Evaluating the fields of periodic dislocation distributions using the Fourier transform

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Abstract | Expressions are developed to describe the stress, strain and displacement fields of discrete dislocations in Fourier space. By expressing the shear stress for a doubly periodic dislocation as a Discrete Fourier Transform, numerical results are obtained that are consistent with direct summation of the analytical expressions.

By similarly calculating the displacement for a doubly periodic dislocation dipole using the DFT, two inconsistencies with the direct summation of the analytical expressions are observed: the displacement discontinuity is aligned with the $x_1$-axis regardless of the orientation of the slip plane and its step size is not equal to the magnitude of the Burgers vector $b$ along the entire segment between the dislocations.

For a dislocation dipole on a slip plane parallel to the $x_1$-axis, two simple potential corrections to the first issue are discussed: a uniform and a linear displacement correction. Neither of these corrections, however, is concluded to be completely satisfactory.
1 Introduction

A large class of solids has a crystalline structure at the microscopic level, being composed of regularly repeating unit cells that each contain the same motif of atoms. Real crystals are never perfect: in real materials the regular pattern is interrupted by defects such as dislocations. If we visualize a crystal in three dimensions as a stack of planes of atoms, an edge dislocation (often denoted by \( \_ \_ \) ) can be thought of as an extra half-plane of atoms inserted into the stack, as has been illustrated in Figure 1.

Plastic deformation at the macroscopic scale is caused by the motion of a large number of dislocations in the microscopic structure. While we can use a continuum model that in essence “averages” over a huge number of dislocations to describe plasticity at large length scales, if we want to model smaller scales we have to take the individual dislocations into account. At the atomic scale we have to use a full atomistic description, but due to the number of degrees of freedom involved this is unsuited for larger simulations. Plasticity at the micron scale, which already involves a large number of dislocations, can be described by neglecting the atomic structure of a dislocation and modeling it as a line defect in a continuum. (van der Giessen and Needleman, 1995; Shilkrot et al., 2002)

The presence of an edge dislocation with Burgers vector in the \( x_1 \)-direction at the origin of a Cartesian coordinate system induces a stress field

\[
\begin{align*}
\sigma_{11} &= \frac{-\mu b}{2\pi(1-\nu)} \frac{x_1(3x_1^2 + x_2^2)}{(x_1^2 + x_2^2)^2}, \\
\sigma_{22} &= \frac{\mu b}{2\pi(1-\nu)} \frac{x_2(x_1^2 - x_2^2)}{(x_1^2 + x_2^2)^2}, \\
\sigma_{12} &= \frac{\mu b}{2\pi(1-\nu)} \frac{x_1(x_1^2 - x_2^2)}{(x_1^2 + x_2^2)^2},
\end{align*}
\]

where \( b = |b| \), the magnitude of the Burgers vector, \( \mu \) is the shear modulus and \( \nu \) is Poisson’s ratio, both material-dependent constants. Dislocations move under the influence of shear stress \( \sigma_{12} \), and the motion of dislocations leads to plastic deformation. As the stress field of a dislocation is inversely

Figure 1: Atoms are displaced from their positions in the perfect lattice around an edge dislocation, as indicated here for a simple cubic lattice.
proportional to the distance, dislocations have a long-range interaction. (Hirth and Lothe, 1982; Hull and Bacon, 1984)

In this thesis we look at a ‘grid’ of dislocations, a motif of periodic edge dislocations repeating every $L_1$ in the $x_1$-direction and every $L_2$ in the $x_2$-direction. This defines a unit cell as depicted in Figure 2. Such periodic boundary conditions are often used in dislocation dynamics simulations because, among other reasons, they eliminate the need to arbitrarily terminate the material. (Cai, 2005)

The stress field induced by a grid of one dislocation per unit cell is simply the sum of the stresses induced by each of the individual dislocations:

$$\sigma_{ij}^{\text{(grid)}}(x_1, x_2) = \sum_{n=-\infty}^{\infty} \sum_{m=-\infty}^{\infty} \sigma_{ij}^{\text{(single)}}(x_1 - nL_1, x_2 - mL_2).$$

Directly evaluating this sum is computationally intensive, which is why we investigate another method to compute these stresses. We will develop expressions for the stress fields in Fourier space and use a numerical Fourier transform to calculate the stress fields in real space.

We will derive expressions for the stress field of an edge dislocation in Fourier space in Section 2 and Section 3. In Section 4 we will derive the expressions for the displacement field and in Section 5 we will present numerical results. We will summarize our findings and discuss some directions for further investigation in Section 6.

In Appendix A we will give a brief overview of the necessary theorems and properties of Fourier analysis. A listing of the MatLab code used for our numerical work is provided in Appendix B.

