Dynamics of a dislocation bypassing an impenetrable precipitate: the Hirsch mechanism revisited

Takahiro Hatano
Earthquake Research Institute, University of Tokyo, Tokyo 113-0032, Japan.

(Dated: March 23, 2022)

PACS numbers: 81.40.Cd, 61.72.Bb, 62.20.Fe

Plastic flow in crystalline materials is mainly dominated by the movement of dislocations. They are curvilinear defects which can move at much lower stress levels than the theoretical strength of a perfect crystal [1]. A dislocation interacts with other lattice defects such as voids or precipitates, which obstruct the dislocation motion to result in hardening. Such dislocation-obstacle interactions dominate plasticity of crystalline materials, and hence they are one of the major concerns in materials science. Until very recently, they were considered exclusively by plausible continuum models [2, 3], which deal with a single glide plane and neglect atomistic discreteness. The recent computer development enables direct molecular dynamics (MD) simulation on dislocation systems, which consist of multi-million atoms. MD simulations have revealed dynamical properties and atomistic details of dislocations. For example, edge dislocations absorb vacancies when they interact with voids [4] or stacking fault tetrahedra [5]. They are good illustrations of the usefulness of MD simulation in the field of dislocation physics. Along the line of these studies, the interaction with an impenetrable precipitate, which has not been investigated by MD simulation, is explored in this Letter.

An interaction between a dislocation and a precipitate is characterized by their shear moduli. When the shear modulus of a precipitate is larger than the bulk’s, the interaction is repulsive so that the precipitate can be impenetrable [6]. In this case, the extent of hardening becomes significant. This is the principle of so-called “particle strengthening”, which is widely utilized in processing stronger materials [7]. There is a mechanism by which a dislocation bypasses impenetrable obstacles, where a dislocation largely bows out to leave a dislocation loop around the obstacle [1]. Note that the loop is on the original glide plane. This process and the resultant dislocation loop are referred to as the Orowan mechanism and an Orowan loop, respectively. However, because the interaction between an Orowan loop and a dislocation is strongly repulsive, theoretical calculations in which Orowan loops are assumed to be persistent predict unreasonably strong work-hardening [8, 9]. To avoid this contradiction, some alternative bypass mechanisms have been presented. Hirsch [10, 11] had pointed out the possibility of prismatic loops formation in a bypass mechanism. This mechanism is named after Hirsch and referred to as the Hirsch mechanism. On the other hand, Brown and Stobbs presented another mechanism where a dislocation loop of a secondary Burgers vector nucleates on the precipitate surface [12]. In both cases, the resultant structure is a row of prismatic loops which was experimentally observed by transmission electron microscopy (TEM) [13]. However, since the dynamical process cannot be observed by TEM, the postulated mechanisms have not been directly tested. In this Letter, we wish to clarify the dynamics of prismatic loops formation and to find out quantitative conditions which determine resultant dislocation loops: Orowan loops or prismatic loops. Along the line of thought, an MD simulation is performed. Let us describe the computational model. We consider fcc copper utilizing a many-body interatomic potential of Finnis-Sinclair [14] and adopt parameters which are determined by Ackland et al [15]. The lattice constant \( a = 3.615 \) Å. The dimensions of the model system are \( x = 23 \times [112] \) (20 nm), \( y = 79 \times [110] \) (40 nm), and \( z = 27 \times [111] \) (17 nm). This system consists of approximately 1.2 million atoms. (In addition to this system, we prepare some smaller systems which have different length in the \( x \) direction.) We introduce an edge dislocation parallel to the \( x \) axis, setting the Burgers vector to be parallel to the \( y \) axis. Note that we focus on an edge dislocation, since a screw dislocation can avoid a precipitate by switching its glide planes via cross-slip [14], which is not our interest here. An impenetrable precipitate is modeled by a set of immobile atoms, which are coherent to the bulk crystal. It mimics a precipitate of the infinite structure is a row of prismatic loops which was experimentally observed by transmission electron microscopy (TEM) [13]. However, since the dynamical process cannot be observed by TEM, the postulated mechanisms have not been directly tested. In this Letter, we wish to clarify the dynamics of prismatic loops formation and to find out quantitative conditions which determine resultant dislocation loops: Orowan loops or prismatic loops. Along the line of thought, an MD simulation is performed. Let us describe the computational model. We consider fcc copper utilizing a many-body interatomic potential of Finnis-Sinclair [14] and adopt parameters which are determined by Ackland et al [15]. The lattice constant \( a = 3.615 \) Å. The dimensions of the model system are \( x = 23 \times [112] \) (20 nm), \( y = 79 \times [110] \) (40 nm), and \( z = 27 \times [111] \) (17 nm). This system consists of approximately 1.2 million atoms. (In addition to this system, we prepare some smaller systems which have different length in the \( x \) direction.) We introduce an edge dislocation parallel to the \( x \) axis, setting the Burgers vector to be parallel to the \( y \) axis. Note that we focus on an edge dislocation, since a screw dislocation can avoid a precipitate by switching its glide planes via cross-slip [14], which is not our interest here. An impenetrable precipitate is modeled by a set of immobile atoms, which are coherent to the bulk crystal. It mimics a precipitate of the infinite shear modulus, which cannot be sheared by dislocations. Periodic boundary conditions are employed in the \( x \) and the \( y \) directions, and the surfaces exist only in the \( \pm z \) directions. In order to cause the shear strain, \((111)\) surface is displaced at a constant velocity. We test two cases, which are referred to as conditions I and II, respectively. In condition I, the upper \((+z)\) surface move towards the
FIG. 1: Successive snapshots of an edge dislocation bypassing an impenetrable precipitate. The radius of the precipitate (blue atoms) is 1.5 nm. A dislocation (red atoms) is visualized by omitting atoms which have 12 nearest neighbors. (a) A dislocation bows out to form a screw dipole. (b) The screw dipole cross-slips. (c) The screw dipole undergoes double cross-slip to annihilate each other at the top of the precipitate. (d) The dislocation has bypassed the precipitate with a superjog. A prismatic loop is left behind.

