Effect of Eshelby's exterior solution on Configurational forces

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1. Introduction

The dynamics of dislocations determines the plasticity of a material. Though there are various reasons for the movement dislocations to get hindered, presence of inhomogeneity plays a very significant role. The presence of inhomogeneity can significantly hinder the dislocations thus strengthening the material. This is the mechanism by which many alloys, including Al-Cu alloys, acquire its strength. Thus, understanding the effect of inhomogeneities on dislocation would enable us to predict the mechanical response of many industrially relevant alloy systems. To understand how inhomogeneities in the matrix affect the dislocation motion, we try to determine the force acting on the dislocation for a given strain boundary condition and compare it with the case where the material is homogeneous.
In this study we consider the following cases:

1. Validation of code for no eigen strain case
2. Quantification of Peach-Köhler force on dislocation due to the presence of eigen strain in the inhomogeneity.
3. Force on a dislocation dipole due to the inhomogeneity.

For case 1,as shown in Figure 1 we position the positive edge dislocation with a burgers vector length of 2.5Å at distance of 125 μm from the center of the inhomogeneity and the negative edge dislocation is held stationary. This is done to make sure that the boundary effects and the effect of inhomogeneity's exterior solution are minimal. In this limit, we get the force to be exactly τb, i.e $\mu_{mat}\gamma \cdot b = 1.29e^{-09} N\mu m^{-1}$.

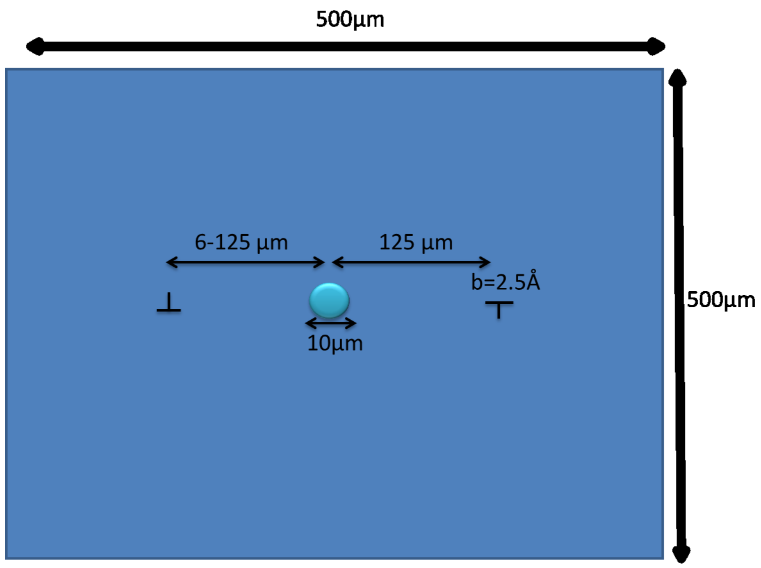

Figure 1. Schematic of the problem setup for validation case

A schematic of case 2 is shown in Figure 2, in which the inhomogeneity is now elastically strained. We study the effects of this elastic strain and its components on the interaction force. The eigen strain is increased from 0 to 0.04 in steps of 0.01.

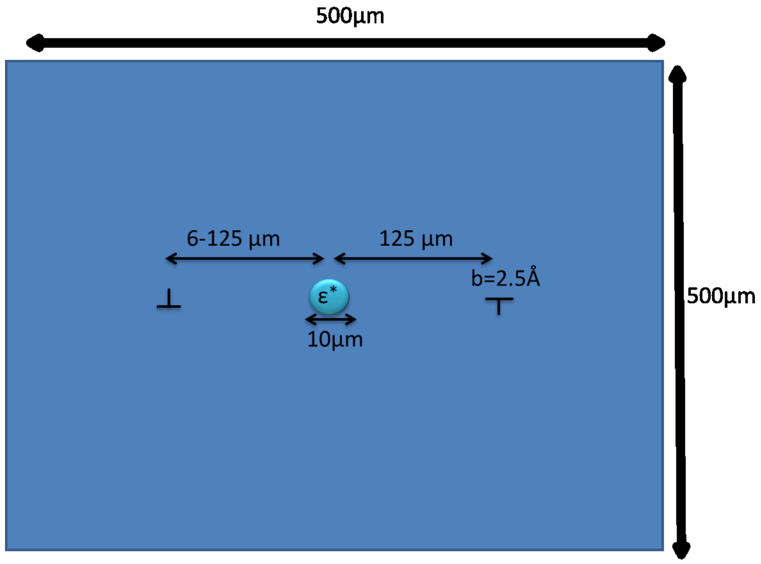

Figure 2. Schematic of the problem setup for eigen strain case

The study is extended to observe the effects of exterior solution with a dislocation dipole. A schematic is shown in Figure 3, where the distance between the dislocations is fixed at 10 μm, and the dipole's distance is varied from 15 to 95 μm relative to the center of the inhomogeneity.