Figure 2: The periodicity of dislocations defines a unit cell of size $L_1$ in the $x_1$-direction by $L_2$ in the $x_2$-direction. Whatever happens at $(x_1, x_2)$ happens at $(x_1 + aL_1, x_2 + bL_2)$ as well, for all integers $a$ and $b$. Note that there is no particular significance in the way these particular dislocations and slip planes are placed, aside from illustrating the fact that the slip planes should also be periodic.
2 Stress field in Fourier space

Kröner (1959) was one of the first to show that a dislocation distribution could be introduced into the compatibility equations as

\[-\varepsilon_{jnm}\varepsilon_{ikl} = \eta_{ij} := \frac{1}{2} \left( \varepsilon_{ikl}\alpha_{jkl} + \varepsilon_{jkl}\alpha_{ikl} \right),\]

where we have used the Einstein summation convention\(^1\), and where \(\varepsilon_{ij}\) is the strain, \(\varepsilon_{ijk}\) is the Levi-Civita permutation symbol, \(\eta_{ij}\) is a source term for internal strains\(^2\) and \(\alpha_{ij}\) is the dislocation density tensor which denotes the density of dislocation lines in the \(x_i\)-direction with net Burgers vector in the \(x_j\)-direction.

Moreover, Kröner (1958) showed that

\[\nabla^4 \psi_{ij} = \eta_{ij}\]

where \(\psi_{ij}\) is a stress function such that

\[\sigma_{ij} = 2\mu \left( \psi_{ij,kk} + \frac{1}{1-\nu} \left( \psi_{kk,ij} - \delta_{ij}\psi_{kk,ll} \right) \right),\]

Taking the Fourier transform of (4), we get \(\nabla^4 \tilde{\psi}_{ij} = \tilde{\eta}_{ij}\). Using the differentiation property of the Fourier transform, (A.1), we find for the left-hand term \(\nabla^4 \tilde{\psi}_{ij} = 16\pi^4 (\pi_k \pi_k)^2 \tilde{\psi}_{ij}\), which implies that

\[\tilde{\psi}_{ij} = \frac{\tilde{\eta}_{ij}}{16\pi^4 (\pi_k \pi_k)^2}\]

We now take the Fourier transform of (5):

\[
\bar{\sigma}_{ij} = 2\mu \left( \bar{\psi}_{ij,kk} + \frac{1}{1-\nu} \left( \bar{\psi}_{kk,ij} - \delta_{ij}\bar{\psi}_{kk,ll} \right) \right)
= -8\pi^2 \mu \left( \pi_k \pi_k \bar{\psi}_{ij} + \frac{1}{1-\nu} \left( \pi_j \pi_k \bar{\psi}_{kk} - \delta_{ij} \pi_k \pi_k \bar{\psi}_{kk} \right) \right)
= -\frac{\mu}{2\pi^2 (\pi_k \pi_k)^2} \left( \pi_k \pi_k \bar{\eta}_{ij} + \frac{1}{1-\nu} \left( \pi_j \pi_k \pi_k \bar{\eta}_{kk} \right) \right)
\]

We will assume that there is a single dislocation in the origin of the \(x_1\)-\(x_2\)-plane that extends infinitely in the \(x_3\)-direction, and that the Burgers vector lies in the \(x_1\)-\(x_2\)-plane as well.\(^3\) Hence, the only non-zero components of the dislocation density tensor are \(\alpha_{31}\) and \(\alpha_{32}\), and all components of the source term vanish except for \(\eta_{33} = \alpha_{31,2} - \alpha_{32,1}\).

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1: Summation is implied over indices that appear twice in an expression.
2: The definition of \(\eta_{ij}\) depends on the exact cause of strain, which in our case is a distribution of dislocations but may also be e.g. a thermal gradient. For a more in-depth discussion we refer to Nye (1953); Bilby et al. (1955) and Kröner (1958, 1959).
3: The same assumptions were used to derive (1), (2) and (3).
For a single dislocation with Burgers vector \( \mathbf{b} = b_1 \mathbf{e}_1 + b_2 \mathbf{e}_2 \), \( \eta_{33} = b_1 \delta(x_1)\delta'(x_2) - b_2 \delta'(x_1)\delta(x_2) \), where \( \delta' \) is the derivative of the delta function. The Fourier transform of \( \eta_{33} \) is
\[
\eta_{33} = b_1 \delta(x_1)\delta'(x_2) - b_2 \delta'(x_1)\delta(x_2) = i2\pi(b_1\tau_2 - b_2\tau_1),
\]
so the stresses in Fourier space are
\[
\begin{align*}
\varphi_{11} &= \frac{i\mu}{\pi(1 - \nu)} \frac{b_1\tau_2 - b_2\tau_1}{(\tau_1^2 + \tau_2^2)^2}, \\
\varphi_{22} &= \frac{i\mu}{\pi(1 - \nu)} \frac{b_1\tau_3 - b_2\tau_1}{(\tau_1^2 + \tau_3^2)^2}, \\
\varphi_{12} &= -\frac{i\mu}{\pi(1 - \nu)} \frac{b_1\tau_2 - b_2\tau_1}{(\tau_1^2 + \tau_2^2)^2}.
\end{align*}
\]

Because of the convolution property, (A.2), we can obtain the stress fields for an array of dislocations that is periodic in \( x_1 \) by multiplying these expressions with \( L_1 \Delta(\tau_1 L_1) \), for a periodic array of dislocations in \( x_2 \) by multiplying with \( L_2 \Delta(\tau_2 L_2) \) or for a doubly periodic array by multiplying with \( L_1 L_2 \Delta(\tau_1 L_1)\Delta(\tau_2 L_2) \), where \( L_1 \) and \( L_2 \) are the lengths at which the dislocation repeats in \( x_1 \) and \( x_2 \), respectively.

