Kinematic Generation of Dislocations

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Abstract

In this letter we present evidence from computer simulations that edge dislocations can be generated by purely kinematic processes, in the absence of more conventional dislocation sources. New dislocation pairs may be generated near high-velocity dislocations. These kinematic processes are only active under high stresses, but may be important under shock loading or under other conditions where a very high strain rate is obtained. This dislocation generation becomes possible because the sign of the force between edge dislocations changes when the dislocation velocity exceeds the Rayleigh velocity.

The dislocation density in a metal under deformation typically increases many orders of magnitude during the deformation process. Understanding the dislocation multiplication phenomena is therefore important for the deformation theory for metals. For normal stresses and strain rates, the dislocation multiplication is believed to be dominated by Frank-Read sources (Frank and Read 1950) and similar well-understood mechanisms (Hirth and Lothe 1982). At high strain rates, e.g. under shock loading, where dislocations may reach high velocities, kinematic mechanisms have been proposed (Hirth and Lothe 1982, sec. 20-7). In this paper we present computer simulations providing evidence for such a kinematic dislocation source.

We have performed Molecular Dynamics simulations of a copper slab with dimensions up to 207Å $\times$ 59Å $\times$ 651Å (725 000 atoms), with periodic bound-

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ary conditions in the y and z directions. The interatomic interactions are described using effective medium theory (Jacobsen, Nørskov and Puska 1987, Jacobsen 1988, Stoltze 1990), which provides a realistic many-body description of the interactions. A notch in the surface of the slab acts as a dislocation source (see figure 1a). The slab is oriented with a $\{100\}$ direction along the z axis, and a $\{110\}$ direction along the x axis, permitting easy relief of a strain in the z direction by edge dislocations moving on the $\{111\}$ planes. The notch surfaces are $\{111\}$ surfaces. The slab is strained by a tensile strain in the z direction, with a strain rate between $5 \cdot 10^7 \mathrm{s}^{-1}$ and $2 \cdot 10^9 \mathrm{s}^{-1}$. This strain rate is high, but the velocities of the atoms are still far below the speed of sound, and should thus easily be realized under shock loading. Due to the high strain rate and the lack of dislocation sources, a very high strain and stress is reached before any plastic deformation occurs. When dislocations finally appear from the notch, they appear pairwise on two different slip systems (a result of the symmetrical initial conditions, see figure 1b), and are quickly accelerated to very high velocities. The dislocations are seen to be split into partials. When a dislocation reaches a velocity of around 2900 $\pm$ 400 m/s a two new dislocations with opposite Burgers' vectors are formed which move quickly away from each other (figure 1c). These new dislocations soon reach the same high velocity, causing a "chain reaction" with formation of more and more dislocations (figure 1d). The rather large uncertainty in the determined velocities comes from the uncertainty of the dislocation positions and the rapid acceleration of the dislocations.

The dislocations are identified using a program that, for each atom, generates tiny Burgers' circuits; if any of the circuits fail to close the atom is considered to be part of a dislocation core. The presence of a stacking fault between two partial dislocations complicates the algorithm significantly, but can be taken into account (Schiøtz 1995). Dislocations with very extended core structures may show up as several parallel lines whose Burgers' vectors add up to the expected Burgers' vector of a partial dislocation.

Looking at the first generation of a new dislocation pair the following picture of the creation process emerges. Close to one of the partials of the original dislocation a pair of partial dislocations of opposite sign and with a connecting stacking fault area is formed. The new partials move away from each other and the stacking fault area expands until a (partial) dislocation loop is nucleated near one of the partials (see figure 2). The dislocation loop expands and thereby removes the stacking fault region. As the loop reaches the other partial they combine so that in total two new dislocations with opposite Burgers' vectors have been formed.

The generation of new dislocations does not seem to depend sensitively on the strain rate within the range $5 \cdot 10^7 \mathrm{s}^{-1}$ to $2 \cdot 10^9 \mathrm{s}^{-1}$. The main effect of increasing the strain rate is that the first dislocation reaches a higher velocity at an earlier stage and that the dislocation does therefore not travel so far before the generation of new dislocations is initiated. If the thickness of the slab in the y-direction is changed from 59 Å to only 15 Å, the generation of new dislocations is still seen. However, the three-dimensional character of the process with the nucleation of small expanding dislocation loops is not so clear. All the simulations show that the generation of new dislocations is initiated when the first dislocation reaches a velocity of 2900 $\pm$ 400 m/s.

The possibility that new dislocations may be generated near rapidly moving dislocations has already been been suggested in the literature (Hirth and Lothe 1982, Sakamoto 1991).