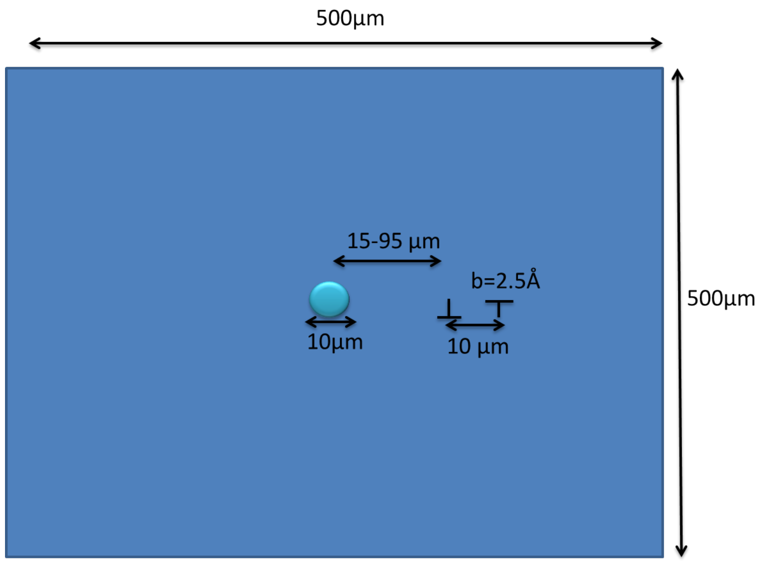

Figure 3. Schematic of the problem setup for dislocation dipole case

Table 1 shows the property data used for running the force calculation. The data pertaining to the matrix is that of Aluminium.

	$\lambda\,(N\mu m^{-2})$	$\mu\,(N\mu m^{-2})$
Matrix (Aluminium)	60.49	25.93
Inhomogeneity (Fictitious)	300.49	125.93

Table 1. Material properties for the matrix and the inhomogeneity

2. Calculation of stress fields throughout the domain

To calculate the force acing on a dislocation, we first need to determine the stress at the location of the dislocation. This is based on the work done by E. van der Giessen and A.Needleman[Van der Giessen and Needleman 1995]. In this method, the stress due to an inhomogeneity and the dislocations are decoupled and are separately calculated. Analytical soluitions are used to calculate these stresses. Since we are more interested in the matrix, Eshelby's exterior soltion[Eshelby 1961] and Volterra's formulation are used to calculate the stress due to an inhomogeneity and dislocation respectively. Both the aforementioned analytical solutions are derived for an infinite domain with homogeneous traction conditions. Since, this is not compatible with the domain we are working on, we calculate the stresses due to these defects on the boundary and then impose conditions on the boundary that are compatible with the boundary conditions we impose on the boundary. We then use the FEM formulation to solve for the displacements in the domain that satisfies eqs. 3.

$$\sigma_{ij,j} = 0, \tag{1}$$

$$\sigma_{ij} = C_{ijkl}\epsilon_{kl}, \tag{2}$$

$$\epsilon_{ij} = \frac{1}{2}\Big(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\Big) \tag{3}$$

The stress by the dislocation can be calculated from using a complex variable approach [Bowler 2009]. For an edge dislocation, the stress is given by eq 6.

$$\sigma_{11} = -\frac{Eb_1(3sin\theta + sin3\theta)}{8\pi(1-\nu^2)r} + \frac{Eb_2(cos\theta + cos3\theta)}{8\pi(1-\nu^2)r}, \tag{4}$$

$$\sigma_{22} = -\frac{Eb_1(sin\theta - sin3\theta)}{8\pi(1-\nu^2)r} + \frac{Eb_2(3cos\theta - cos3\theta)}{8\pi(1-\nu^2)r}, \tag{5}$$

$$\sigma_{12} = \frac{Eb_1(cos\theta + cos3\theta)}{8\pi(1-\nu^2)r} - \frac{Eb_1(sin\theta - sin3\theta)}{8\pi(1-\nu^2)r} \tag{6}$$

Thus, the stress at a location can be found by summing the contributions of above mentioned stresses.