### 3 Expressing the stress field as a DFT

To find the stress field in real space for a dislocation grid, we apply the inverse Fourier transform. For the shear stress this reads

\[
\sigma_{12}^{(\text{grid})} = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \sigma_{12}^{(\text{single})} \exp(\pm i2\pi(x_1\tau_1 + x_2\tau_2)) \, d\tau_1 \, d\tau_2
\]

\[
= L_1 L_2 \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \sigma_{12}^{(\text{single})} \Delta(\tau_1 L_1) \Delta(\tau_2 L_2) \exp(\pm i2\pi(x_1\tau_1 + x_2\tau_2)) \, d\tau_1 \, d\tau_2
\]

\[
= L_1 L_2 \sum_{n=-\infty}^{\infty} \sum_{m=-\infty}^{\infty} \sigma_{12}[m, n] \exp(\pm i2\pi(x_1 n/L_1 + x_2 m/L_2))
\]

where we have defined
\[
\sigma_{12}[m, n] := \left[ \sigma_{12}^{(\text{single})} \right]_{\tau_1=n/L_1, \tau_2=m/L_2} = \left[ -\frac{i\mu(b_1\tau_2 - b_2\tau_1)}{\pi(1 - \nu)} \frac{\tau_1\tau_2}{(\tau_1^2 + \tau_2^2)^2} \right]_{\tau_1=n/L_1, \tau_2=m/L_2}
\]

the \( m \)-th sample out of the shear stress in Fourier space for a single dislocation, from (10), with sampling intervals \( 1/L_1 \) and \( 1/L_2 \). We can similarly sample the real stress \( \sigma_{12}^{(\text{grid})} \) at intervals of \( l_1 \) and \( l_2 \), if we are not interested in features smaller than these intervals. We denote this sampled stress \( \sigma_{12}^{(\text{grid})}[u, v] := \sigma_{12}^{(\text{grid})}(ul, vl) \). The classic Nyquist-Shannon sampling theorem from information theory states that a function specified at points spaced a distance \( l \) apart contains no frequencies higher than \( 1/2l \) (Shannon, 1949). Hence, the highest relevant frequencies in \( \sigma_{12}^{(\text{grid})}[u, v] \) are \( 1/2l_1 \) and \( 1/2l_2 \) and we can truncate the summation in (11) to find

\[
\sigma_{12}^{(\text{grid})}[u, v] := L_1 L_2 \sum_{n=-\frac{N}{2}}^{\frac{N}{2} - 1} \sum_{m=-\frac{M}{2}}^{\frac{M}{2} - 1} \sigma_{12}[m, n] \exp(\pm i2\pi(um/N + vm/M))
\]

4: Typically, we are not interested in length scales in the order of magnitude of a few times \( l \), because at that length scale the linear elastic approach breaks down anyway.
where $N := [L_1/l_1]$ and $M := [L_2/l_2]$. This expression is the definition of the two-dimensional inverse discrete Fourier transform (inverse DFT) as given by Bracewell (2000), so we can numerically calculate the stresses in real space by using a DFT algorithm.

Up to this point, we have assumed that the dislocation was located at the origin of the Cartesian coordinate system. Due to the shift property of the Fourier transform, moving the dislocation from $(0, 0)$ to $(x'_1, x'_2)$ is equivalent to multiplying by a phase factor $\Xi(x'_1, x'_2) := \exp(-i2\pi(mx'/L_1 + nx'/L_2))$ within the double summation in (12). This exponential satisfies $\Xi(x_1 + aL_1, x_2 + bL_2) = \Xi(x_1, x_2)$ for integers $a$ and $b$, so that we get the same results for a dislocation at $(x_1, x_2)$ as for one at $(x_1 + aL_1, x_2 + bL_2)$. This periodicity is illustrated in Figure 2.

Moreover, we have assumed that there was only a single dislocation in each unit cell. Introducing multiple dislocations is as simple as adding together the relevant expressions for each dislocation, either before or after taking the inverse Fourier transform. This is because we have assumed linear elasticity and because the Fourier transform is linear as well.

All in all, this implies that we can get the stress field in Fourier space for any number of dislocations by replacing the factor $(b_1^1 \pi_2 - b_2^1 \pi_1)$ in the expressions for a single dislocation by $\sum_k (b_1^k \pi_2 - b_2^k \pi_1) \Xi(x^k_1, x^k_2)$.

