# Dislocation jumping over the sound barrier in tungsten

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It is commonly believed that dislocations cannot surmount the sound barrier at the shear wave velocity. This letter presents results of molecular dynamics simulation showing the contrary, namely that a stationary dislocation can be accelerated above the sound barrier provided that the theoretical shear strength is reached at the dislocation core and the total energy of a subsonic perfect dislocation is sufficiently high to cause its dissociation into transonic partial dislocations.  [DOI: 10.1063/1.1473865]

Linear elasticity theory with a ''relativistic'' treatment[1] predicted that the dislocation velocity can reach a sizable fraction of the transverse acoustic wave velocity $C_T$, but cannot reach $C_T$ because the energy required to drive such a dislocation becomes infinitely large at this speed.[2] Recent molecular dynamics (MD) simulations in tungsten[3] have shown that dislocations can move faster than the speed of sound if they are created at high speed at a strong stress concentration and subjected to high shear strain. The propagation of transonic and supersonic shear cracks has been observed in high-speed impact tests.[4] However, whether or not a subsonic dislocation can be accelerated to a supersonic one remains unknown. In this letter, we demonstrate that a stationary dislocation can be accelerated to a supersonic one in MD simulation.

In our MD simulation, metal tungsten was chosen. Finnis–Sinclair potential[5,6] was used for tungsten. A block of tungsten single crystal with a bcc structure was arranged as in Fig. 1. The $x$ axis of the block is along the [111] direction, the $y$ axis along the $[2\bar{1}\bar{1}]$ direction, and the $z$ axis along the $[01\bar{1}]$ direction. The length of the crystal along the $x$ direction is $L=90\times\sqrt{3}\ a_0\approx 49.3$ nm, the width along the $y$ direction is $W=30\times\sqrt{6}\ a_0\approx 23.3$ nm, and the thickness along the $z$ direction is $B=3\times\sqrt{2}\ a_0\approx 1.3$ nm, where $a_0=0.3165$ nm is the lattice constant. A periodic condition was applied in the $x$ and $z$ directions. An edge dislocation was created by cutting out half an atomic plane in the crystal and relaxing the system to equilibrium with the top edge fixed to avoid crystal deflection. The top edge of the crystal was allowed to move only horizontally along the $+x$ direction, while the bottom edge of the crystal was allowed to move only horizontally along the $-x$ direction as shown in Fig. 1. A constant shear rate was applied. The moving speed of the top and bottom edges was $\pm 37.5$ m/s. The motions of all the atoms were followed in MD simulation at a time step of 2 fs. The temperature of the crystal was started at 10 K and raised continuously to about 100 K during the shear loading. The size of the crystal was doubled and it was found that there is no size effect on the results.

The dislocation velocity as a function of time and shear strain is presented in Fig. 2. As the shear loading proceeds, the dislocation quickly approaches a speed of around 2 km/s that is about 0.7 $C_T$. After propagating at this velocity for a while, it then jumps over both the transverse wave speed and the longitudinal wave speed ($C_L$) within a rather narrow time span. The transverse and longitudinal wave speeds of tungsten are 2.85 and 5.4 km/s, respectively. When the sampling of dislocation velocity was taken more frequently, as shown in Fig. 2, between 16 and 24 ps, it was found that the dislocation velocities actually fluctuated. It was observed that, when the shear strain is less than 0.07, the dislocation propagates at around the Rayleigh wave speed, that is about 0.93 $C_T$ with maximum velocities below the sound barrier. The plateau at 0.7 $C_T$ is actually the average velocity of the dislocation movement as indicated in Fig 2. At about 21 ps, the dislocation is clearly accelerated to a supersonic one, and the corresponding shear strain of the system is about 0.076.

The distribution of the potential energy around the moving dislocation is shown in Fig. 3. It can be seen that in the subsonic regime, the dislocation is, in fact, carrying the deformation field along with it, as shown in Figs. 3(a)–3(c). After the dislocation surmounts the sound barrier at the shear wave velocity, it outruns the deformation field and leaves the distorted lattice behind. It thus gets a boost in velocity as if it has suddenly got rid of the dragging hindrance, as shown in Figs. 3(d)–3(f). When the dislocation propagates at

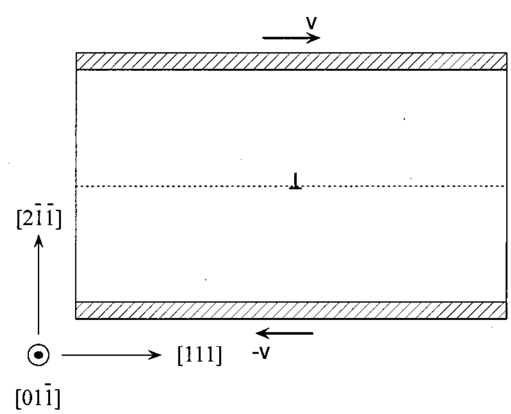


FIG. 1. Schematic plot of crystal tungsten with an edge dislocation in MD simulation.

