Green's function molecular dynamics meets discrete dislocation plasticity

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Abstract. Metals deform plastically at the asperity level when brought in contact with a counter body even when the nominal contact pressure is small. Modeling the plasticity of solids with rough surfaces is challenging due to the multi-scale nature of surface roughness and the length-scale dependence of plasticity. While discretedislocation plasticity (DDP) simulations capture size-dependent plasticity by keeping track of the motion of individual dislocations, only simple two-dimensional surface geometries have so far been studied with DDP. The main computational bottleneck is the description of the elasticity-mediated interactions of dislocations with each other and with the prescribed boundary conditions. We address this issue by combining two-dimensional DDP [1] with Green's function molecular dynamics (GFMD) [2]. The resulting method allows for an efficient boundary-value-method based treatment of elasticity in the presence of dislocations. We demonstrate that our method captures plasticity quantitatively from single to many dislocations and that it scales more favorably with system size than conventional methods. We also derive the relevant Green's functions for elastic slabs of finite width allowing arbitrary boundary conditions on top and bottom surface to be simulated.

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1. Introduction

Modeling the contact mechanics of solid bodies assuming realistic surface roughness is highly relevant to tribology, the science of friction. It is found experimentally that metallic surfaces have roughness covering many decades of length scales and exhibit self affinity within length scales ranging from 100 μ m to 50 nm [1,2]. In the past years, various theories of rough surface contact have been presented [3,4], the most notable of which being Persson's theory [4–6]. The main improvement of Persson's theory compared with classical theories of the past century, like Greenwood and Williamson's [7], is that it accounts for long-range elastic interactions. It accurately predicts contact stress distributions, contact areas and gap functions for frictionless as well as adhesive contacts, in good agreement with experiments as well as simulations. However, the validity of Persson's analysis of plastic contacts [5] in the range where plasticity is size-dependent [8–11] has not yet been shown.

Numerical simulations of contact between rough surfaces are made possible through several techniques. Of particular interest are the boundary-element based approaches [12, 13] such as Green's function molecular dynamics (GFMD) [14–18], which calculate the response of a solid to contact loading by modeling only the surface. These methods are suitable to study large systems where the surface roughness can be described by many orders of length scale [16, 19, 20]. Additionally, GFMD has the advantage that it can be extended to a multi-scale method [21] where the surface layer can be described atomistically and the body underneath can be treated with harmonic approximation. Pastewka *et al.* [21] have shown that the GFMD coefficients can be quickly computed from interatomic potentials and a seamless coupling to the atomic region can be derived even for interactions going beyond nearest-neighbor interactions. GFMD has been successfully used to model the contact response of semi-infinite elastic solids [20, 22, 23], while plasticity was neglected.

Size-dependent plasticity in metal crystals has been successfully predicted by discrete dislocation plasticity (DDP) [24] simulations, which for simple problems, as the tensile response of free-standing metal films, give results in quantitative agreement with experiments [25]. In the context of contact mechanics, DDP has been used to study indentation of flat surfaced single crystals with single indenters [26, 27], periodic indenters [28, 29], as well as an indenter with self-affine surface modeled as a collection of Hertzian contacts [30]. The only DDP studies, in which the plastically deforming bodies were not approximated to be flat, involved the flattening of simple sinusoidal surfaces [31–33]. Results showed that the contact area increases in a patchy fashion, due to the discreteness of the dislocations exiting the surface and as a consequence the local contact pressure presented high spikes, at odds with the pressure profiles predicted by classical plasticity. The study of size-dependent plasticity for realistic surface geometries is computationally very expensive. To overcome this limitation we here combine the accurate description of plasticity offered by DDP with the fastly converging elastic solution delivered by GFMD, in a modeling technique which we name Green's function dislocation dynamics (GFDD).

We begin the paper by briefly introducing DDP in section 2 and GFMD in section 3. We then present the methodology of the new model in section 4. The results obtained using the new GFDD model are compared with DDP in section 5 and 6. Section 7 summarizes the advantages and potential of the new model.

2. Discrete dislocation plasticity

Discrete dislocation plasticity is a numerical technique to solve boundary-value problems (b.v.p), which treats plasticity as the collective motion of discrete dislocations [24]. The

dislocations are modeled as line defects in an elastic continuum. The solution at each time step of the simulation is obtained by the superposition of two linear elastic solutions: The elastic fields for dislocations in a homogeneous infinite solid, and the solution to the complementary elastic b.v.p., which corrects for the boundary conditions. The methodology is illustrated for the indentation of a single crystal by an array of flat rigid indenters in figure 1. The elastic dislocation fields are represented by a superscript (^d), the fields solving the complementary b.v.p. by a superscript (^). The elastic dislocation fields are given analytically. The solution to the b.v.p. is traditionally obtained using the finite-element method FEM. The rigid indenter is modeled implicitly by imposing boundary conditions on the deformable body.



Figure 1: Schematic representation of the DDP methodology: The boundary-value problem for a body containing dislocations is decomposed into two parts: the fields of the dislocations in an infinite medium and the solution to the elastic boundary-value problem which corrects for the boundary conditions.

The total stress and displacement fields obtained at a given time increment are used along with a set of constitutive rules for dislocation nucleation, dislocation motion, dislocation annihilation and pinning of dislocation at obstacles to determine the plastic behavior of the solid. Dislocations can exit the domain through the free surface leaving behind a displacement step of $\pm b/2$ along the slip direction at the surface, where b is the magnitude of the Burger's vector.