### 4 Strains and displacements in Fourier space

Using a similar approach as for the stress field above, we can derive expressions for the strain and displacement field. For isotropic materials, the strain field in Fourier space is related to the stress field as

$$
2\mu\varepsilon_{11} = (1 - \nu)\sigma_{11} - \nu\sigma_{22},
$$

$$
2\mu\varepsilon_{22} = (1 - \nu)\sigma_{22} - \nu\sigma_{11},
$$

$$
2\mu\varepsilon_{12} = \sigma_{12},
$$

where we have dropped those expressions that are trivially zero for our problem. From (8), (9), (13) and (14) we can obtain the following expressions for the displacement field:

$$
\pi_1 = \frac{\varepsilon_{11}}{i2\pi x_1} = \frac{\pi_1}{b_1^1 \pi_2 - b_2^1 \pi_1},
$$

$$
\pi_2 = \frac{\varepsilon_{22}}{i2\pi x_2} = \frac{\pi_2}{b_1^2 \pi_1 - b_2^2 \pi_1},
$$

up to some constant in $x_1$ and $x_2$, respectively, where we have used the integration property of the Fourier transform and the fact that $\varepsilon_{11} := u_{1,1}$ and $\varepsilon_{22} := u_{2,2}$. Using Mathematica we have verified that the inverse transforms of (15) and (16) for $b = b_1 e_1$ equal the real displacement field (Hirth and Lothe, 1982)

$$
u_1 = \frac{b}{4\pi(1 - \nu)} \left( \frac{x_1 x_2}{x_1^2 + x_2^2} - 2(1 - \nu) \arctan \frac{x_1}{x_2} \right),
$$

$$
\nu_2 = \frac{b}{4\pi(1 - \nu)} \left( \frac{x_2^2}{x_1^2 + x_2^2} - \frac{1}{2} \ln \frac{x_1^2 + x_2^2}{b^2} \right).
$$

A rigorous proof that the expressions for $\nu_1$ and $\pi_1$ and for $\nu_2$ and $\pi_2$ are transform pairs using the definition of the Fourier transform is beyond the scope of this report.
5 Numerical results

5.1 General | We calculated stresses and displacements from the expressions derived in the previous sections using the DFT (see Listing 1) for a number of ensembles of dislocations, taking different values of \( b, L_1, L_2, l_1 \) and \( l_2 \). The numerical results for the stresses \( \sigma_{ij} \) were found to depend linearly on \( b/L_1 \) and \( b/L_2 \), as we expect from the scaling of \( (1), (2) \) and \( (3) \). The numerical results for the displacement \( u_i \) were found to depend linearly on \( b \), in agreement with the scaling of \( (17) \) and \( (18) \).

We will take \( L_1 = L_2 = 1000b \) in the remainder of this work without qualitative loss of generality. Furthermore, we will use the same resolution in the \( x_1 \)- and \( x_2 \)-direction, so \( l_1 = l_2 = l \). The effects of decreasing the resolution \( 1/l \) on the DFT output are plotted in Figure 3. Up to \( l \approx 10b \), the results are not noticeably deteriorated by using a lower resolution. However, as using a high resolution does not lead to prohibitively higher computation time (less than 0.3 s in all cases), we will simply set \( l = b \).

5.2 Shear stresses | The shear stress for a single doubly-periodic array of dislocations with Burgers vectors \( b = b e_1 \) (i.e., one dislocation per unit cell) was evaluated using the DFT and by directly summing the real stress \( (3) \) over a number of unit cells. The numerical results of the direct summation are plotted in Figure 4 for different numbers of unit cells. Upon increasing the number of cells over

![Figure 3: Shear stress \( \sigma_{12} \) divided by \( \mu/2\pi(1 - \nu) \) for a single doubly-periodic array of dislocations with Burgers vectors \( b = b e_1 \), calculated using the DFT with different resolution \( 1/l \). The contours correspond to values of \( 2\pi(1 - \nu)\sigma_{12}/\mu = -4 \cdot 10^{-3}, -3 \cdot 10^{-3}, \ldots, 4 \cdot 10^{-3} \).](image)

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5: \( b \) is usually in the order of one atomic distance (\( b \approx 1 \text{ Å} - 1 \text{ nm} \)).
Figure 4: Shear stress $\sigma_{12}$ divided by $\mu/2\pi(1 - \nu)$ for a single doubly-periodic array of dislocations with Burgers vectors $b = be_1$, directly calculated by summing over $N \times N$ unit cells. The contours correspond to values of $2\pi(1 - \nu)\sigma_{12}/\mu = -4 \cdot 10^{-3}, -2 \cdot 10^{-3}, 2 \cdot 10^{-3}, 4 \cdot 10^{-3}$. The computation time is approximately proportional to $N^2$, compared to less than 0.3 s for the DFT. While the difference between successive summations is small, even for very large $N$ the summations still show a discontinuity at $x_1/b = \pm 500$. 

(a) $N = 1$. Time: 0.1 s
(b) $N = 2$. Time: 1 s
(c) $N = 4$. Time: 2 s
(d) $N = 16$. Time: 27 s
(e) $N = 128$. Time: 26 minutes.
(f) $N = 512$. Time: 9.4 hours.
Figure 5: Shear stress $\sigma_{12}$ divided by $\mu/2\pi(1-\nu)$ for a homogenous dislocation pileup (a) and wall (b), calculated using the DFT. The contours correspond to the same values as in Figure 3. The spacing between dislocations is $2b$. The zooms show that the shear stresses of neighboring dislocations partly cancel.
which we sum, the results for the direct calculation seem to approach those obtained by using the DFT, however, they do so only very slowly: the average difference between $N = 128$ and $N = 512$ is in the order of $10^6 \times \mu/2\pi(1 - \nu)$ (ie. 1%), while there is still a large discontinuity at $x_1/b = \pm 500$.