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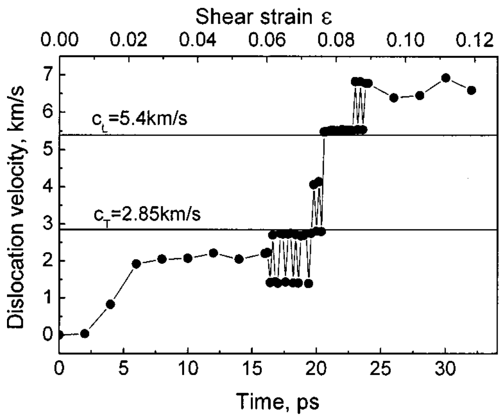


FIG. 2. The change of dislocation velocity as a function of time. The velocity values were measured every 0.2 ps between 16 and 24 ps, while others were taken every 2 ps.

supersonic velocity, it can be seen from Fig. 3(f) that it is moving as if in a deformation-free lattice environment.

In linear elasticity theory, the dislocation is described as a stress singularity,[2] while in reality, stresses at the dislocation core can only be finite. Recent pseudopotential calculations[7] have found an ideal relaxed shear strength of 26.3±0.8 GPa for a ⟨111⟩{112} anti-twinning slip system in bcc tungsten. A detailed examination of our MD simulation shows that the maximum shear stress at the dislocation core fluctuates, as shown in Fig. 4. At 19.4 ps, when the dislocation has just started to accelerate over the sound barrier, the shear stress at the dislocation core reached 24.2 GPa and was maintained at high level for a while. The 24.2 GPa in our simulation is comparable to 26.3 GPa in Ref. 7, given the fact that the two theoretical approaches are very diffferent. At this moment, the strain energy stored in the crystal was very high because of the large shear strain (average elastic strain energy density was in the order of $\frac{1}{2}G\epsilon_{xy}^2 \approx 0.45 \times 10^9$ J/m$^3$, with a shear modulus of $G = 160$ GPa for tungsten). Once the dislocation velocity has overcome the sound barrier, i.e., in the transonic (above $C_T$) or supersonic (above $C_L$) regime, the maximum shear stress at the dislocation core decreased to lower level again.

It is also important to note that at the moment when the dislocation jumped over the sound barrier, the dislocation core was extended, see Fig. 3(c) and compare to Fig. 3(b). The elongation of dislocation core may be accomplished by