The aim of this work is to replace the FEM solution to the complementary b.v.p. with GFMD, while the constitutive rules that control the dislocation dynamics remain unchanged.

3. Green's function molecular dynamics

GFMD is also a boundary-value method to study the elastic response of a body subjected to contact loading [20]. In GFMD, only the surface of the deformable body is modeled explicitly and discretized using equi-spaced grid points as seen in figure 2. The unknown surface displacement field $\tilde{\boldsymbol{u}}(q) = (\tilde{u}_1(q), \tilde{u}_3(q))$ for each mode with wavenumber q are calculated in Fourier space and hence the different modes are uncoupled.



Figure 2: Schematic representation of the boundary-value problem studied using GFMD.

The elastically deformable body represented by the system of grid points is loaded by a rigid indenter that is not modeled explicitly, but its effect is included by means of a hard-wall potential. To satisfy static equilibrium the following condition must hold:

$$\tilde{\boldsymbol{F}}^{\text{ext}}(q) + \tilde{\boldsymbol{F}}^{\text{el}}(q) + \tilde{\boldsymbol{F}}^{\text{if}}(q) = 0, \qquad (1)$$

where $\tilde{\boldsymbol{F}}^{\text{ext}}(q)$ is the external force and $\tilde{\boldsymbol{F}}^{\text{if}}(q)$ is the interfacial force ensuring the nonoverlap constraint, which are imposed "by hand" after each time step. $\tilde{\boldsymbol{F}}^{\text{el}}(q)$ is the elastic restoring force, which can be written as:

$$\tilde{\boldsymbol{F}}^{\mathrm{el}}(q)/A_0 = \tilde{\boldsymbol{G}}^{-1}(q)\tilde{\boldsymbol{u}}(q) = \nabla_{\tilde{\boldsymbol{u}}} v_{\mathrm{el}}.$$
(2)

Here, A_0 is the total surface area and $\tilde{\boldsymbol{G}}^{-1}(q)$ is the inverse Green's function, the evaluation of which involves the knowledge of the areal elastic energy density $v_{\rm el}$.

The condition for static equilibrium is reached by means of damped dynamics, where a damping force of the form:

$$\tilde{\boldsymbol{F}}^{\text{damp}}(q) = \eta(\tilde{\boldsymbol{u}}^{n-1}(q) - \tilde{\boldsymbol{u}}^n(q))$$
(3)

is used in the position-Verlet algorithm to solve for the displacement fields at each increment (n + 1),

$$\tilde{\boldsymbol{u}}^{n+1}(q) = 2\tilde{\boldsymbol{u}}^n(q) - \tilde{\boldsymbol{u}}^{n-1}(q) + \left(\tilde{\boldsymbol{F}}^{\text{el}}(q) + \tilde{\boldsymbol{F}}^{\text{ext}}(q) + \tilde{\boldsymbol{F}}^{\text{damp}}(q)\right)\tau^2,$$
(4)

where τ is the discrete time step used in the simulation.

The hard-wall potential is employed at the end of each iteration to ensure there is no inter-penetration, i.e., in real space,

$$z_{\text{punch}}(x) \le z_{\text{substrate}}(x),$$
 (5)

where z_{punch} and $z_{\text{substrate}}$ are the z- coordinates of the punch and substrate surface, respectively. Notice that the method is not bound to use a hard-wall potential. Finiteinteractions can be accounted for, however, we have here chosen for a hard-wall potential for the sake of comparison to conventional DDP.

When the surface equilibrates to the final deformed configuration, the body fields are calculated from the discrete surface fields using closed-form analytical solutions [34].

4. Green's function dislocation dynamics

The Green's function dislocation dynamics method is based on the same decomposition concept as used in DDP except that, now, the image fields are found using GFMD instead of FEM. The methodology is schematically presented in figure 3.



Figure 3: Decomposition of the problem for the dislocated body similar to figure 1 except for the complementary problem, which is solved using GFMD.

When solving the complementary b.v.p., both tractions and displacements caused by the dislocations on the top and bottom boundary of the body need to be simultaneously prescribed at a given time increment. Tractions are imposed in Fourier space as described in the previous section by using $\hat{t}(q)$ as external force $\tilde{F}^{\text{ext}}(q)$ before stepping forward in time. Here $\hat{t}(q)$ is the Fourier transformation of the discontinuous function $\hat{t}(r)$ at point r = (x, z):

$$\hat{\boldsymbol{t}}(\boldsymbol{r}) = \boldsymbol{t}(\boldsymbol{r}) - \boldsymbol{t}^{\mathrm{d}}(\boldsymbol{r}) \qquad \text{if } \boldsymbol{r} \in S_{\mathrm{t}}, \\
\hat{\boldsymbol{t}}(\boldsymbol{r}) = 0 \qquad \qquad \text{if } \boldsymbol{r} \in S_{\mathrm{u}},$$
(6)

where S_t and S_u are traction- and displacement-prescribed boundaries, respectively. Unlike tractions, displacements are imposed in real space by setting the equilibrium position of the hard-wall to the required position:

$$\hat{\boldsymbol{u}}(\boldsymbol{r}) = \boldsymbol{u}(\boldsymbol{r}) - \boldsymbol{u}^{\mathrm{d}}(\boldsymbol{r}) \quad \text{if } \boldsymbol{r} \in S_u.$$
 (7)

The hard-wall is not applied to the boundaries where traction is prescribed S_t .

