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Response to "Shear Impossibility—Comments on 'Void Growth by Dislocation Emission' and 'Void Growth in Metals'"

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We thank the authors of Ref. [1] for their comments and interest in our work [2–6]. We agree that the emission of shear loops on one single shear plane cannot lead to void growth. However, our simulations suggest that coordinated shear on non-parallel planes can lead to void growth/shrinkage [3–5]. Detailed descriptions of this process are still being worked out and represent an exciting area for future research. Thus, there seem to be two separate dislocation mechanisms operating either sequentially or simultaneously: shear and prismatic loop emission. Whereas prismatic loops are well known and have been extensively documented, the postulation of "special" shear loops is novel. The authors [1] have correctly pointed out that special restrictions need to be applied to these shear loops, something not mentioned in Refs. [2–6].

On the subject of shear impossibility, the authors [1] bring some good points in their comments of our papers. Indeed, the closed loop emitted from the surface of the void does not by itself expand the void. This is obvious from our papers, in which we considered a growth of a cylindrical void by emission of an edge dislocation [2], and a collapse of the void by an emission of an opposite-signed edge dislocation [5]. Thus, if both (positive and negative) dislocations were emitted (which is a 2-D counterpart of a dislocation loop), no net effect on the void growth would take place. Void growth takes place by the outward transfer of the material, which is possible even in an incompressible case due to the outward movement of the remote boundary of the body (the plastically deformed region around the void is surrounded by an elastically deformed region). Eq. (1) of the Comments on our papers [1] nicely states that the net amount of added material associated with the creation of a closed loop entirely within a single slip plane (with its Burgers vector in that plane) is zero. However, while shear on a single plane cannot expand a void, coordinated shear can, because it is able to account for the mass transfer from the surface of the void, without violating mass conservation. This is clear from Figure 13 of Ref. [2], where the material removed from the surface of the void is compensated by the material associated with the emitted dislocation dipole, consisting of a positive and negative edge dislocation at two parallel slip planes.

We agree that shear deformation is an isochoric process. The manifestation of this is the value of Poisson's ratio (0.5) in plastic deformation. However, coordinated shear in two and more planes can create openings in a material, as is shown by the simple 2-D analog presented in Figure 1a. Let us imagine a body with rectangular section composed of four trapezoidal blocks and let us assume that the four inclined interfaces are cohesive (i.e. they can slide but cannot separate) and that the vertical interface is free. When tractions are applied vertically as shown in Figure 1b, the two trapezoidal blocks move laterally through shear along the four glissile interfaces. In doing so, they produce a lateral extrusion of material and the creation of an internal void. It should be noted that the same configurational change could be produced by horizontal tractions. Volume constancy is obeyed. Figure 1c shows the same case when we have numerous glissile interfaces along two non-parallel shear planes. Coordinated shear along these interfaces produces the same lateral transfer of material. These unit glide processes, which are in this case confined in the material, can be considered as dislocations. Each one creates a step on the void surface. In the general tridimensional case, several (five or more) slip systems can be activated simultaneously or sequentially, creating the necessary material transfer operation. In continuum mechanics, one refers to the region with dislocations as the plastic annulus