FIG. 2: Geometry of the primary cross-slip from (111) to (11̅1). (a) A [11̅1] projection. (b) A [111] projection.

Let us turn to the simulation results. First, we focus on the dynamics and the geometry. The configuration is shown in Fig. 1, where a dislocation does not leave an Orowan loop but two prismatic loops. At the first stage, a dislocation bows out to form a screw dipole of opposite signs. The main difference between the Orowan mechanism and the mechanism observed here lies in the behavior of this screw dipole. It cross-slips onto a (11̅1) plane (see FIG. 2), and then undergoes double cross-slip onto another (111) plane, on which the screw dipole eventually annihilates each other. In FIG. 1(d), a prismatic loop is formed on the left side of the precipitate and a superjog is formed on the opposite side. Then the superjog is dragged by the dislocation for a while, and is eventually separated to form the secondary prismatic loop as shown in Fig. 3(a). If the primary cross-slip takes place towards the extra atomistic half plane which constitutes the edge dislocation, the prismatic loop created before the precipitate is interstitial and the secondary loop after the precipitate is vacancy. (If the primary cross-slip goes opposite, the order is reversed). Note that the resultant prismatic loops have the same Burgers vector as that of the original edge dislocation. Indeed, this mechanism is identical to the Hirsch mechanism [11]. We stress that this is the first case where the Hirsch mechanism is dynamically observed, while TEM observations have detected only the resultant structures. Note that the mechanism of Brown and Stobbs [12] has not been observed in the conditions investigated here. More importantly, it is found that the Hirsch mechanism always occurs for the condition I, while the Orowan mechanism is realized for the condition II. To clarify the underlying physics, we have to investigate the quantitative aspect.

We investigate the critical resolved shear stress for the Hirsch mechanism, which we will call the “Hirsch stress”. The shear stress is defined as the area-averaged force acting on the surfaces. The Hirsch stress is defined as the maximum shear stress during a bypass process. It is realized just before the primary cross-slip, by which the Hirsch stress is determined. Behaviors of the Hirsch stress with respect to the precipitate radius and to the precipitate spacing are shown in Fig. 4, where we find the Hirsch stress is described by the following logarithmic law.

$$\sigma_{yz} = \frac{A}{L} \log \left( \frac{1}{0.5r^{-1} + L^{-1}} \right) B,$$

where $A$ and $B$ denote material-dependent parameters, $r$ is the radius of a precipitate, and $L$ is the precipitate spacing in the $x$ direction. Namely, $L = L_x - 2r$, where $L_x$ denotes the system size in the $x$ dimension. Note that $A = 6.5 \text{ N/m}$ and $B = 0.5 \text{ nm}$ in the present sys-
interrelated as the critical stress on the spacing of the precipitates, where
the line tension is estimated as \[\tau = \frac{\gamma}{\rho b}.\] (2)

Note that \(\gamma\) denotes the line tension, which depends on the configuration of a bending dislocation. When an edge dislocation bends to form a screw dipole at a pinning point, the line tension is estimated as \[\gamma = \frac{Gb^2}{4\pi} \log \frac{1}{B} \left( \frac{1}{2r} + \frac{1}{L} \right)^{-1}.\] (3)