Notice that the elastic energy required for the evaluation of the Green's function, which is needed in the calculation of the restoring elastic force, was derived in [34] but only for the case of an isotropic slab with an undulated top layer and a fixed bottom. This allows a b.v.p. to be solved for a mixed boundary condition at the top, however, with the restriction of the bottom displacement to be zero. Here, however, we need to impose mixed boundary conditions also at the bottom. To this end, the areal elastic energy is required for a solid with both top and bottom undulation as seen in figure 4. This will be dealt with in the subsequent section.

4.1. Elastic energy of an elastic layer loaded at both surfaces

A linear elastic isotropic body in a slab geometry is considered. The equilibrium condition for the case of no body forces can be written as $\partial_{\alpha}\sigma_{\alpha\beta}(\mathbf{r}) = 0$, where $\sigma_{\alpha\beta}(\mathbf{r})$ is the stress at point (x, z) represented by vector \mathbf{r} and $\partial_{\alpha} \equiv \partial/\partial r_{\alpha}$. This can be written in Voigt notation as:

$$[C_{11}\partial_1^2 + C_{44}\partial_3^2]u_1(\mathbf{r}) + (C_{44} + C_{12})\partial_1\partial_3u_3(\mathbf{r}) = 0,$$

$$[C_{11}\partial_3^2 + C_{44}\partial_1^2]u_3(\mathbf{r}) + (C_{44} + C_{12})\partial_3\partial_1u_1(\mathbf{r}) = 0,$$
(8)

where C_{ij} denotes the coefficients of the elastic tensor. The in-plane wavenumber q is a scalar for the two-dimensional body considered here.



Figure 4: Periodic unit cell of an isotropic slab of height $z_{\rm m}$ represented by the shaded region is undulated at the top and bottom surfaces in lateral and normal directions.

It is shown in Appendix A that for the system of differential equations (8) the solutions of the in-plane cosine transform of the lateral u_1 displacement field couples to the in-plane sine transform of the normal u_3 displacement and vice versa. Thus, we can write:

$$u_{1}^{c}(x,z) = \cos(qx)\tilde{u}_{1}^{c}(q,z), u_{3}^{s}(x,z) = \sin(qx)\tilde{u}_{3}^{s}(q,z).$$
(9)

Solutions satisfying the following boundary conditions:

$$\widetilde{u}_{1}^{c}(q,0) = u_{1}^{bot},
\widetilde{u}_{3}^{s}(q,0) = u_{3}^{bot},
\widetilde{u}_{1}^{c}(q,z_{m}) = u_{1}^{top},
\widetilde{u}_{3}^{s}(q,z_{m}) = u_{3}^{top}$$
(10)

and equation (8) are then obtained to satisfy

$$\begin{bmatrix} \tilde{u}_{1}^{c}(q,z)\\ \tilde{u}_{3}^{s}(q,z) \end{bmatrix} = \begin{bmatrix} h_{1}(q,z) & h_{2}(q,z) & -h_{3}(q,z) & -h_{4}(q,z)\\ h_{3}(q,z) & h_{4}(q,z) & h_{5}(q,z) & h_{6}(q,z) \end{bmatrix} \begin{bmatrix} A_{1}\\ A_{2}\\ A_{3}\\ A_{4} \end{bmatrix}$$
(11)

with

$$h_{1}(q, z) = (1 - r)\cosh(qz) + rqz\sinh(qz),$$

$$h_{2}(q, z) = \sinh(qz) + rqz\cosh(qz),$$

$$h_{3}(q, z) = r(qz\cosh(qz) - \sinh(qz)),$$

$$h_{4}(q, z) = rqz\sinh(qz),$$

$$h_{5}(q, z) = (1 + r)\cosh(qz) - rqz\sinh(qz),$$

$$h_{6}(q, z) = \sinh(qz) - rqz\cosh(qz),$$
(12)

where $r = \frac{1-s}{1+s}$ and $s = C_{44}/C_{11}$. A_i can be found by applying the boundary conditions in equation (10):

$$\begin{bmatrix} A_1 \\ A_2 \\ A_3 \\ A_4 \end{bmatrix} = \frac{1}{f(q, z_{\rm m})} \begin{bmatrix} \frac{f(q, z_{\rm m})}{(1-r)} & 0 & 0 & 0 \\ k_1(q, z_{\rm m}) & k_2(q, z_{\rm m}) & k_3(q, z_{\rm m}) & k_4(q, z_{\rm m}) \\ 0 & \frac{f(q, z_{\rm m})}{(1+r)} & 0 & 0 \\ k_5(q, z_{\rm m}) & k_6(q, z_{\rm m}) & k_7(q, z_{\rm m}) & k_8(q, z_{\rm m}) \end{bmatrix} \begin{bmatrix} \tilde{u}_1^{\rm c}(q, 0) \\ \tilde{u}_3^{\rm s}(q, 0) \\ \tilde{u}_1^{\rm c}(q, z_{\rm m}) \\ \tilde{u}_3^{\rm s}(q, z_{\rm m}) \end{bmatrix}$$
(13)