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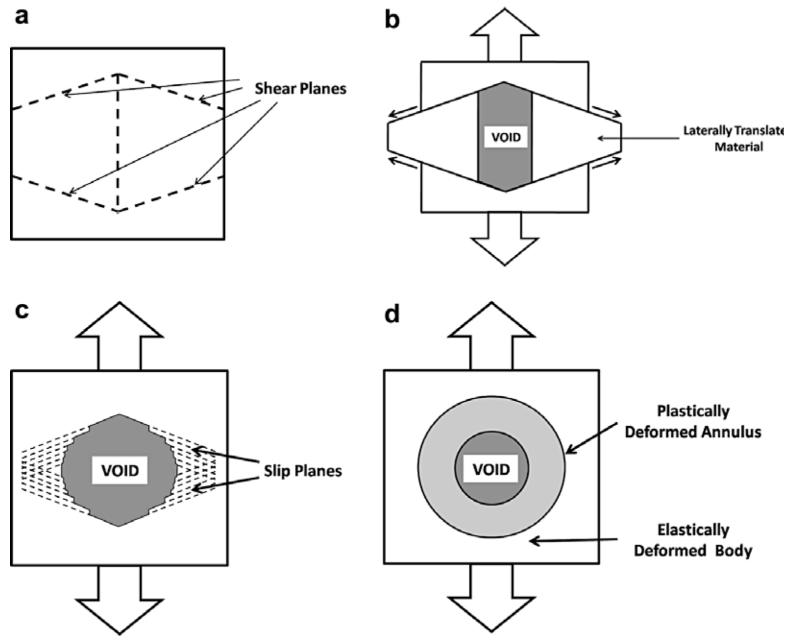

Figure 1. (a) Initial configuration of material decomposed into cohesive sliding trapezoidal blocks; (b) coordinated shear of blocks generating void and translating material outwards; (c) coordinated shear by dislocations terminating in body; (d) schematic continuum representation of void growth with plastic deformation annulus and elastically deformed area.

(which has a radius that is a multiple of the void radius). This plastic annulus is surrounded by the elastically deformed material, a classic plasticity problem [7]. Figure 1d shows the two regions (for isotropic remote tension, the plastic annulus around a spherical void is fully symmetric; for uniaxial tension, it is symmetric around the loading axis and the horizontal plane of symmetry).

Upon unloading, the vast majority of dislocations does not recede to the surface of the void, but remains in the region around the expanded void, because of the locking interaction mechanisms which prevent their reversible slip, in spite of the attractive image forces from the surface of the void. This is observed by optical microscopy of the region around the plastically expanded void, as shown in Figure 2a, where slip markings indicate localized dislocation activity associated with the expansion of the void. Using the concept of geometrically necessary dislocations [3], we calculated the dislocation density in the plastically deformed annulus to be on the order of 10^{11}–$10^{13}\,\mathrm{cm}^{-2}$, consistent with a highly work-hardened metal.

A related classical problem involving the shear loop emission is in fracture mechanics: the blunting of the crack tip is produced by shear (semi) loop emission, which carries the material and opens up the space between by crack faces [8,9].

Independently of semantic discussions regarding loops, the fact remains that in our molecular dynamics (MD) simulations in Cu (a face-centered cubic (fcc) metal), the void volume changes dramatically due to the emission of shear loops along different planes. Voids are completely closed (disappear) under compression [5] and multiply their volume multiple times under tension [3,4]. When the tension or compression is released, the situation does not reverse. Partial dislocations are

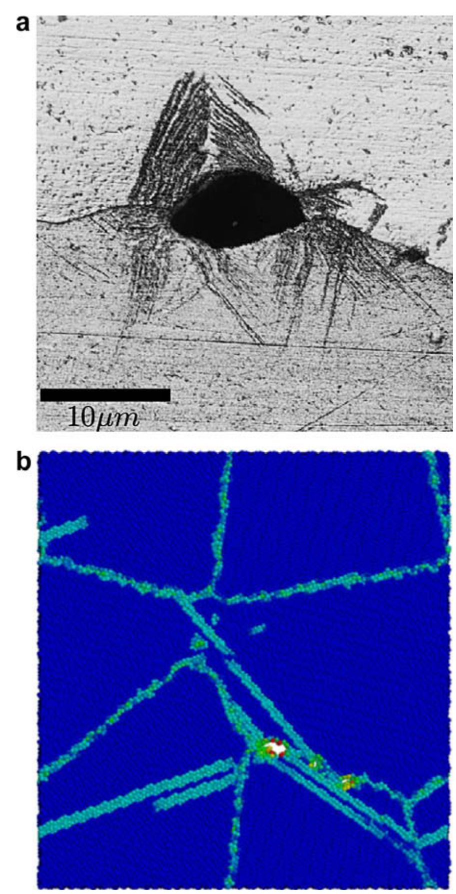

Figure 2. (a) Slip activity emanating from void at grain boundary (from Ref. [4]); (b) voids forming at grain boundary in nanocrystalline nickel; notice partial dislocations emanating from incipient voids (from Ref. [4]).