For dislocations with Burgers vectors $b = b e_1$, we have calculated the shear stress of a periodic homogeneous dislocation pileup (a row of edge dislocations in the $x_1$-direction) and of a homogeneous dislocation wall (a column of edge dislocations in the $x_2$-direction), with the spacing between dislocations equal to $20b$. The shear stress of these dislocation configurations falls off very quickly because the stress fields of neighboring dislocations partly cancel, a feature we also see in the numerical results plotted in Figure 5. These numerical results agree with the analytical expressions (Hirth and Lothe, 1982; van der Giessen and Needleman, 1995) and illustrate that we can use the DFT to calculate the stress field for a large number of dislocations per unit cell at once.

In Figure 6 we have plotted the results for a single doubly-periodic array of dislocations with Burgers vectors $b = \cos \theta e_1 + \sin \theta e_2$, with $\theta = \pi/16, \pi/8, 3\pi/16, \pi/4$. These numerical results agree with those obtained by direct summation of the appropriately transformed versions of (1), (2) and (3) (not shown). This illustrates that when we use the DFT to calculate the stresses, we can set the Burgers vector (and hence, the slip plane) at any angle with respect to the directions of periodicity.

![Figure 6](https://example.com/figure6.png)

**Figure 6:** Shear stress $\sigma_{12}$ divided by $\mu/2\pi(1 - \nu)$ for a single doubly-periodic array of dislocations with Burgers vectors $b = \cos \theta e_1 + \sin \theta e_2$, calculated using the DFT. The contours correspond to the same values as in Figure 3.
5.3 Displacements | The displacement $u_1$ for a dislocation dipole\(^6\), a pair of dislocations with Burgers vectors $\mathbf{b} = \pm b \mathbf{e}_1$ located at $x_1 = \pm 100b$, is plotted in Figure 7, for $\nu = 1/2$, $\nu = 1/3$, $\nu = 0$ and $\nu = -1$\(^7\). Regardless of the value of $\nu$ we see the same main characteristic: the discontinuity in the horizontal displacement $u_1$ along the entire slip plane. We can see in Figure 8 that the discontinuity in $u_1$ is distributed over the two paths between the dislocation pair and that, as we move the dislocations, the discontinuity changes in step size.

In reality, this discontinuity is always located between the dislocations and the step size is equal to $b$, as we can see from the plots in Figure 9, that were obtained by directly summing (17) over a number of unit cells. The reason for this difference is that we have not made any assumptions about where the dislocations came from in deriving the expressions for $u_1$, so there is no term that specifies that the output of the DFT should have a discontinuity between the dislocations within the boundaries unit cell rather than across the boundaries of the unit cell. The discontinuity is therefore distributed: denoting the shortest-path distance between dislocations with $D$ and the unit cell size in the $x_1$-direction with $L_1$, there will be a discontinuity with approximate step size $(1 - D/L_1) b$ along the shortest path between dislocations and a discontinuity with approximate step size $(D/L_1) b$ along the longer path.

In order to remove the superfluous discontinuity $u_1\text{(disc.)}$, we add a displacement correction $u_1\text{(corr.)}$ that has the opposite discontinuity along the slip plane. In Figure 10(b) we have sketched the effect of

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\(^6\) We will work with dipoles from here on, because the displacements become infinite if the net Burgers vector in a unit cell is non-zero.

\(^7\) Poisson’s ratio cannot be greater than $\nu = 1/2$, nor smaller than $\nu = -1$. 

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Figure 7: Displacement $u_1/b$ for a dislocation pair located at $\pm 100b$. 
Figure 8: The discontinuity in the horizontal displacement $u_1/b$ is distributed over the two paths between the dislocation pair, i.e. one inside the cell, the other between neighboring cells. As we move the dislocations from $x_1 = \pm 100b$ to $x_1 = \pm 400b$ in, the discontinuities change height so that the displacement in (d) is the exact opposite of (a), shifted $500b$ in $x_1$.

Figure 9: Directly calculated displacement $u_1/b$ for a periodic unit cell (b-d).
adding a displacement correction that has such a discontinuity but is otherwise constant,

\[ u_{1}^{(\text{corr.})} = u_{1}^{(\text{disc.})} (2H(x_2) - 1), \]

where \( H(x_2) \) is the Heaviside step function

\[ H(x_2) := \begin{cases} 1 & \text{if } x_2 > 0, \\ 0 & \text{if } x_2 < 0. \end{cases} \]

As the derivative of this correction vanishes everywhere, it corresponds to a shear strain \( \varepsilon_{12}^{(\text{corr.})} := u_{1,2}^{(\text{corr.})} = 0 \) and shear stress \( \sigma_{12}^{(\text{corr.})} = 2\mu\varepsilon_{12}^{(\text{corr.})} = 0 \). The displacement field we so obtain is plotted in Figure 11(a). The displacement in the vertices of the unit cell, listed in Table 1 and graphed as a function of the distance between the dislocations in Figure 12(a), are useful in determining macroscopical deformation.