with

$$k_{1}(q, z_{\rm m}) = rqz_{\rm m} - \sinh(qz_{\rm m})\cosh(qz_{\rm m}),$$

$$k_{2}(q, z_{\rm m}) = -\frac{r}{1+r}(\cosh^{2}(qz_{\rm m}) - 1 + r(qz_{\rm m})^{2}),$$

$$k_{3}(q, z_{\rm m}) = h_{6}(q, z_{\rm m}),$$

$$k_{4}(q, z_{\rm m}) = h_{4}(q, z_{\rm m}),$$

$$k_{5}(q, z_{\rm m}) = \frac{r}{1-r}(\cosh^{2}(qz_{\rm m}) - 1 - r(qz_{\rm m})^{2}),$$

$$k_{6}(q, z_{\rm m}) = -rqz_{\rm m} - \sinh(qz_{\rm m})\cosh(qz_{\rm m}),$$

$$k_{7}(q, z_{\rm m}) = -h_{4}(q, z_{\rm m}),$$

$$k_{8}(q, z_{\rm m}) = h_{2}(q, z_{\rm m}),$$
(14)

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and

$$f(q, z_{\rm m}) = \cosh^2(qz_{\rm m}) - (rqz_{\rm m})^2 - 1$$

= $\frac{1}{2} \left\{ \cosh(2qz_{\rm m}) - 2(rqz_{\rm m})^2 - 1 \right\}.$ (15)

Similarly, the in-plane sine transform of u_1 and cosine transform of u_3 can be obtained from:

$$\begin{bmatrix} \tilde{u}_{1}^{s}(q,z) \\ \tilde{u}_{3}^{c}(q,z) \end{bmatrix} = \begin{bmatrix} h_{1}(q,z) & h_{2}(q,z) & h_{3}(q,z) & h_{4}(q,z) \\ -h_{3}(q,z) & -h_{4}(q,z) & h_{5}(q,z) & h_{6}(q,z) \end{bmatrix} \begin{bmatrix} B_{1} \\ B_{2} \\ B_{3} \\ B_{4} \end{bmatrix}$$
(16)

with

$$\begin{bmatrix} B_1 \\ B_2 \\ B_3 \\ B_4 \end{bmatrix} = \frac{1}{f(q, z_{\rm m})} \begin{bmatrix} \frac{f(q, z_{\rm m})}{(1-r)} & 0 & 0 & 0 \\ k_1(qz_{\rm m}) & -k_2(qz_{\rm m}) & k_3(qz_{\rm m}) & -k_4(qz_{\rm m}) \\ 0 & \frac{f(q, z_{\rm m})}{(1+r)} & 0 & 0 \\ -k_5(qz_{\rm m}) & k_6(qz_{\rm m}) & -k_7(qz_{\rm m}) & k_8(qz_{\rm m}) \end{bmatrix} \begin{bmatrix} \tilde{u}_1^{\rm s}(q, 0) \\ \tilde{u}_3^{\rm c}(q, 0) \\ \tilde{u}_1^{\rm s}(q, z_{\rm m}) \\ \tilde{u}_3^{\rm c}(q, z_{\rm m}) \end{bmatrix} .$$
(17)

From equation (11), the strains are calculated as:

$$\widetilde{\epsilon}_{1}^{s}(q,z) = -q\widetilde{u}_{1}^{c}(q,z),
\widetilde{\epsilon}_{3}^{s}(q,z) = \partial_{3}\widetilde{u}_{3}^{s}(q,z),
\widetilde{\epsilon}_{5}^{c}(q,z) = \partial_{3}\widetilde{u}_{1}^{c}(q,z) + q\widetilde{u}_{3}^{s}(q,z).$$
(18)

Stresses are then obtained as usual through Hooke's law:

$$\sigma_i = C_{ij}\epsilon_j. \tag{19}$$

Gathering all contributions to the elastic energy leads to

$$v_{\rm el} = \frac{C_{11}q}{2} \left[s\tilde{\epsilon}_5^{\rm c}(q, z_{\rm m})\tilde{u}_1^{\rm c}(q, z_{\rm m}) + \{\tilde{\epsilon}_3^{\rm s}(q, z_{\rm m}) + (1 - 2s)\tilde{\epsilon}_1^{\rm s}(q, z_{\rm m})\} \tilde{u}_3^{\rm s}(q, z_{\rm m}) \right. \\ \left. + s\tilde{\epsilon}_5^{\rm c}(q, 0)\tilde{u}_1^{\rm c}(q, 0) + \{\tilde{\epsilon}_3^{\rm s}(q, 0) + (1 - 2s)\tilde{\epsilon}_1^{\rm s}(q, 0)\} \tilde{u}_3^{\rm s}(q, 0) \right] \\ = \frac{C_{11}q}{2} \left[\tilde{u}_1^{\rm c}(q, 0) \quad \tilde{u}_3^{\rm s}(q, 0) \quad \tilde{u}_1^{\rm c}(q, z_{\rm m}) \quad \tilde{u}_3^{\rm s}(q, z_{\rm m}) \right] \left[H_{ij}(q, z_{\rm m}) \right] \begin{bmatrix} \tilde{u}_1^{\rm c}(q, 0) \\ \tilde{u}_3^{\rm s}(q, 0) \\ \tilde{u}_3^{\rm s}(q, z_{\rm m}) \\ \tilde{u}_3^{\rm s}(q, z_{\rm m}) \end{bmatrix} \right]$$
(20)

