to be branched to the dislocation. This gives rise to two types of sawtooth configurations (Figure 4) whose nature differs according to whether the impacted loops are piled up (ST_1) or they belong to a string (ST_2) but in each case the resulting debris is nothing but a helical dislocation[6, 10, 14].

It is worth noting that locally, the resulting helix turn looks like a dipolar hairpin trailed by a jogged mobile dislocation. This uncertainty can be easily ruled out when the configuration shows two pinning points ahead of the dipole and one behind (left-hand side box in Figure 4(*b*)).

Multipoles are frequent in TiAl as well as in Cu alloys[15] deformed in single slip. Branches with opposite signs are often paired as part of an elongated prismatic loop, and then the multipole results from the piling-up of such loops. Another configuration is when the branches are interconnected, continuously snaking from between the two extremities of the multipole. The second case is the result of the intersection of piled-up loops by a mobile dislocation. An intriguing and not yet explained property of multipoles is that their extremities are very often aligned in the screw direction.

Recovery

All the loops of a string can be partly or totally eliminated at once by an impacting dislocation through a process that involves glide exclusively. Partial elimination, that is, loop refinement, takes place when the slip plane intersects the jogs, whereas total elimination requires that the slip plane be coplanar with the upper or lower edge dictated by signs (Figure 6). Whether this process or the above formation of sawtooth configurations takes place depends on the angle of impact between the dislocation and the string [14]. As seen above, a near-screw dislocation will engender accordion-like multipoles whereas an impacting dislocation with pronounced mixed character promotes loop refinement.

The preceding loop refinement process will take place between a dislocation and any ensemble of loops provided the loops are all of the same nature. Clearly, the process cannot be envisaged to explain loop elimination in fatigue walls which, for some time, has been thought of as resulting from fast climb between very close segments of opposite signs [16]. There is however an alternative manoeuvre, not involving diffusion, that allows for total or partial elimination of a random distribution of loops of both signs [17]. The loops are indeed pushed towards each other by the new dislocation portions that impinge the wall as a result of the back and forth motion of the screw portions in the channels. Statistically, loops of both signs merge under these internal stresses and/or by elastic attraction and the loop parts corresponding to two overlapping loop surfaces will mutually annihilate provided of course that the loops are of different nature.

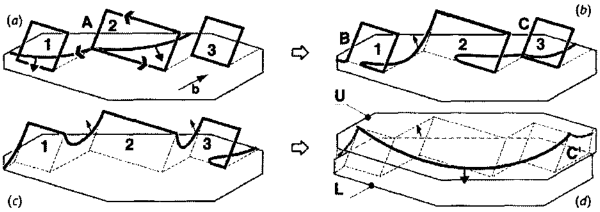

Figure 6. The total elimination of a loop string by a gliding dislocation. (*a*) The dislocation impacts the string in the habit plane of the lower edges. (*b*) It annihilates with these forming a crenellated configuration. (*c*) Once segments 1-3 have relaxed in the screw direction they slip up in the cross-slip plane. (*d*) The resulting configuration is a portion entirely glissile in plane U.

Dislocation patterning

Dislocation patterning has been recently explained in terms of loop string genesis in consistency with observations in TiAl [14]. In this scenario, a loop string constitutes an obstacle to mobile dislocations approaching from above or from below the string. The dislocation is bound to the string and whether or not the ensemble drifts is unimportant in the explanation. Sooner or later another dislocation with opposite sign arrives and interacts with the awaiting dislocation to form a second loop string. The second string is expected to adopt a stepped shape that resembles that of the first string, as frequently attested by observations. The string pair has a larger cross-section for capture of a fresh impacting dislocation and the process of capture/annihilation repeats itself. Hence, the microstructure bifurcates from homogeneous to heterogeneous distribution upon the formation of the first string. The scenario remains valid in the case of a sawtooth-forming intersection.

The situation in Al and Cu alloys is thought to be similar to that identified in TiAl although, as mentioned above, there is no clear evidence for well-defined loop string arrangements. It is believed that, in those cases, loops are more readily swept by mobile dislocations than in TiAl, yielding rapid re-shuffling of the loop ensembles. This is consistent with the fact that in Al within sub-tangles, the loops are in general larger and with rather irregular shapes.

MULTIPLICATION

Prismatic source and dislocation multiplication

The fact that prismatic loops are destroyed under stress and that such configurations can operate as dislocation sources of the Frank-Read type has been suggested very early (see [3]). Source operation is a function of loop height, which determines the stress to destroy the dipole, and of loop length which is conversely related to the Frank-Read stress. Even though the applied stress, σ, is enough to split apart an infinitely long dipole of given height, it cannot destroy a loop of equal height whose length is less than $\alpha\mu b/\sigma$. Given this height though, when two or several consecutive loops of a string merge to form one single prismatic loop, as a result for