formed, rather than perfect dislocations. In many cases the leading partial is not followed by the trailing partial, and a maze of stacking faults is produced. We never saw the reaction of shear loops leading to a prismatic loop which glides away in our copper simulations. We do not discard the possibility that, for other materials or with the application of further stress, prismatic loops might be freed and glide away from such a dislocation tangle, which seems to remain attached to void sizes. Indeed, Rudd [10] recently modeled the growth of voids in body-centered cubic (bcc) metals by MD and showed the emission of "prismatic" loops in molybdenum.

As a final example for void growth without the need of prismatic loops, the nucleation and growth of voids was also modeled in nanocrystalline metals and found to take place at grain boundaries [4]. In this case, Figure 2b shows a section through such a void in our MD simulations. All lattice atoms are dark blue whereas the stacking fault atoms are light blue. Figure 2b shows significant dislocation activity surrounding the void. The lines correspond to stacking faults. Dislocations traverse the grains and are annihilated at the opposite grain boundaries. Generally, if the void has reached a critical size, the stacking fault network precludes the closure of the voids once stress is released.

In none of the simulations in fcc metals were the telltale dislocation quadrilaterals, indicative of prismatic loops, observed. All dislocations were still connected to the surface of the voids through their extremities. In this sense the shear loops that we postulated are original and different from conventional shear loops. We recognize that we did not explicitly state in Refs. [2–6] that these loops need to remain attached to the surface of the voids for the process of shear loop expansion to be operational. A forthcoming paper will deal with this in greater detail and rigor [11]. In our case, the dislocation interactions become quite complex and a plastic deformation annulus is formed, the dislocations being trapped in it.

The fact that we did not observe prismatic loops does not preclude their formation, probably as an evolution from two biplanar shear loops as shown in Figure 1 of Ref. [1]. Indeed, Figure 1 of Ref. [1] concurs with us: two shear loops form and connect with two other ones, leading to the formation of a "cage". This is termed a prismatic loop, although at the genesis there were clearly two biplanar shear loops. Our MD simulations revealed the biplanar loops but failed to show the more advanced stage shown in Figure 1c–f of Ref. [1]. Figures 4–6 of Rudd [10] show the formation of prismatic loops totally detached from the void. However, in fcc metals primarily partial dislocations were formed, whereas in bcc metals Rudd [10] showed, for molybdenum and tantalum, the formation of perfect dislocations, which can slip on three planes, {1 1 0}, {1 1 2} and {1 2 3}, creating quite different configurations.

In conclusion, the discussion presented in Ref. [1] is in greater agreement with our results than apparent and helps to elucidate the mechanism (or mechanisms) for the initiation and growth of voids. Figure 1a and b of Ref. [1] and Figure 8(a) of Ref. [3] are almost identical. It is tacitly assumed [1] that shear loops can initiate the process. We proposed a dislocation mechanism for void growth [2] and obtained confirmation through MD calculations [3]. As highlighted in the Comments [1], to which this reply was written, it is important to point out that these loops are different from conventional shear loops in the sense that their extremities have to remain connected to the void so that the attached segment creates the necessary step for expansion or contraction. Resolving the detailed processes will require experimentation and characterization by transmission electron microscopy.

We recognize that we did not explicitly state in Refs. [2–6] that these loops need to remain attached to the surface of the voids for the process of shear loop expansion to be operational and we thank the authors of Ref. [1] for providing us with the opportunity to clarify this.

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