with

$$H_{11}(q, z_{\rm m}) = H_{33}(q, z_{\rm m}) = (1 - r) \frac{\sinh(qz_{\rm m})\cosh(qz_{\rm m}) - rqz_{\rm m}}{f(q, z_{\rm m})}$$

$$-H_{12}(qz_{\rm m}) = H_{34}(qz_{\rm m}) = \frac{1 - r}{1 + r} \frac{(1 - r)\sinh^2(qz_{\rm m}) - 2(rqz_{\rm m})^2}{f(q, z_{\rm m})},$$

$$H_{13}(q, z_{\rm m}) = (1 - r) \frac{rqz_{\rm m}\cosh(q, z_{\rm m}) - \sinh(qz_{\rm m})}{f(q, z_{\rm m})},$$

$$-H_{14}(q, z_{\rm m}) = H_{23}(q, z_{\rm m}) = (1 - r) \frac{rqz_{\rm m}\sinh(qz_{\rm m})}{f(q, z_{\rm m})},$$

$$H_{22}(q, z_{\rm m}) = H_{44}(q, z_{\rm m}) = (1 - r) \frac{\sinh(qz_{\rm m})\cosh(qz_{\rm m}) + rqz_{\rm m}}{f(q, z_{\rm m})},$$

$$H_{24}(q, z_{\rm m}) = -(1 - r) \frac{rqz_{\rm m}\cosh(q, z_{\rm m}) + \sinh(qz_{\rm m})}{f(qz_{\rm m})}.$$

(21)

The complete elastic energy density containing the complex Fourier transform of the displacement with wavenumber q reads

$$v_{\rm el} = \sum_{q} \frac{C_{11}q}{2} \begin{bmatrix} \tilde{u}_{1}^{*}(q,0) & \tilde{u}_{3}^{*}(q,0) & \tilde{u}_{1}^{*}(q,z_{\rm m}) & \tilde{u}_{3}^{*}(q,z_{\rm m}) \end{bmatrix} \begin{bmatrix} H_{ij}(q,z_{\rm m}) \end{bmatrix} \begin{bmatrix} \tilde{u}_{1}(q,0) \\ \tilde{u}_{3}(q,0) \\ \tilde{u}_{1}(q,z_{\rm m}) \\ \tilde{u}_{3}(q,z_{\rm m}) \end{bmatrix}$$
(22)

with

$$\begin{bmatrix} H_{ij}(q, z_{\rm m}) \end{bmatrix} = \begin{bmatrix} H_{11}(q, z_{\rm m}) & -iH_{12}(q, z_{\rm m}) & -iH_{13}(q, z_{\rm m}) & -iH_{14}(q, z_{\rm m}) \\ iH_{21}(q, z_{\rm m}) & H_{22}(q, z_{\rm m}) & -iH_{23}(q, z_{\rm m}) & -iH_{24}(q, z_{\rm m}) \\ iH_{31}(q, z_{\rm m}) & iH_{32}(q, z_{\rm m}) & H_{33}(q, z_{\rm m}) & -iH_{34}(q, z_{\rm m}) \\ iH_{41}(q, z_{\rm m}) & iH_{42}(q, z_{\rm m}) & iH_{43}(q, z_{\rm m}) & H_{44}(q, z_{\rm m}) \end{bmatrix}.$$
(23)

The body fields are obtained through the closed-form analytical expressions in equation (11) and (16). The displacement fields hence obtained are compared with those obtained by FEM in figures 5 and 6. It has to be noted that periodic boundary conditions in GFMD are intrinsically enforced through the periodicity of the Fourier transforms. In FEM periodicity can be imposed using various methods, including the penalty method, as done in this study, or Lagrangian multipliers, but is never exact.



Figure 5: Lateral displacement u_1 in an elastic layer with undulations $u_1^{\text{bot}}/L_x = 0$, $u_3^{\text{bot}}/L_x = \frac{0.5 \times 10^{-4}}{12}$, $u_1^{\text{top}}/L_x = 0$ and $u_3^{\text{top}}/L_x = \frac{1 \times 10^{-4}}{12}$ obtained using (a) GFMD and (b) FEM.



Figure 6: Normal displacement u_3 in an elastic layer with undulations $u_1^{\text{bot}}/L_x = 0$, $u_3^{\text{bot}}/L_x = \frac{0.5 \times 10^{-4}}{12}$, $u_1^{\text{top}}/L_x = 0$ and $u_3^{\text{top}}/L_x = \frac{1 \times 10^{-4}}{12}$ obtained using (a) GFMD and (b) FEM.

The elastic energy density in equation (22) is extended to the case of a semiinfinite half-space in Appendix B. This opens up the possibility of modeling the plastic contact response of a semi-infinite body using dislocation-dynamics simulations. This is beneficial to study the plastic response of a body under contact loading without the effect of its bottom, *i.e.*, an increase in contact pressure caused by dislocations piling up at the bottom of the body.

5. Preliminary results: a simple static solution

In this section, the new GFDD model is compared to DDP when computing the image fields for the simplest case scenario: a single dislocation pinned in an isotropic slab with Young's modulus E = 70 GPa and Poissons ratio $\nu = 0.33$. The magnitude of the Burger's vector is b = 0.25 nm.