Adding a correction of this form, however, violates our assumption of double periodicity, as the displacement at \( x_2 = -500b \) is not equal to the displacement at \( x_2 = 500b \), although it should be noted that the displacement we obtain by adding a constant correction has the same characteristics as the displacement field we get by direct calculation from (17) for a dislocation pair that is periodic only in \( x_1 \), as we can see from Figure 9(b).

![Figure 10: When we use the DFT to calculate the displacement field of the dislocation dipole shown in (a), there is an extraneous displacement discontinuity with step size \( (D/L) b \) that deforms the outline of the unit cell as illustrated in the first frame of (b) and (c). At the corners of the unit cell, the displacement is exactly zero. To remove this discontinuity, we add a displacement field that has a discontinuity of the same magnitude but opposite sign. The effect of two possible corrections on the deformation of the outline of the unit cell are schematically drawn above. Note that the displacement of the edge and the unit cell size are not to the same scale.](image)

![Figure 11: Horizontal displacement for a dislocation dipole located at \( \pm 100b \) that was corrected using a constant correction in (a) and using a linear correction in (b). The first of these violates the assumption of periodicity, the second introduces a stress term with no physical source.](image)
Dislocation distance $D/L$ & 0.1 & 0.2 & 0.3 & 0.4 & 0.5 & 0.6 & 0.7 & 0.8 & 0.9 \\
Vertex displacement $2u_1^{(\text{corr})}/b$ & 0.12 & 0.23 & 0.35 & 0.47 & 0.58 & 0.70 & 0.82 & 0.93 & 1.04 \\
Step size $2u_1^{(\text{max})}/b$ & 1.04 & 1.06 & 1.08 & 1.09 & 1.11 & 1.12 & 1.13 & 1.14 & 1.14 \\

Table 1: Dependence of maximum displacement step size $2u_1^{(\text{max})}/b$ and relative vertex displacement $2u_1^{(\text{corr})}/b$ on the distance $D/L$ between dislocations.

To illustrate a displacement that does satisfy double periodicity, in Figure 10(c) we have drawn the effect of a linear correction: a displacement field

$$u^{(\text{cor})}_1 = u^{(\text{disc})}_1 \left( 2H(x_2) - 1 - \frac{x_2}{L_2} \right).$$

(19)

This gives a total displacement field that is continuous at every point of the unit cell boundary (see Figure 11(b)) and therefore does not violate our assumption of periodicity. Cai et al. (2003) have shown that a similar linear correction is needed to make a direct summation of the displacement field for a screw dislocation absolutely convergent.

Adding a correction of this form, however, introduces a constant shear strain $\gamma^{(\text{cor})}_{12} := u^{(\text{cor})}_{1,2} = u^{(\text{disc})}_1/L_2$, i.e. a shear stress $\sigma_{12} = 2u^{(\text{disc})}_1/L_2$. The Fourier transform of this additional constant stress is a delta peak at the origin in Fourier space, which we have assumed to be zero in the previous part of this report, as there appears to be no physical source for this term.

Comparing both corrected displacements in Figure 11 with the directly calculated displacements in Figure 9, we see that the general shape of the displacement field is reproduced fairly well, but there is still a disagreement at the slip plane. While the step size in the displacement along the slip plane is supposed to be exactly equal to $b$, in the DFT output the maximum step size is slightly larger than $b$ by a factor that depends on the distance between the dislocations (see Table 1 and Figure 12(b)). We have found no simple correction that makes these results agree more.

Apart from these features, we do get fairly sensible results from the DFT regardless of where the dislocation pair is located, but only if the dislocations have the same $x_1$-coordinate if their Burgers vectors are in the $x_2$-direction, or vice versa. The DFT does not converge if the slip plane is inclined so that the slip plane itself is not periodic, i.e. if it does not connect with an equivalent slip plane.

![Figure 12](image.png)

Figure 12: Dependence of relative vertex displacement $2u_1^{(\text{max})}/b$ and relative vertex displacement $2u_1^{(\text{corr})}/b$ on the distance $D/L$ between dislocations.
from another unit cell. Note that we generally cannot solve this by choosing the unit cell differently, as such a unit cell exists only if the angle between the slip plane and the $x_1$-axis is $r\pi$, where $r$ is a ratio of integers. Furthermore, the DFT does not converge if the dislocations are not on the same slip plane.

If the slip plane is in itself periodic, the DFT may converge, but as illustrated in Figure 13 for a slip plane at a $\pi/4$ angle, this does not provide results that agree with a direct calculation from (17). We have not been able to find a simple correction that makes the fit between these results better.

![Figure 13](image)

Figure 13: Horizontal displacement for a dislocation dipole on a slip plane oriented at a $\pi/4$ angle with respect to the coordinate axes.

6 Conclusions
From the partial differential equations that govern the elastic fields of dislocations in real space, we can easily derive expressions in Fourier space for the stress field induced by a discrete edge dislocation look similar to their real-space equivalents. From these, we can derive expressions in Fourier space for the real displacements.

The output of the DFT for the stress fields is very similar to that obtained by direct summation over a large number of unit cells, however using the DFT is much faster. Using the DFT to calculate the stress and strain fields yields sensible results regardless of the number of the dislocations or their orientation.

