Nucleation and propagation of dislocations near a precipitate using 3D discrete dislocation dynamics simulations

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Abstract. A 3D dislocation dynamics code linked to the finite element procedures is used to simulate the case of a matrix containing a cubical precipitate. Since the matrix and the precipitate do not have the same elastic moduli and thermal expansion coefficients, a heterogeneous stress field is generated in the whole volume when the sample is submitted to a temperature change. In many cases this may nucleate dislocations in the matrix as experimentally observed. Here, the phenomenon of dislocations nucleation in the matrix is simulated using dislocation dynamics and the first results are presented. In a first time, a glissile loop has been put surrounding a precipitate. The equilibrium position of the glissile loop is investigated in terms of the image stress field and the line tension of the loop. In a second time, the dislocations are introduced as a prismatic loop admitting a Burgers vector perpendicular to the plane containing the loop. The prismatic loops are moving in the sample according to the heterogeneous stress field resulting from the summation of the internal stress field generated by the dislocations and the stress field enforcing the boundary conditions, which is computed by the finite element method. The latter takes into account the presence of the precipitate as well as the interactions between the precipitate and the dislocations. The equilibrium configuration of the rows of prismatic loops is analysed and the spacing of loops is compared to the analytic solution.

1. INTRODUCTION

Since the prismatic punching model was first described by Seitz [1], dislocation generation phenomena around precipitates or artificially produced particles have been studied both experimentally and theoretically. Dislocations produced around precipitates can affect physical properties of two-phase materials, that is, the structure of the dislocations around precipitates affects the subsequent deformation of the two-phase materials and the generated dislocation changes the strain energy of the system.

Experimentally, it has been observed that stresses induced by differential thermal expansion or volume change of a precipitate can generate dislocations around the precipitate. The generation of dislocations can relieve the stresses and reduce the total system energy. The investigations showed that prismatic dislocation loops [2-4], dislocation climb sources [5] and dislocation tangles [6] formed around a precipitate.

The generation of prismatic loops has been studied with respect to the energy or the stress of the system. Critical radius of the precipitate to generate the prismatic dislocation loop was considered on the condition that the energy of the system should decrease if the prismatic loop is generated [7] and critical stress was proposed as a necessary condition for the prismatic loop generation [8]. It was suggested that spacing of the loops relates to the diameter of adjacent loops and that the critical shear stress to move the loop can be deduced from the measured spacing of loops [9]. All the theoretical approaches above have been based on the linear, isotropic, elastic solution, and the interaction between dislocation loops and between the precipitate and the loop was approximated because of the complexity of the stress field involved.

3D discrete dislocation dynamics (DDD) simulation has proven to be a powerful numerical tool to investigate the plasticity of single crystals [10,11]. And complex boundary conditions can be applied to the DDD simulation code by coupling the code to the finite element method (FEM) [12,13]. It is possible to calculate long-range elastic interactions of dislocation loops and image stresses on the loops by a free surface numerically.
The aim of this work is to present a calculation of image stresses due to a precipitate by using the DDD-FEM code and to present the first results of nucleation and subsequent propagation of dislocation loops near a precipitate. Two physical situations are investigated. First, an equilibrium position of a glissile loop around a cubical precipitate is investigated by considering the line tension of the loop and the image stress field between the precipitate and the loop. And second, a spacing of several co-axial prismatic loops is calculated when the loops are nucleated in the vicinity of the precipitate and the result is compared to the experimental observations and the analytic approach.

2. DESCRIPTION OF SIMULATION MODEL

2.1 3D Discrete Dislocation Dynamics

The DDD simulation involves a discretization of dislocation line, which is a continuous curve in reality, as discrete dislocation segments of edge and screw type. The discrete segments move on the simulation network similar to the crystal lattice but larger in lattice spacing. In FCC metals, edge dislocation segment with <112> line direction and <110> Burgers vector glides in direction of Burgers vector and screw segment with <110> line direction glides on possible two slip planes in direction of <112> vector. Details of discretization of the dislocation lines can be found in [12]. The dislocation segments move according to a resolved shear stresses acting on it. The resolved shear stress on each segment comes from three different components:

i) the applied stress field \( \sigma_{\text{app}} \) which is a summation of internal stress field \( \sigma \) produced by all the other dislocation segments present and stress field \( \sigma \) compensated for the boundary conditions,

ii) the lattice frictions due to the Peierls forces on the segment \( \tau_{\text{Peierls}} \),

iii) the line tension stresses of dislocation lines \( \tau_l \).