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Simulations are carried out for a unit cell with the bottom fixed and a traction free top surface, i.e.,

$$u_x(x,0) = u_z(x,0) = 0,$$

$$\sigma_{xz}(x, z_{\rm m}) = \sigma_{zz}(x, z_{\rm m}) = 0.$$
(24)

The stress distribution obtained using GFDD is compared with DDP in figure 7. The displacements at the top surface, where tractions are zero, and the tractions at the bottom surface, where displacement are zero, are shown in figure 8 and figure 9.



Figure 7: Stress fields for a dislocated elastic layer with a traction free top surface obtained using (a) GFDD and (b) DDP.



Figure 8: (a) Normal displacement u_z and (b) lateral displacement u_x at the traction free surface of an elastic layer containing a pinned edge dislocation obtained using GFDD and DDP.



Figure 9: (a) Lateral traction t_x and (b) normal traction t_z at the bottom surface of the elastic layer containing a pinned edge dislocation obtained using GFDD and DDP.



Figure 10: Lateral traction t_x at the bottom surface (a) before and (b) after the removal of ringing artifacts.

It is found that the tractions at the surface obtained using GFDD suffer from ringing, also known as Gibb's phenomenon (see figure 10). This is because the discontinuities in the displacement imposed at the surfaces cause the higher harmonics of the traction to have higher amplitudes than the lower harmonics. To remove the ringing artifacts the results displayed in figure 9 are obtained after multiplying the traction t(q)with a sinc function $sinc(qa_0)$, where a_0 is the discretization length. This is equivalent to convolving in real space the traction suffering from ringing with a rectangular box of unit height and width equal to the discretization length. Notice, however, that ringing affects only surface tractions, not surface displacements, from which the body fields are calculated.

6. Indentation by an array of flat rigid punches

This benchmark problem is used to compare GFDD to classical DDP. The simulations are carried out for a unit cell that is indented by a rigid punch as in Fig. 11.



Figure 11: Boundary-value problem.

6.1. Boundary-value problem

The indentation is prescribed by specifying the normal displacement rate along the contact of length L_x^p :

$$\dot{u}_z(x, z_{\rm m}) = -\dot{u}_z^0, \quad x \in \left[\frac{L_x - L_x^{\rm p}}{2}, \frac{L_x + L_x^{\rm p}}{2}\right].$$

A sticking contact is modeled in DDP by taking the lateral displacement $u_x = 0$ in the contact region. In GFDD, the lateral movement in the contact region is constrained horizontally through the hard-wall potential. The non-contact part of the top surface of the unit cell is taken to be traction-free,

$$\sigma_{xz}(x, z_{\rm m}) = \sigma_{zz}(x, z_{\rm m}) = 0.$$

This is achieved in GFDD by letting the contact points relax to equilibrium without any constraints. Finally, the bottom of the unit cell, z = 0 is fixed:

$$u_x(x,0) = u_z(x,0) = 0.$$

In GFDD this is implemented by constraining the lateral and normal motion of grid points at the bottom surface using the hard-wall potential.

6.2. Choice of parameters

Calculations are carried out for crystals with aspect ratio $a = z_m/L_x = 1/2$, contact fractions $L_x^p/L_x = 1/12$ and $L_x = 12 \ \mu m$. The elastic constants are chosen to represent aluminum: the Young's modulus is E = 70 GPa and Poissons ratio $\nu = 0.33$.

For the DDP simulations, the slab is discretized using a uniform mesh of square elements. The number of degrees of freedom is $n_{dof} = 2nnx \times nnz$, where nnx is the number of nodes in x-direction, and nnz the number of nodes in z-direction. For the GFDD simulations, the surface is discretized using nx equi-spaced grid points, with nx = nnx.

In GFDD, the center-of-mass mode is critically damped or slightly under-damped for quick convergence. The damping factor η is

$$\eta \propto \frac{1}{\tau \sqrt{nx}},\tag{25}$$

where τ is the time step used in the simulation. The number of iterations used to reach convergence scales as $n_{\rm it} \propto \sqrt{anx}$ and the time step is $\tau=0.25$.

The dislocations can glide on three sets of parallel slip planes, with slip plane orientations: 0°, 60° and 120° to the top surface. The discrete slip planes are spaced at 200b where b = 0.25 nm is the length of Burger's vector. The Frank-Read sources and obstacles are randomly distributed in the crystal with a density $\rho_{\rm nuc} = 30 \ \mu {\rm m}^{-2}$ and $\rho_{\rm obs} = 30 \ \mu {\rm m}^{-2}$ in an initially dislocation free crystal. The strength of the sources follows a Gaussian distribution with mean strength $\tau_{\rm nuc} = 50$ MPa and standard deviation of 10 MPa. The critical time for nucleation is $t_{\rm nuc} = 0.1$ ns. The strength of the obstacles is taken to be 150 MPa. Dislocations of opposite sign in the same slip plane annihilate when the distance between them is below $L_{\rm ann} = 6b$.

6.3. A simple dislocation dynamic simulation: a single Frank-Read source

In this section a simple problem is considered where a rigid flat punch indents a crystal containing a single Frank-Read source as shown in figure 12(a). In order to observe appreciable plastic deformation in the material, the magnitude of the Burger's vector is magnified four times, *i.e.* b = 1.0 nm. The mean contact pressure obtained using both methods is displayed in figure 12(b). While the flat rigid punch indents the layer, the source keeps generating dislocation dipoles, causing periodic kinks in the pressure-displacement curve. The difference in mean contact pressure in figure 12(b) is not seen to the naked eye.