Since a fully bending dislocation forms a semi-arc between two pinning points, the radius of curvature is \(\rho = L/2\). Inserting this relation and Eq. (3) into Eq. (2) immediately leads to the logarithmic law.

\[\tau = \frac{Gb}{2\pi L} \log \frac{1}{B} \left( \frac{1}{2r} + \frac{1}{L} \right)^{-1}.\] (4)

Although Eqs. (1) and (4) are of the same form, the quantitative discrepancy is considerable. Namely, \(Gb/2\pi = 1.96 \text{ N/m}\) in Eq. (1), while the corresponding factor in Eq. (4) is \(A = 6.5 \text{ N/m},\) which is three times larger than \(Gb/2\pi\). There are at least two reasons for this disagreement. The first is that dissociation of dislocations is not taken into account in deriving Eq. (1). It takes much more stress to bend two partial dislocations simultaneously \(\text{(a)}\). The second is the high dislocation density. Since the glide of a single dislocation causes large strain relaxation in small systems, the critical depinning stress may depend on the initial position of a dislocation in MD simulations.

Then we discuss the difference between the Hirsch and the Orowan mechanisms, both of which are realized in the present simulation depending on the boundary conditions. It should be remarked that the Orowan stress is almost the same as the Hirsch stress, and therefore we must refine the analysis. Recalling that the Hirsch mechanism is realized by displacing only the upper surface, inhomogeneity of the shear strain may play a key role. In order to see the inhomogeneity more explicitly, we calculate the average atomistic displacements in the \(y\) direction for each mechanism. We define

\[\delta y(z) = \frac{1}{n(z)} \sum_i [y_i(t) - y_i(0)] ,\] (5)

where the subscript \(i\) denotes the \(i\)-th atom. We take the sum regarding all the atoms that belong to the layer of \(z < z_i(t) < z + 1.89 \text{ A}\). Then \(n(z)\) is the number of atoms in the layer, and \(t\) is the time just before each bypass mechanism begins (i.e. when the shear stress becomes maximum.) FIG. 5 shows \(\delta y(z)\) for each mechanism. For the Hirsch mechanism, the gradient of \(\delta y\) is different with respect to the glide plane. Because the cross-slip which precedes the Hirsch mechanism occurs towards the larger stress region, it is concluded that the strong spatial inhomogeneity of the shear stress is essential to the Hirsch mechanism. This spatial inhomogeneity is attributed to the existence of the precipitate. Because the precipitate consists of immobile atoms, it inhibits the deformation caused by the boundary displacement. Therefore, if the

FIG. 4: The critical resolved shear stresses for the Hirsch mechanism (denoted by the red × symbols). Note that the Orowan stress is almost the same as the Hirsch stress. The green dashed lines represent Eq. (1) with \(A = 6.5 \text{ N/m}\) and \(B = 0.5 \text{ nm}\). (a) Dependence of the critical stress on the precipitate radius, where \(L_z = 20.4 \text{ nm}\). (b) Dependence of the critical stress on the spacing of the precipitates, where \(r\) is 1.5 nm.

FIG. 5: Spatial profiles of the average atomistic displacement in the \(y\) direction when the shear stress becomes maximum. The red solid line represents \(\delta y(z)\) for the Hirsch mechanism, while the green dashed line denotes that for the Orowan mechanism. The gradient of \(\delta y(z)\) for the Hirsch mechanism is asymmetric with respect to \(z = 95 \text{ A}\) (the glide plane). System parameters \(r = 1.5 \text{ nm}\) and \(L = 20.4 \text{ nm}\).
upper (or lower) surface is displaced, the elastic strain tends to localize on that side \[21\]. When the both surface is equivalently displaced, the elastic strain becomes symmetric to realize the Orowan mechanism. The above discussion further leads us to the speculation that Orowan loops become unstable for the larger shear strain. They can be decomposed into two prismatic loops via double cross-slip of the screw component, which is essentially the same manner as the Hirsch mechanism. For example, in the system shown in FIG. 5, the shear strain of 0.103 is enough to destabilize Orowan loops.

While the discussions so far involve a single bypass process, for the rest of this Letter, iteration of the Hirsch mechanism is briefly investigated. Namely, we consider the dynamics of subsequent dislocations which successively interact with a precipitate. It involves the relevance of the Hirsch mechanism to work-hardening. Although prismatic loops can move under an appropriate stress field (prismatic punching), they cannot move in the simple shear condition to be stagnant near the precipitate. However, they do not cause hardening since subsequent dislocations can easily penetrate them. For example, when \(L_x = 20.4 \text{ nm}\) and \(r = 1.5 \text{ nm}\), it takes less than 180 MPa for dislocations to penetrate prismatic loops, which is much smaller than the Hirsch stress itself, 560 MPa. Plastic flow is maintained by repetition of the Hirsch mechanism, which yields a row of prismatic loops as is shown in Fig. 3(b). This is what has been observed in the experiments \[11\] \[12\] \[13\]. By contrast, the loops on the right side of the precipitate do not form an apparent row. Because the prismatic loops move towards the \(+y\) direction (the left in FIG. 3) when they are sheared by dislocations, the loops on the \(-y\) (the right) side of the precipitate cannot move across the precipitate to collide each other there. This phenomenon may be related to plastic cavitation which is often observed near precipitates \[11\], and also to the rotational plastic flow around a nondeformable particle \[21\].