The effective resolved shear stresses \( \tau \) on the segment with the unit Burgers vector \( b \) and the unit line vector \( l \) is calculated with these stresses.

\[
\tau = [(\sigma_{\text{app}}) \cdot b \cdot l] \cdot b + \tau_l - \tau_{\text{Peierls}} \tag{1}
\]

The applied stress \( \sigma_{\text{app}} \) is calculated using the superposition principle [12] and decomposed into two parts (see Figure 1.)

\[
\sigma_{\text{app}} = \sigma + \sigma \tag{2}
\]

\( \sigma \) is the internal stress field by dislocation segments that are assumed to be in infinite medium and \( \sigma \) is the complementary solution which is purely elastic solution of dislocation-free volume with imposed boundary conditions modified by the forces and the displacements generated by the dislocations in the volume on the corresponding boundaries. The calculation of the internal stress \( \sigma \) is based on the De Wit formula and the simplified formula can be found in [14]. \( \sigma \) is calculated using the finite element method. The method to incorporate the image stress by a precipitate to dislocations is detailed in subsection 2.2. The line tension stress \( \tau_l \) is computed with the local curvature of the dislocation line

\[
\tau_l = \frac{\alpha G b}{R} \tag{3}
\]

where \( G \) is the shear modulus of a medium, \( b \) is the magnitude of Burgers vector, \( R \) is the local curvature radius and \( \alpha \) is the parameter set to be 0.63.

The velocity of dislocation segments \( v \) is related to the resolved shear stress \( \tau \) and the phonon drag coefficient \( B \).

\[
v = \frac{\tau b}{B} \tag{4}
\]
For each simulation time step, the velocity of each segment is calculated and the glide distance of the segment is determined from the calculated velocity and time step $\delta t$.

During the movement of dislocation segments, each segment can meet another segment. Several local rules are adapted to account for the local interaction of dislocation segments, such as junction formation, annihilation and cross-slip of screw dislocation segments. The parameters for such local phenomena, such as junction strength and probability of cross-slip, are adapted from experimental observations [10,12].

### 2.2 Image stresses by precipitate

The presence of free surfaces and precipitates induces image stresses on dislocations. The image stresses by the free surface could be computed from the fact that the free surface is traction free. The forces by the dislocations in the volume are computed onto the free surface, and appropriate point forces are applied to compensate for these forces [15].

In case of a precipitate, stresses and displacements should be continuous across the boundary between the precipitate and the matrix. One possible method to calculate the image stresses by the precipitate is again using the decomposition of the problem into the problem of dislocations in infinite medium and the complementary problem of finite dislocation-free volume, which, in this case, consists of the matrix and the precipitate. The extension of decomposition of the problem to two-phase problem was performed by E. van der Giessen et al. [16] and applied to 2D problem. The method of calculation of the complementary problem using FEM is briefly described here. The stresses by dislocations on the points in the volume representing the precipitate, e.g. stress integration Gauss points, are calculated and the so-called polarization stresses $(L' : L') : \sigma$ are computed using the fourth-order stiffness tensor of the matrix $(L)$ and the precipitate $(L')$. $I$ is the fourth-order unit tensor and $\sigma$ is the stresses at the stress integration points of precipitate meshes. The calculated polarization stresses are changed to nodal force fields and these forces are applied to the volume representing the precipitate.

The complementary inhomogeneous problem that incorporates the image stresses between the precipitate and the dislocations is solved using the finite-element code CASTEM2000 developed at the Commissariat à l’Energie Atomique of Saclay (France).