Figure 12: (a) Schematic representation of the problem with a single Frank-Read source (b) Mean contact pressure for nx = nnx = 256. The dislocation structure and stress distribution is shown at three different depth of indentations: (1) when the first pair of dislocation is nucleated, (2) when the first dislocation exits and (3) when the second dipole is nucleated.

The surface fields obtained using both methods at $u_z = 0.01 \mu \text{m}$ are shown in figure 13. The displacement steps formed due to the exiting of dislocations can be clearly seen close to $x/L_x = 0.6$.

Note that in figure 13(a) the curves for the u_z displacement overlap since in zdirection displacement boundary conditions are imposed. The difference between the curves representing u_x stems from the numerical difference in calculating the resolved shear stress acting on the source and the location of the dislocations in the two numerical schemes. The calculated stress field depends not only on boundary conditions when the simulation is elastic, but also on the location of other dislocations in the crystal when there is plasticity. Therefore, the differences builds up with increasing dislocation density. However, relative differences between the two methods remain below 8%.



Figure 13: (a) Displacement at the top surface and (b) traction at the bottom surface obtained using GFDD and DDP at the final indentation depth $u_z = 0.01 \ \mu m$. The green curve in (a) overlaps with the blue-dashed curve since displacement boundary conditions are prescribed in the z-direction.

6.4. Dislocation dynamics simulation with many sources and obstacles

In this section the indented crystals contain a density of Frank-Read sources $\rho_{\rm nuc} =$ $30 \ \mu m^{-2}$ and a density of obstacles $\rho_{obs} = 30 \ \mu m^{-2}$. The simulations are carried out with DDP and GFMD on crystals containing the same realization of sources and obstacles, *i.e.*, the location as well as the strength of sources and obstacles are identical. Figure 15 shows the stress state and dislocation distribution at final indentation depth. Note that there is no one-to-one correspondence between the dislocations and therefore also not in terms of stress distribution. This is not surprising given that a tiny difference in the evolution of the dislocation structure, like a small delay in the nucleation of a dislocation or in the formation of a junction would trigger an avalanche of differences in the following dislocation dynamics [35]. The overall features such as the shear bands emitted by the contact are captured by both methods. This is also testified by the mean contact pressure in figure 14(a) for the simulation presented in figure 15 and for a different realization. While DDP and GFDD do not produce identical mean pressures as a function of displacement for a given realization of Frank-Read sources, differences tend to be larger within one method from one realization to the next. In figure 14(b) are presented the average between the two realizations.



Figure 14: Mean contact pressure $P_{\rm m}$ obtained using GFDD and DDP for nx = nnx = 512 are plotted for (a) two different initial realizations of dislocation structure and (b) average of three different realizations.



Figure 15: Stress and dislocation distribution in the crystal for the first realization obtained using (a) GFDD and (b) DDP for an indentation depth $u_z = 0.1 \ \mu m$ and nx = nnx = 512.

6.5. Simulation time

The computational complexity involved in solving the elastic b.v.p. using GFDD is only $O(nx\sqrt{nx} \log nx)$ [34], while it is $O(nx^2B^2)$ [36] in DDP, where B is the mean bandwidth of the stiffness matrix, which cannot exceed nx.

The time consuming part in 2D dislocation dynamics is the calculation of the resolved shear stress $\tau_{\rm res}$ at the location of objects, *i.e.*, sources, dislocations and

obstacles. In DDP, this requires searching the element where the object is located and subsequently calculating the stress and interpolating it to the location of the object. This procedure scales as $O(nx^2)$. In GFDD, instead, the resolved shear stress can be evaluated directly at the points of interest, *i.e.*, at dislocations, sources and obstacles, which requires a smaller computational effort, scaling with O(nx). This is because the body field is calculated based on surface displacements $\tilde{\boldsymbol{u}}(q)$ using nx/2 modes.

The simulation time required for elasticity and for the calculation of the resolved shear stress is displayed in figure 16, and shows in both cases how the computational advantage of using GFDD increases with increasing discretization. The simulations performed on a single Intel Xeon(R) 3.10 GHz processor with 31.3 Gbytes of RAM.

The dislocation dynamics is computed using the same algorithm in both methods and takes therefore the same amount of time and resources. The time required for the dynamics is independent of the discretization and increases with dislocation density. For the DDP simulations performed here, the time consumed by the dislocation dynamics is a negligible fraction of the time required to compute the resolved shear stress. GFDD is thus computationally more efficient than DDP independently of dislocation density.



Figure 16: (a) Simulation time for the elastic boundary-value problem and calculating resolved shear stress $\tau_{\rm res}$ are plotted separately, (b) total simulation time for GFDD vs DDP for the full simulation.

It has to be noted that the maximum number of surface nodes chosen for this study is only 2⁹. If one intends to study the contact response of a realistic self-affine surface where roughness scales over three orders of magnitude ranging in scale from 50 nm to 100 μ m [1], the surface has to be discretized by at least 2¹³ points (or even more depending on the thermodynamic and continuum limit [20]). In this case the computational advantage of GFDD becomes even more appreciable.