3. Peach Koehler force

Any arbitrary state of deformation even though it satisfies boundary value problems won't be in thermodynamic equilibrium because of the strong interactions between the dislocations. This non equilibrium will cause re-distribution of dislocations by motion of these dislocations along their slip systems.

To study these dynamics it is important to calculate the force acting on the dislocation in a particular slip plane. Considering f^i is the force acting on the dislocation, the change in potential energy ($\delta\Pi$) can be written as,

$$\delta\Pi = -\sum_i \int_{l^i} f^i.\delta s^i dl \tag{7}$$

where s^i is the displacement cause due f^i the so called Peach Koehler force.

Now we need to correlate this Peach Koehler force on the dislocation to the stress at the dislocation site. To do this we introduce a small core region C^i around each dislocation loop i, which is formed by a torus of radius r_o along the dislocation line, cut open internally by the slip plane and bounded by two surfaces S^i_+ and S^i_-. The total surface of the core region, including S^i_+ and S^i_-, is denoted by ∂C^i. Then, the volume of the body excluding the core region C^i is $\hat{V}^i = V \setminus C^i$. The body volume excluding all core regions $\widetilde{C} = U^i C^i$ is $\hat{V} = V \setminus \widetilde{C}$. The potential energy ($\pi$) for the dislocated body is then found as the potential energy of the volume $\hat{V}$ excluding all core volumes, while the core energies are accounted for through the work of tractions on the interfaces ∂C^i of $\hat{V}$. It follows the below equation,

$$\pi = \frac{1}{2}\int_v \hat{\sigma} : \hat{\epsilon} dV + \frac{1}{2}\int_v (\hat{\sigma} : \widetilde{\epsilon} + \widetilde{\sigma} : \hat{\epsilon}) dV + \frac{1}{2}\sum\sum_{j\neq i}\int_v \sigma^j : \epsilon^k dv + \sum_i \left[\frac{1}{2}\int_{\hat{V}^i} \sigma^i : \epsilon^i dv + \frac{1}{2}\int_{\partial C^i} T^i.u^i dv\right] - \int_{S_f} T_0.(\hat{u} + \widetilde{u}) dS \tag{8}$$

Now we write the differential potential energy of the body in terms of the local stress state and compare it with 7. This gives,

$$f^i = t^i \times \left[\left(\hat{\sigma} + \sum_{j\neq i}\sigma^j\right).b^i\right] \tag{9}$$

The component of the force in the direction $t^i \times n^i$ in the slip plane and normal to the dislocation is found as,

$$f^i = n^i.\left(\hat{\sigma} + \sum_{j\neq i}\sigma^j\right).b^i \tag{10}$$

The force described by 10 will determine the motion of the dislocation in its dislocation.

4. Validation of the calculation

The positions of the dislocations were so chosen such that the dislocations were not affected by the inhomogeneity at the same time care was taken to ensure that they were not close to boundary either. Fig. 4 calculates the force as a function of distance from the inhomogeneity.

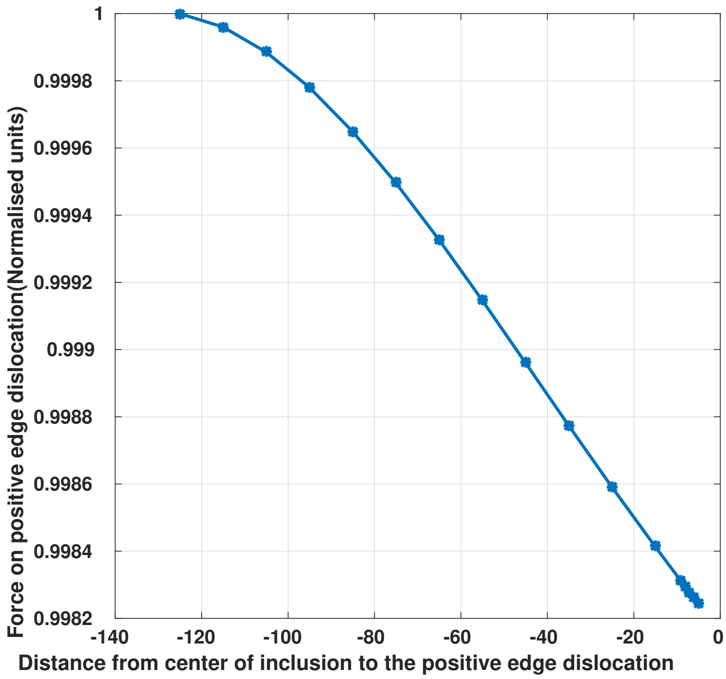

Figure 4. Validation plot

5. Results and discussion

5.1. Effect of eigen strain

The eigen strain was varied by imposing different strains in the inclusion. The force experienced by the dislocation for different normal strains in the inhomogeneity is given in Fig. 6. The force experienced by the dislocation for different shear strains in the inhomogeneity is given in Fig. 5.