![Figure 1. Decomposition of the problem into the problem of dislocations in infinite media and the complementary problem of inhomogeneous finite volume without dislocations](image)

### 3. MODELLING OF DISLOCATION LOOPS AND A PRECIPITATE

#### 3.1 Materials

Aluminium matrix containing a cubical silicon carbide particle is considered. The elastic constants of the aluminium are set to 27GPa for the shear modulus $(G)$ and 0.347 for the Poisson ratio. The thermal expansion coefficient $(\alpha)$ is set to be $23.6 \times 10^{-6} \text{K}^{-1}$. The shear modulus of a particle $(G^p)$ is $6.4 \times G$, and Poisson’s ratio is 0.19. The thermal expansion of particle $(\alpha^p)$ is set to 0.2 times the thermal expansion coefficient of the matrix. The magnitude of Burgers vector is 2.86 Angströms for the aluminium.
3.2 Geometry and initial configuration of dislocations

In Figure 2(a), a cubic with a side length of 3 µm is meshed with 8-nodes three-dimensional elements. The cubical particle with a side length of 0.6 µm is meshed at the centre of the matrix. The mesh is refined near to the boundary of the particle so that the high gradient of stress field near the particle can be represented correctly. The displacement of bottom surface is set to be zero in normal direction of the surface in order to remove the trivial rigid body solution and there are no specific boundary conditions on the other surfaces.

To investigate the equilibrium position of a dislocation loop, a glissile loop is put around the precipitate. The line tension of the loop will make the loop shrink and the image stress will force back the loop from the precipitate. The balance of these two stresses will determine the equilibrium position of the dislocation loop. Figure 2(b) shows the initial configuration of the loop with Burgers vector of [-101] and the precipitate seen at the direction of (1-11).

Secondly, prismatic dislocation loops are put near to the precipitate to calculate the equilibrium spacing of the prismatic loops. The Burgers vector of the prismatic loop is [-101] and the segments of each prismatic loop lie on the active glide systems. The size of the prismatic loop is about 0.5 µm in Figure 2(c).

3.3 Propagation of dislocation segments

The image force by the precipitate is calculated for every step of dislocation movement and the resulting heterogeneous stress field is computed. The resolved shear stress on each dislocation segment is calculated using the interpolated stress through polynomial functions and the internal stress between dislocation segments. The simulation stops if there is no significant change in the configuration of dislocation segments.

![Figure 2](image.png)

Figure 2. (a)-Meshes of the two-phase material (half view). (b)-Glissile loop and the cubical precipitate (seen along direction (1-11)). (c)-Two prismatic loops at the vicinity of the precipitate

4. RESULTS

4.1 A glissile loop around a cubical precipitate

A glissile loop is put around a cubical precipitate as shown Figure 2(b). The loop has the segments with the screw line direction of [-101] and the edge line direction of [121], two of the segments are edge types and the others are screw types. The initial segments length for the loop is approximately 1.3 µm. No specific boundary condition is applied except for the image force between the precipitate and the
The aim of this work is to present a calculation of image stresses due to a precipitate by using the DDD-FEM code and to present the first results of nucleation and subsequent propagation of dislocation loops near a precipitate. Two physical situations are investigated. First, an equilibrium position of a glissile loop around a cubical precipitate is investigated by considering the line tension of the loop and the image stress field between the precipitate and the loop. And second, a spacing of several co-axial prismatic loops is calculated when the loops are nucleated in the vicinity of the precipitate and the result is compared to the experimental observations and the analytic approach.

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i) the applied stress field \( \sigma_{\text{app}} \) which is a summation of internal stress field \( \tilde{\sigma} \) produced by all the other dislocation segments present and stress field \( \tilde{\sigma} \) compensated for the boundary conditions,

ii) the lattice frictions due to the Peierls forces on the segment \( \tau_{\text{Peierls}} \),

iii) the line tension stresses of dislocation lines \( \tau_h \).