When calculating displacements the DFT converges only if the net Burgers vector within a unit cell is zero and only if all dislocation dipoles lie on periodic slip planes. Even then, we see a discontinuity in the displacement along the coordinate axes. For slip planes that are parallel to either of the coordinate axes, we can add a displacement correction to make the output of the DFT agree more with the results obtained by directly summing the real displacements.

We have described the effects of two such corrections on a dislocation dipole with Burgers vectors in the $x_1$-direction. Adding a constant displacement correction gives a displacement that looks similar to the displacement we get by directly summing over a number of unit cells for a dislocation dipole that is periodic only in the $x_1$-direction; i.e. it violates the assumption of double periodicity that we needed to express the displacement as a discrete Fourier transform. It does, however, provide a relative displacement of the vertices of the unit cell equal to the height of the superfluous discontinuity, which is useful in determining the macroscopic deformation.
Adding a linear displacement correction gives a proper doubly periodic displacement field, but it necessarily introduces a stress term that has no physical source.

Finally, regardless of which of these two corrections we apply, the displacement we get from the DFT does not have a constant step size equal to $b$ on the line segment between dislocations. The maximum step size is dependent on the distance between the dislocations.

All in all, we conclude that more work is needed to make the DFT approach for calculating the displacement fields agree with the real results. We expect that an investigation on the convergence of the infinite sum of the real displacements will provide more insight in the corrections needed – either as a priori corrections to the expressions in Fourier space or a posteriori to the DFT output.

For inclined slip planes in real space, we perform a change of coordinates to make the discontinuity of the arc tangent lie along the slip plane. We expect that a similar coordinate transformation in Fourier space will make the DFT results for angled slip planes agree closer to the real results.

Given the speed of the DFT compared to a direct summation, we expect that a DFT-based approach to calculating the elastic fields of dislocations may prove very useful in modeling mechanical behavior. The approach we have taken here, deriving the expressions in Fourier space from the dislocation density, can be quite naturally extended to three dimensions, which opens the door to including screw dislocations as well.

References


A Properties of the Fourier transform

The Fourier transform is an operator that decomposes a function into its constituting frequencies. In this section we will give some basic properties of the Fourier transform. We will not give proofs or derivations; for a more in-depth discussion we refer to e.g. Bracewell (2000).

A.1 Definition

We will use the following definition of the one-dimensional Fourier transform and its inverse:

$$\varphi(\pi) = \int_{-\infty}^{\infty} \varphi(x) \exp(-i2\pi x\pi) \, dx \quad \text{and} \quad \varphi(x) = \int_{-\infty}^{\infty} \varphi(\pi) \exp(+i2\pi x\pi) \, d\pi.$$  

For the sake of notational simplicity, we use $\pi$ to denote the analog in Fourier space of some real $\alpha$, whatever their physical interpretation may be. For example, if $x$ is a spatial coordinate, then $\pi$ is a spatial frequency, and if $\varphi(x_1, x_2, \ldots)$ is any function in real space, then $\varphi(\pi_1, \pi_2, \ldots)$ is a function of spatial frequencies in Fourier space.

Of particular interest are the Fourier transform of the Dirac delta function, $\delta(x) = 1$, and that of the Dirac comb $\Delta(x/L) := \sum_{n=-\infty}^{\infty} \delta(x - nL)$. The latter is a sequence of Dirac delta peaks which often represents sampling at intervals of $L$. Its Fourier transform is $\Delta(x/L) = L \Delta(x L)$.

A.2 Symmetry

If the Fourier transform $\varphi(\pi)$ of $\varphi(x)$ is $\varphi(\pi) = \chi(\pi)$, then the Fourier transform of $\chi(x)$ is $\chi(\pi) = \varphi(-\pi)$. If two functions $\varphi$ and $\chi$ are related through a Fourier transform they are commonly called a Fourier transform pair. For example, we have mentioned that the Fourier transform of the Dirac comb is $\Delta(x/L) = L \Delta(x L)$, so the Dirac comb in $x$ and the Dirac comb in $\pi$ are a transform pair.

A.3 Linearity

For any constants $a$ and $b$, $a\varphi + b\chi = a\varphi + b\chi$. This property will be used so often that we will not explicitly call attention to it.

A.4 Shift

Shifting $\varphi(x) \rightarrow \varphi(x - x')$ in real space is equivalent to multiplying its Fourier transform $\varphi$ by $\exp(-i2\pi x'\pi)$.

A.5 Differentiation

Using $\varphi_k$ to indicate the partial derivative of $\varphi$ with respect to $x_k$ in real space, the Fourier transform of $\varphi_k$ is

$$\varphi_k = i2\pi x_k \varphi,$$  \hfill (A.1)

i.e. differentiating $\varphi$ in real space is equivalent to multiplying its Fourier transform $\varphi$ by $i2\pi x_k$. Conversely, taking the antiderivative of $\varphi$ in real space is equivalent to dividing $\varphi$ by $i2\pi x_k$.

---

8: Talking about the symmetry property using notation that differentiates between Fourier space and real space is a great way to illustrate the shortcomings of that notation.