Notice also that the benchmark problem chosen in this work involves a constant contact area. For contact problems where the area is not constant, DDP becomes even slower since finding the correct contact area by means of the FEM requires many iterations as well as updating the boundary conditions at each time increment. GFDD is inherently impervious to such issues since it employs an interaction potential between the contacting surfaces.

7. Concluding Remarks

In this work we present a modeling technique, Green's function dislocation dynamics, which combines Green's function molecular dynamics with discrete dislocation plasticity. We firstly extended the existing Green's function molecular dynamics model such that it can simulate an elastic layer with arbitrary loading at both the top and bottom surfaces. To this end we derived the areal elastic energy for the case of an isotropic layer with sinusoidal loading at both ends. In addition, we derived the body fields required to capture the evolution of the dislocation structure. The results obtained using GFDD are compared with conventional DDP for a benchmark problem: periodic indentation of a single crystal by flat punches.

The mean contact pressure during indentation using the two methods is found to differ less than two different realizations using the same method. Here by realization is intended a given initial distribution of dislocation sources and obstacles. The differences between the two methods stems from the evaluation of the fields using different discretizations: GFDD discretizes only the surface, DDP also the body.

The new GFDD model has various advantages compared to classical DDP. First, it is faster and opens up the possibility of studying realistic rough surfaces by exploiting a larger number of degrees of freedom. Next, GFDD employs an interaction potential between the contacting bodies, and does not involve time-consuming algorithms to keep track of the evolution of the contact area. Also, the periodicity in GFDD is intrinsically enforced through Fourier transforms, making it a better candidate than DDP to study contact problems by exploiting the periodicity of the unit cell on which the analysis is performed. Obviously, this is also a limitation of the GFDD model, which is currently not suitable to study non-periodic problems. Extension of the model to overcome this limitation seems an interesting avenue for future research. Additionally, the GFDD model has the potential to serve as a platform for multi-scale modeling where the surface has an explicit atomistic description and the bulk can be treated as a dislocated continuum.

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Appendix A. Lateral-normal displacement coupling

It was shown in [34] that assuming an in-plane undulation of the top surface of an isotropic layer with a real-valued wavenumber q, equation (8) can be solved with the factorization

$$u_{\alpha}(x,z) = u_{\alpha}^{0} \exp(iqx) \exp(\pm qz).$$
(A.1)

Substituting equation (A.1) in the equilibrium condition (8), it can be rewritten in Fourier space as

$$C_{11}\tilde{u}_1(q,z) - C_{44}\tilde{u}_1(q,z) - i(C_{12} + C_{44})\tilde{u}_3(q,z) = 0$$

$$C_{11}\tilde{u}_3(q,z) - C_{44}\tilde{u}_3(q,z) - i(C_{12} + C_{44})\tilde{u}_1(q,z) = 0.$$
(A.2)

Equation (A.2) then reduces to

$$\tilde{u}_1(q,z) = i\tilde{u}_3(q,z). \tag{A.3}$$

This implies that

$$\tilde{u}_{1}^{c}(q,z) - i\tilde{u}_{1}^{s}(q,z) = i\tilde{u}_{3}^{c}(q,z) + \tilde{u}_{3}^{s}(q,z).$$
(A.4)

This explains how the solutions of the in-plane cosine transform of the lateral u_1 displacement field couples to the in-plane sine transform of the normal u_3 displacement, and vice versa.

Appendix B. Asymptotic analysis

For the limiting case in which the height of the slab tends to infinity, $H(q, z_m)$ can be written as:

$$H_{11}(qz_{\rm m} \gg 1) = H_{33}(qz_{\rm m} \gg 1) = \frac{2s}{1+s},$$

$$-H_{12}(qz_{\rm m} \gg 1) = H_{34}(qz_{\rm m} \gg 1) = \frac{2s^2}{1+s},$$

$$H_{13}(qz_{\rm m} \gg 1) = 0,$$

$$-H_{14}(qz_{\rm m} \gg 1) = H_{23}(qz_{\rm m} \gg 1) = 0,$$

$$H_{22}(qz_{\rm m} \gg 1) = H_{44}(qz_{\rm m} \gg 1) = \frac{2s}{1+s},$$

$$H_{24}(qz_{\rm m} \gg 1) = 0.$$
(B.1)

In the limiting case of short wave-numbers, we find

$$qH_{11}(qz_{\rm m} \ll 1) = qH_{33}(qz_{\rm m} \ll 1) = \frac{C_{44}}{z_{\rm m}},$$

$$-qH_{12}(qz_{\rm m} \ll 1) = qH_{34}(qz_{\rm m} \ll 1) = 0,$$

$$qH_{13}(qz_{\rm m} \ll 1) = -\frac{C_{44}}{z_{\rm m}},$$

$$-qH_{14}(qz_{\rm m} \ll 1) = qH_{23}(qz_{\rm m} \ll 1) = 0,$$

$$qH_{22}(qz_{\rm m} \ll 1) = qH_{44}(qz_{\rm m} \ll 1) = \frac{C_{11}}{z_{\rm m}},$$

$$qH_{24}(qz_{\rm m} \ll 1) = -\frac{C_{11}}{z_{\rm m}}.$$
(B.2)

In the case of bottom undulation going to zero $\boldsymbol{u}(q,0) \to 0$, we recover the elastic energy for a fixed bottom derived in [34].

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