To conclude, the present study indicates that the dynamics of dislocation-obstacle interaction is much richer than considered before. Cross-slip plays the crucial role in a bypass mechanism which is quite different to the Orowan mechanism. We have clarified the condition that determines which bypass mechanism occurs. Namely, the shear stress which is asymmetric with respect to the glide plane causes cross-slip of the screw dipole and the Hirsch mechanism follows. Further development along the line of the present study will be the relevance of the Hirsch mechanism to macroscopic plasticity. A three-dimensional continuum approach, which is referred to as "dislocation dynamics", is now developing to compute the many-body dynamics of dislocations and obstacles \[22\]. It may be fruitful that the present results are suitably incorporated to such continuum approaches. In addition, it should be remarked that the dislocation dynamics is closely related to the interface dynamics in the quenched disorder, which is extensively investigated in the field of nonlinear physics \[23\]. Dislocation physics would be much richer in communication with the different research field.

The author gratefully acknowledges helpful discussions with Yuhki Satoh, Hideki Matsu, and Hideo Kaburaki.

[1] J. Friedel, Dislocations (Pergamon Press, Oxford, 1964).
[2] D. J. Bacon, U. F. Kocks, and R. O. Scattergood, Phil. Mag. 28, 1241 (1973).
[3] R. O. Scattergood and D. J. Bacon, Acta Metall. 30, 1665 (1982).
[4] Yu. N. Osetsky and D. J. Bacon, J. Nucl. Mater. 323, 268 (2003).
[5] B. D. Wirth, V. V. Bulatov, and T. Diaz de la Rubia, J. Eng. Mater. Tech. 124, 329 (2002).
[6] Although incoherency is an important ingredient that causes impenetrability in many alloy systems, we do not consider incoherent precipitates here.
[7] A. S. Argon, Physics of Strength and Plasticity (MIT Press, Cambridge, MA, 1969).
[8] M. F. Ashby, in Oxide Dispersion Strengthening, proceedings of the Second Bolton Landing Conference, Bolton Landing, New York, 1966, edited by G. S. Ansell, T. D. Cooper, and F. V. Lenel (Gordon and Breach, New York, 1968), p. 143.
[9] L. M. Brown and W. M. Stobbs, Phil. Mag. 23, 1185 (1971).
[10] P. B. Hirsch, J. Inst. Metals 86, 7 (1957).
[11] F. J. Humphreys and P. B. Hirsch, Phil. Mag. 318, 73 (1970).
[12] L. M. Brown and W. M. Stobbs, Phil. Mag. 23, 1201 (1971).
[13] A. M. Wusatowska-Sarneck, H. Miura, and T. Sakai, J. Mater. Sci. 34, 5477 (1999).
[14] Although edge dislocations can also avoid impenetrable precipitates by the local climb motion, this process requires long-range self-diffusion and is irrelevant to materials at room temperatures.
[15] M. W. Finnis and J. E. Sinclair, Phil. Mag. A 50, 45 (1984).
[16] G. J. Ackland, D. J. Bacon, A. F. Calder, and T. Harry, Phil. Mag. A 75, 713 (1997).
[17] J. Li, Modelling Simul. Mater. Sci. Eng. 11, 173 (2003).
[18] T. Hatano and H. Matsui, Phys. Rev. B 72, 094105 (2005).
[19] Y. Satoh, T. Yoshiie, H. Mori, and M. Kiritani, Mater. Sci. Eng. A 350, 44 (2003).
[20] L. M. Brown, Phil. Trans. R. Soc. Lond. A 355, 179 (1997).
[21] Although the model precipitate of immobile atoms is somewhat artificial, the asymmetric shear stress may be realized if other lattice defects exist near the precipitate, such as dislocations or grain boundary.
[22] H. M. Zbib, M. Rhee, J. P. Hirth, and T. D. de La Rubia, J. Mech. Behavior Mater. 11, 251 (2000).
[23] M. Kardar, in Fundamental Problems in Statistical Mechanics, edited by H. van Beijeren, Phys. Rep. 301, 85 (1998).