When dislocations are accelerated to velocities approaching the transverse sound wave velocity (C_t), the stress field is contracted in the direction of motion similarly to the well-known Lorenz contraction in the special theory of relativity. The behavior of screw dislocations is equivalent to the relativistic behavior, with C_t entering the equations in place of the velocity of light. The behavior of edge dislocations is somewhat more complicated, since both the transverse and longitudinal sound wave velocities enter the problem. At the Rayleigh wave velocity (C_R), slightly below C_t, the sign of the shear stress in the glide plane changes sign, causing the interaction between two edge dislocations in the same glide plane to change sign (Weertman 1961).

This change of sign of the interaction can also be seen from the following energy argument (Weertman 1960). Consider two dislocations of unlike sign approaching at a high velocity (v_0). The energy of each dislocation can be written as a sum of the potential energy in the elastic fields (E_{pot}) and the kinetic energy of the atoms in the field (E_{kin}). When the dislocations are far from each other, they do not interact and the total energy is just $2\,(E_{pot} + E_{kin})$. When the dislocations meet (with the new velocity v_1) the displacements and stresses go to zero (E_{pot} vanishes), but the velocities of the atoms in the fields are doubled, ie. the kinetic energy is quadrupled. Energy conservation thus requires:

$$2\Big(E_{pot}(v_0) + E_{kin}(v_0)\Big) = 4E_{kin}(v_1) \qquad (1)$$

For low-velocity dislocations, $E_{kin} < E_{pot}$, and equation 1 tells us that $E_{kin}(v_1) > E_{kin}(v_0)$, and thus $v_1 > v_0$ (assuming that E_{kin} is an increasing function of the dislocation velocity), indicating an attractive interaction. If however $E_{kin} > E_{pot}$, the opposite will be the case. A similar argument can be made for two dislocations of like sign. We can thus conclude that if the kinetic energy of the dislocations become larger than the potential energy, the interaction between them changes sign. For screw dislocations the potential energy is always greater than the kinetic energy, but for a pure edge dislocation the kinetic energy becomes larger than the potential energy for dislocation velocities above the Rayleigh velocity (Weertman 1961). Crystal anisotropy will generally narrow the velocity range somewhat (Teutonico 1962, Weertman 1962, van Hull and Weertman 1962).

If a dislocation with Burgers' vector $\vec{b}$ undergoes a core fluctuation $\vec{b} \rightarrow 2\vec{b} - \vec{b}$ generating a dislocation/anti-dislocation pair in or very near the core, the oppositely signed dislocations will normally attract and annihilate. A dislocation core is thus stable with respect to this kind of fluctuation. But if the dislocation is moving with velocities exceeding the Rayleigh velocity, the oppositely signed dislocations will repel, and the newly generated dislocation pair will separate, resulting in the generation of new dislocations.

A similar dislocation multiplication mechanism has been observed in simulations of a two-dimensional simple cubic lattice using a linear force field, where the atomic motion was constrained to be one dimension (Weiner and Pear 1975).

From our simulations we find that the generation of new dislocations begins when the dislocation velocity is 2900 ± 400 m/s. This is consistent with the suggestion that the critical velocity should be the Rayleigh velocity (which is approximately 2700 m/s as calculated from the elastic constants for the Copper potential). It should be noted, however, that even at dislocation velocities slightly below the Rayleigh velocity the attractive interaction between the dislocations in the pair is significantly reduced, and may be overcome by the oppositely directed, very large forces on the two dislocations caused by the large stress in the crystal. At the observed stress (10 GPa) a pair of partial dislocations should only be separated by one lattice constant before the forces from the deformation stress in the crystal exceed the attractive interaction between the dislocations.

We can conclude that under shock loading and similar conditions, dislocations may be accelerated to such high velocities that the interaction forces between the dislocations change sign, and new dislocations can be generated through a kinematic pair-generation process. This process will only be active if the stress is high enough to accelerate dislocations to the Rayleigh velocity, but under such conditions it may be a very important source for new dislocations.