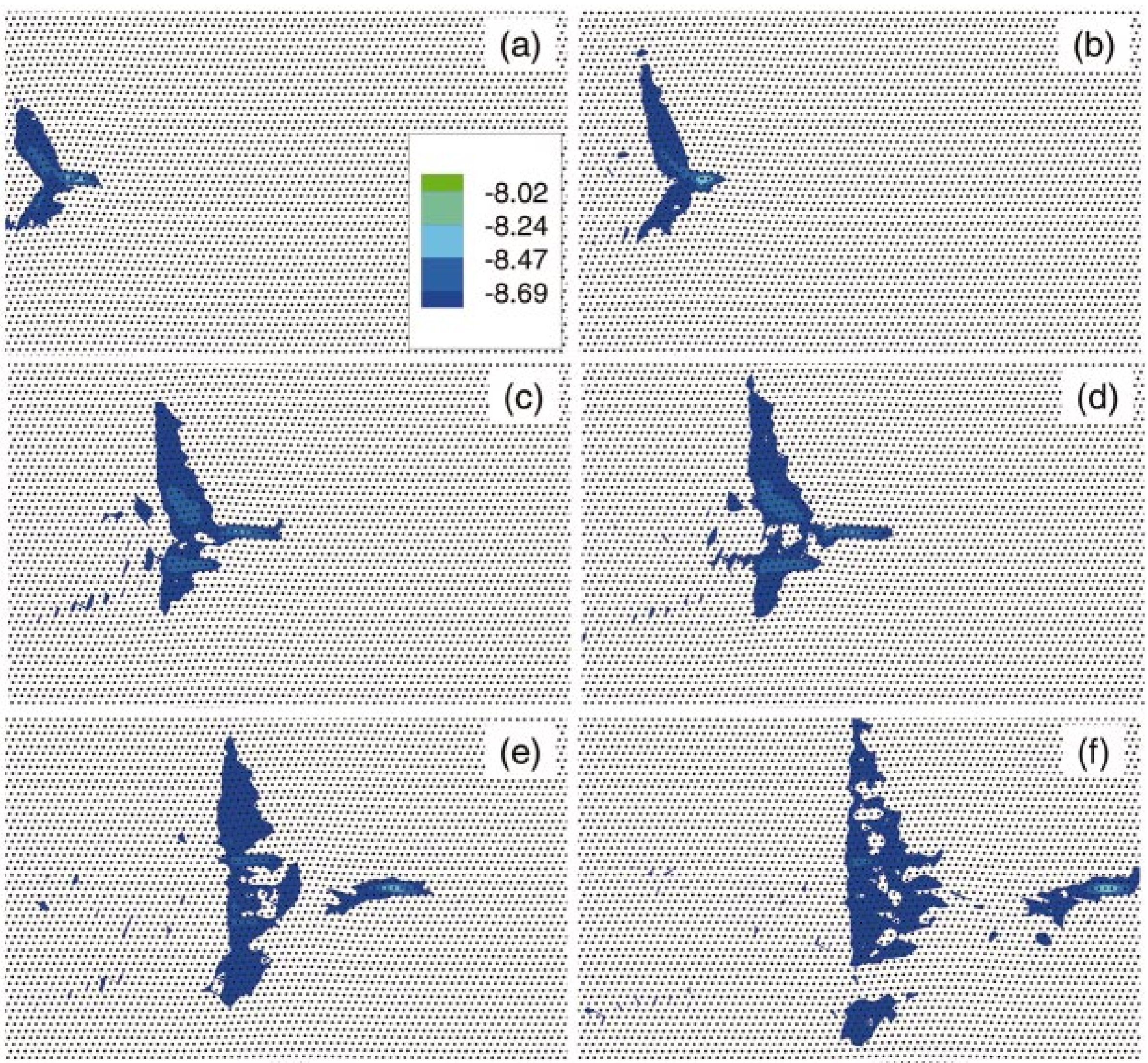


FIG. 3. (Color) Distribution of potential energy and atomic configuration around the dislocation core at (a) 17 ps, (b) 18 ps, (c) 19.6 ps, (d) 20 ps, (e) 21 ps and (f) 22 ps. The values in the figure legends are in units of eV.

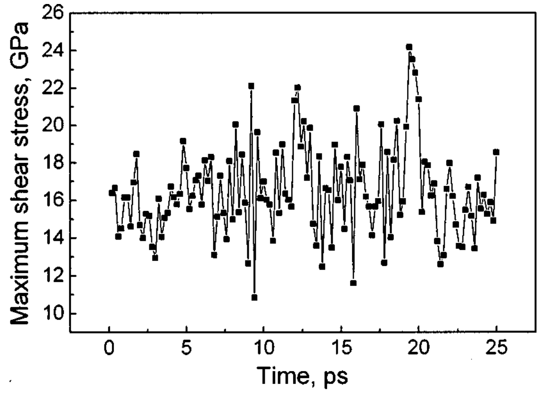


FIG. 4. Maximum shear stress at the dislocation core vs time; the points were taken every 0.2 ps.

dissociation of a perfect $\frac{1}{2}[111]$ dislocation into two partials of the type $\frac{1}{6}[111]$ and $\frac{1}{3}[111]$, or even three $\frac{1}{6}[111]$ partials, with stacking faults between them.[2] It is very likely that the total energy of the subsonic perfect $\frac{1}{2}[111]$ dislocation can reach a sufficiently high level as its speed approaches the sound barrier[1] so that it dissociates into a few transonic partial dislocations for a short moment. Later these partials recombine to form a transonic perfect dislocation again. In such a way the sound barrier is overcome. It is not absolutely clear due to resolution that the oscillation in dislocation velocity in Fig. 2 was all caused by oscillation between partials in a dumbbell fashion with the stacking faults acting as ''springs.''

As the dislocation jumped over the sound barrier and attained the longitudinal wave speed at about 20.6 ps, two pairs of shock wave fronts were observed as a Mach cone emanating from the moving dislocation. Figure 5 gives an example at 26 ps. These shock fronts correspond to two types of sound waves generated around the moving dislocation. In more general terms, ''signals'' carried by a supersonic dislocation travel faster than the speed of sound.

If the shear load is maintained until 34 ps (corresponding to a shear strain of 0.13), the crystal becomes unstable and some new dislocations pop up. These new dislocations can be explained by a kinematical mechanism of dislocation generation.[8]

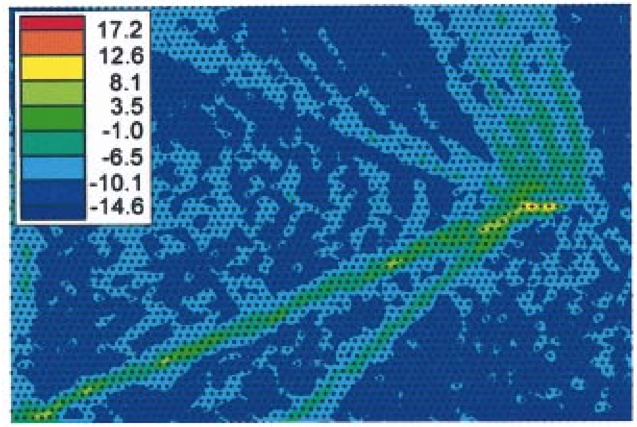


FIG. 5. (Color) Distribution of shear stress and atomic configuration around the dislocation core at 26 ps. The speed of the moving dislocation is about 6.4 km/s. The values of the figure legend are in units of GPa.

If the shear load is removed at 28 ps (i.e., to set the shear velocity$=0$), the supersonic dislocation will maintain its momentum and propagate at the supersonic wave speed for some time, and then suddenly jump back to $0.7\,C_T$. The dislocation will continue to travel at the $0.7\,C_T$ plateau for a much longer time until the shear strain of the crystal is released, and then finally relax to its normal equilibrium status—a stationary dislocation.

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