The effective resolved shear stresses \( \tau \) on the segment with the unit Burgers vector \( b \) and the unit line vector \( l \) is calculated with these stresses.

\[
\tau = [(\sigma_{\text{app}} \cdot b^\alpha l) \cdot b + \tau_h - \tau_{\text{Peierls}}]
\] (1)

The applied stress \( \sigma_{\text{app}} \) is calculated using the superposition principle [12] and decomposed into two parts (see Figure 1.)

\[
\sigma_{\text{app}} = \tilde{\sigma} + \bar{\sigma}
\] (2)

\( \tilde{\sigma} \) is the internal stress field by dislocation segments that are assumed to be in infinite medium and \( \bar{\sigma} \) is the complementary solution which is purely elastic solution of dislocation-free volume with imposed boundary conditions modified by the forces and the displacements generated by the dislocations in the volume on the corresponding boundaries. The calculation of the internal stress \( \tilde{\sigma} \) is based on the De wit formula and the simplified formula can be found in [14]. \( \bar{\sigma} \) is calculated using the finite element method. The method to incorporate the image stress by a precipitate to dislocations is detailed in subsection 2.2.

The line tension stress \( \tau_h \) is computed with the local curvature of the dislocation line

\[
\tau_h = \frac{\alpha G b}{R}
\] (3)

where \( G \) is the shear modulus of a medium, \( b \) is the magnitude of Burgers vector, \( R \) is the local curvature radius and \( \alpha \) is the parameter set to be 0.63.

The velocity of dislocation segments \( v \) is related to the resolved shear stress \( \tau \) and the phonon drag coefficient \( B \).

\[
v = \frac{\tau b}{B}
\] (4)
On the basis of the experimental observations, several square prismatic loops with the segments 0.424 \( \mu\text{m} \) long in [121] and [-12-1] direction have been generated on the (-101) plane near the cubical precipitate with the side length of 0.6 \( \mu\text{m} \). The centre position of the nucleation point is chosen to be at the distance of \( \sqrt{3}/\sqrt{2} \) times the half side length of the precipitate from the centre of the precipitate [18].

The matrix and the precipitate are assumed to be subject to temperature change of -50\(^\circ\)C, which corresponds to the stress-free strain of 0.945\(\times10^{-3}\), and the resulting thermal stress is remained constant through the simulation. After one prismatic loop is nucleated, the image stress field is calculated and the loop glides along the glide cylinder for \( N_{\text{move}} \) steps. The image stress field is calculated at every step. Another prismatic loop is nucleated at the same nucleation position, and now two loops glide for \( N_{\text{move}} \) steps. New loop is nucleated at every \( N_{\text{move}} \) step and total ten prismatic dislocation loops are nucleated successively. The number of emitted prismatic dislocation loops should be determined from a criterion of minimization of elastic energy, but in this study ten loops are emitted so that the result is compared with the analytic solution [9].

The analytic solution of equilibrium positions of ten loops is presented in Figure 4 for the value of dimensionless parameter \( \nu \) given in equation (5). In analytic solution, the stress field of a single prismatic loop was derived and only the interaction with first and second neighbours was considered to compute the shear stress of the loop. The critical shear stress \( \tau_{\text{crit}} \) to move the loop was set as the parameter to determine the final configuration.

\[
\nu = \frac{4\pi(1-v)}{bG} \tau_{\text{crit}}
\]

(5)

Here \( r \) is the loop radius, \( b \) is the Burgers vector magnitude, \( v \) the Poisson's ratio and \( G \) the shear modulus of the matrix material.

In DDD calculation, the value of \( \tau_{\text{crit}} \) is assumed to be equal to \( \tau_{\text{Points}} \) because the nucleated prismatic loop has four segments although each segment is discretized to several segments during subsequent gliding. The value of \( \tau_{\text{Points}} \) has been changed to 2.24MPa(8.3\(\times10^{-5}\)G), 1.13MPa(4.2\(\times10^{-5}\)G), and 0.224MPa(0.83\(\times10^{-5}\)G), which are supposed to correspond to \( \nu = 0.5 \), \( \nu = 0.25 \) and \( \nu = 0.05 \) respectively. The equilibrium configuration of ten loops is calculated considering the image stresses, the internal stresses by all prismatic loops and the thermal stresses. The calculated loop spacing ratio (0.5\(\times\pi/r \)) of the loops is represented in Figure 4, where loop number 1 is the closest loop to the precipitate in a given row of loops. The trend of change of loop spacing ratio calculated by DDD-FEM is similar to that of the analytic solution, that is, as the critical shear stress to move a loop decreases, the spacing between adjacent loops increases as shown in Figure 5 and also the loop spacing ratio increases.