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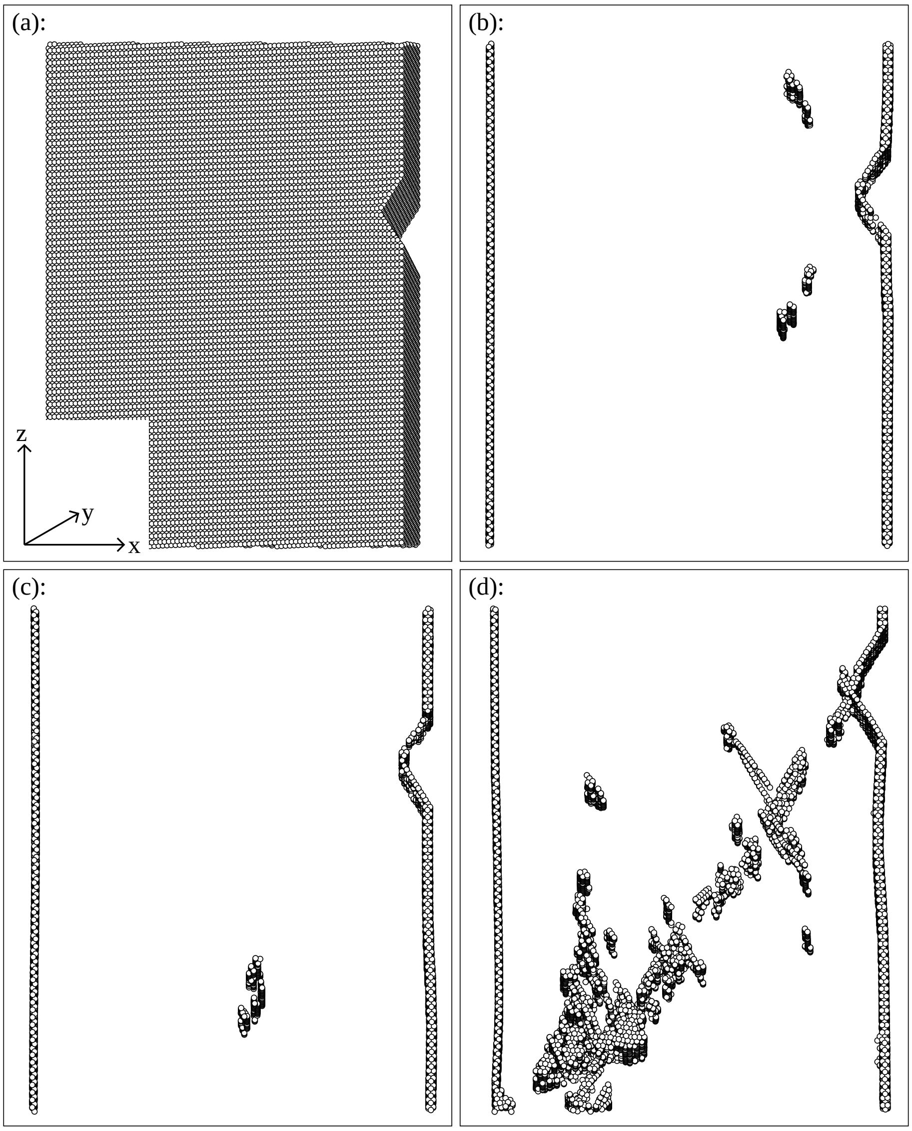

Figure 1: Simulation of the stretching of a copper single crystal. The strain rate is $5 \cdot 10^7 \mathrm{s}^{-1}$. In subfigure (a) all atoms are shown, in (b–d) only atoms at the surface or in a dislocation core are shown. (a) The "initial" configuration. (b) Two dislocations are emitted from the notch. Each dislocation is split in two partials with rather extended core structures. (c) A pair of new dislocations is generated near the high-velocity dislocation. (d) A "chain-reaction" leads to a high dislocation density.

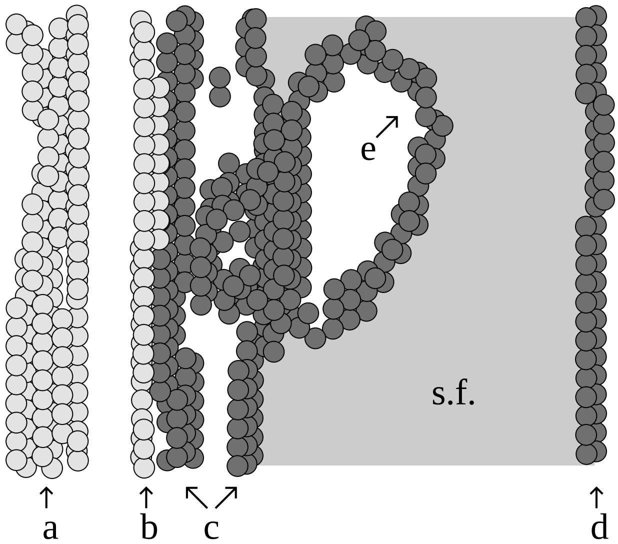

Figure 2: Snapshot of the nucleation process, a few time steps later than figure 1c. The nucleation process is viewed from the side, ie. the y axis is down, and the glide plane is in the plane of the paper. The original dislocation (moving left) is shown in light gray, the leading partial is marked (a), the trailing partial (b). Two partial dislocations with opposite Burgers' vectors are nucleated as discussed in the text, they are marked (c) and (d) and are moving away from each other. The (c) partial has a rather extended core structures and shows up as two lines. A stacking fault (shaded) is present between the partials. When the partials have separated sufficiently, a dislocation loop forms (e), removing the stacking fault as it expands.