9: Technically, we should also add a constant of integration in the form of $\varphi(0)\delta(\pi)$, but this ‘zero-frequency’ contribution will always vanish here, because the functions we integrate are odd.
A.6 Convolution | The Fourier transform of the convolution of \( \phi \) and \( \chi \)

\[
(\varphi * \chi)(x) := \int_{-\infty}^{\infty} \varphi(\xi) \chi(\xi - x) \, d\xi.
\]

is the product of their respective Fourier transforms,

\[
\mathcal{F}(\varphi * \chi) = \mathcal{F}(\varphi) \cdot \mathcal{F}(\chi).
\]  \hfill (A.2)

In general, it is not an easy task to decompose a function into its convolution factors, but functions \( \phi \) that are equal to a periodic sum of some other function \( \varphi \)

\[
\phi(x) = \sum_{n=-\infty}^{\infty} \varphi(x - nL)
\]  \hfill (A.3)

are easily deconvoluted into \( \phi = \varphi * \Delta(x/L) \).

A.7 Periodicity | As a direct consequence of the convolution property, a function has a discrete Fourier transform if and only if it is periodic, and vice versa.\(^{10} \) Because of this, any numerical Fourier transform, necessarily operating on a finite, discrete set of values, will always give a periodic, discrete set of output values.

B MatLab source code

We used the MatLab function in Listing 1 to compute the stresses and displacements illustrated in this report. As the expressions for \( \sigma_{ij}, \varepsilon_{ij} \) and \( \pi_i \) are all composed of a factor \( (\pi_1^2 + \pi_2^2)^{-2} \), a factor \( (b_1 \pi_2 - b_2 \pi_1) \Xi(x'_1, x'_2) \) that depends on orientation and position of the dislocation and some factor determined by the type of field we want to evaluate, we calculate these three factors separately before applying the DFT.

It should be noted that there are several definitions of the inverse DFT in common use that may give different limits for the summation compared to (12) or use a scaling factor that differs from \( L_1L_2 \). Hence, we have to multiply by \( l^2 \) to make the MatLab output agree with the definitions we used in this report.

Listing 1: disfield.m

```matlab
function field = disfield(xpos,ypos,xb,yb,L1,L2,1,mode,mu,nu)

% Compute stress, strain or displacement field for a
% number of dislocations.

% xpos : x1-positions of the dislocations
% ypos : x2-positions of the dislocations
% xb   : b1-components of Burgers vectors
```

---

10: Periodic functions, e.g. \( \exp(i2\pi x) \), functions that do not vanish in the infinite limit, e.g. constant functions, and functions that have an infinite discontinuity, e.g. \( \delta(x) \), strictly speaking have no Fourier transforms, because the integral in (A.1) does not converge for all \( \pi \). Physically, they constitute waveforms with infinite energy. Their Fourier transforms exist only as a limit, e.g. the Fourier transform of a sequence that approaches \( \delta(x) \) is a sequence that approaches unity.
% yb : b2-components of Burgers vectors
% L1,L2: size of unit cell
% l : gridsize
% mode : - 'stress11', normal stress in x1-direction
% - 'stress22', normal stress in x2-direction
% - 'stress12', shear stress
% - 'strain11', normal strain in x1-direction
% - 'strain22', normal strain in x2-direction
% - 'strain12', shear strain
% - 'disp1', displacement in x1-direction
% - 'disp2', displacement in x2-direction
% mu : Shear modulus
% nu : Poisson's ratio

if (L1*L2/l.^2 > 1e7) % To stay within memory.
    field = NaN ;
    return
end

X = -.5/l:1/L1:.5/l ;
Y = -.5/l:1/L2:.5/l ;
X = X(1:end-1) ;
Y = Y(1:end-1) ;

[x,y] = meshgrid(X,Y,'single') ;

if strcmp(mode,'stress11')
    field = (1i*mu)/(pi*(1-nu)) * y.^2 ;
end
if strcmp(mode,'stress22')
    field = (1i*mu)/(pi*(1-nu)) * x.^2 ;
end
if strcmp(mode,'stress12')
    field =-(1i*mu)/(pi*(1-nu)) * x.*y ;
end
if strcmp(mode,'strain11')
    field = 1i*2*pi*(y.^2-(nu/(1-nu))*x.^2) ;
end
if strcmp(mode,'strain22')
    field = 1i*2*pi*(x.^2-(nu/(1-nu))*y.^2) ;
end
if strcmp(mode,'strain12')
    field =-1i/(2*pi*(1-nu)) * x.*y ;
end
if strcmp(mode,'disp1')
field = (y.^2-(nu/(1-nu))*x.^2)./(x*4*pi^2) ;
end
if strcmp(mode,'disp2')
    field = (x.^2-(nu/(1-nu))*y.^2)./(y*4*pi^2) ;
end
d = 0*x ;
for n = 1:length(xpos)
    d = d + (xb(n)*y-yb(n)*x) * exp(-1i*2*pi*(xpos(n).*x+ypos(n).*y)) ;
end
field = d.*field./((x.^2+y.^2).^2 ;
field(isnan(field)) = 0 ; % Zero frequency component
field = l.^2*real(ifft2(fftshift(field))) ;
end