![Figure 4. Variation in loop spacing ratio for ten prismatic dislocation loops. (Solid symbols: DDD-FEM results. Line symbols: analytic solution [9])](image-url)
In the results of DDD-FEM, the variation of loop spacing ratios of number one and number two is smaller than that of the analytic solution. It is because there are thermal stresses and the image stresses around the precipitate in case of DDD-FEM calculation. The heterogeneous stress field around the precipitate pushes first loop away from the precipitate and as a result, the shape of the curve obtained by DDD-FEM calculation is different significantly at the low number loop from the curve obtained by analytic solution.

If it is assumed that the critical shear stress is equal to \( \tau_{\text{Peierls}} \), the curve with circle symbol in Figure 4 corresponds to the value of \( \nu = 0.25 \). The difference between the analytic result and the DDD-FEM result of \( \nu = 0.25 \) case can be explained with the fact that in the analytic solution, the resultant shear stress of a loop is determined from the interactions of its first and second neighbour loops. This assumption is based on the fact that the stress field of a loop decreases rapidly. But as mentioned in [9], when the critical shear stress is high, the loops become closely spaced. In this case, the analytic solution based on the assumption mentioned above will be different to the results, which calculate the interactions of all the loops. And the reason of difference can also be attributed to the assumption that the critical shear stress is equal to \( \tau_{\text{Peierls}} \). For example if it is assumed that the critical shear stress is set to \( 1.5 \times \tau_{\text{Peierls}} \), the results of DDD-FEM calculation is comparable to the analytic solution. And thermal stresses and image stresses are not taken into account in the analytic solution. But the effects of these stresses are expected to be short ranged because the image stresses and thermal stresses decreases rapidly as the distance from the centre of the precipitate increases. The equilibrium configurations of ten loops in each case are shown in Figure 5. The loop in the centre of the cubic represents the nucleation position of prismatic dislocation loop.

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\[ \begin{array}{ccc}
\text{(a)} & \text{(b)} & \text{(c)} \\
\end{array} \]

**Figure 5.** Equilibrium configurations for row of ten loops with \( \tau_{\text{Peierls}} \) of (a) \( 8.3 \times 10^{-5} \)G (b) \( 4.2 \times 10^{-5} \)G (c) \( 0.83 \times 10^{-5} \)G

5. CONCLUSIONS AND PERSPECTIVES

The image stresses between dislocations and a precipitate have been calculated based on the formulation proposed in [16] using DDD-FEM code. Interaction between dislocations and a cubical precipitate are presented.

The equilibrium position of a glissile dislocation loop around a precipitate has been investigated by accounting for the image forces. The magnitude of the shear image stress is comparable to the analytic solution of infinite screw dislocation near an internal interface. It is found that the stress field around the precipitate only by the image force is large enough to stop the glissile loop from shrinking by its line tension. This shows that the gliding dislocation can be stopped near the hard particle or precipitate by the image stresses and explains one of the mechanisms of hardening by precipitates or particles.

Several prismatic dislocation loops are nucleated near the cubical precipitate and the spacing of the loops is computed. A criterion for the generation of the loop is not taken into account and only the spacing of the loops by the image force is considered. The size and the position of the nucleated loop are determined from experimental observations. Bullough and Newman [9] have formulated the spacing of circular prismatic loops, and the calculated loop spacing ratio is compared to their results. The trend of loop spacing ratio calculated by DDD-FEM is comparable to the result of analytic solution, and
differences of two results can be attributed to the image stress fields and thermal stresses. The significant
differences of two methods when the value of $u$ increases are attributed to the fact that the assumption of
considering only first and second neighbour loops cannot be justified when the loops are closely spaced,
and that the definition of the critical shear stress to move a loop is ambiguous.

This work will be extended to a different shape of precipitate and an interface separating two
materials of differing elastic constants, such as hard coatings at the surface of thin films. In the future, the
full scale simulation of the nucleation and propagation of prismatic dislocation loops near a particle will
be analysed in terms of stress field and strain energy and be compared to the experimental transmission
electron microscopy observations.

References