5.2. Effect of distance on the dislocation dipole

The dislocation dipole initially placed at 15.11 units (distance of dislocation 1 from the centre of inhomogeneity) is varied in the units of 10 until 95.11 units. The force on both of the dislocation is computed at all these locations and is plotted as a function of distance in Figure 7). Figures 8 and 9 show shear stress contours.

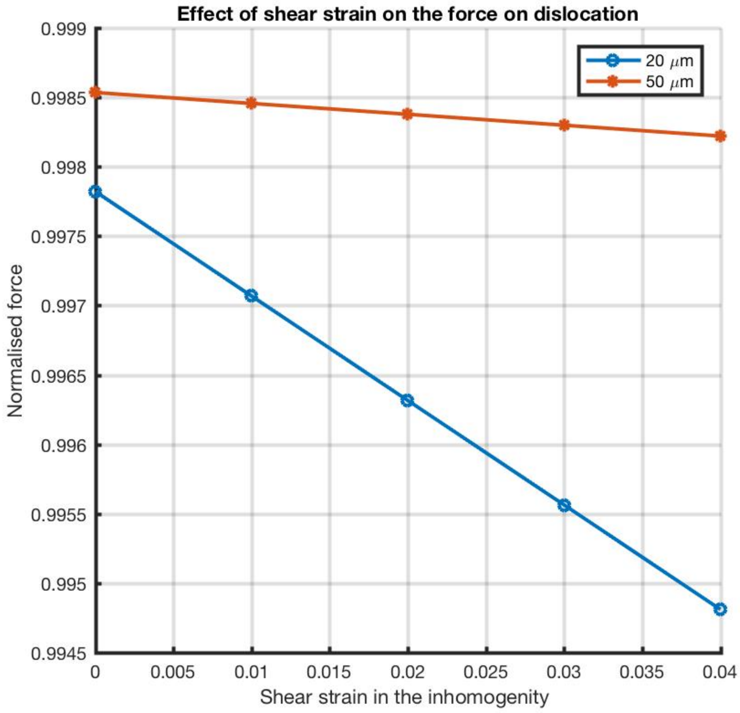

Figure 5. Effect of shear strain on the force on dislocation

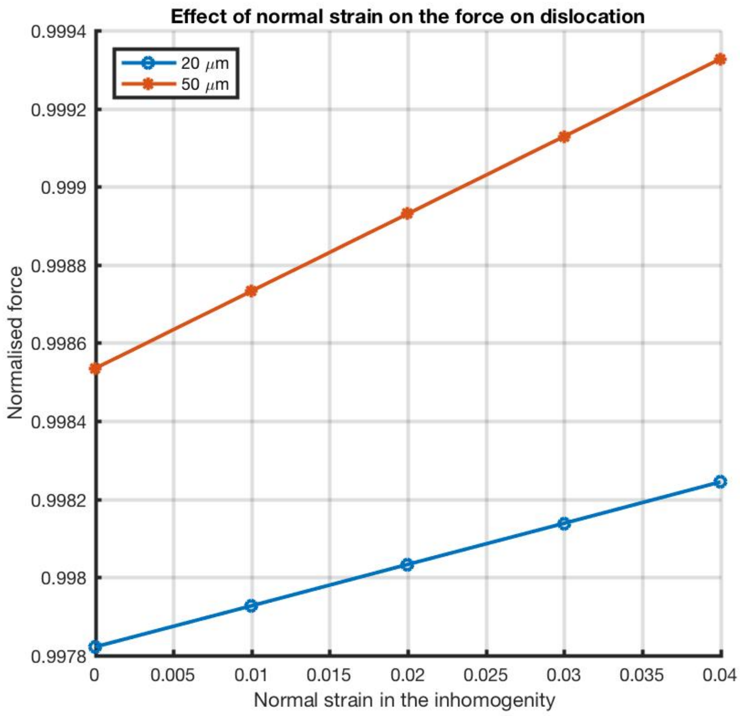

Figure 6. Effect of normal strain on the force on dislocation

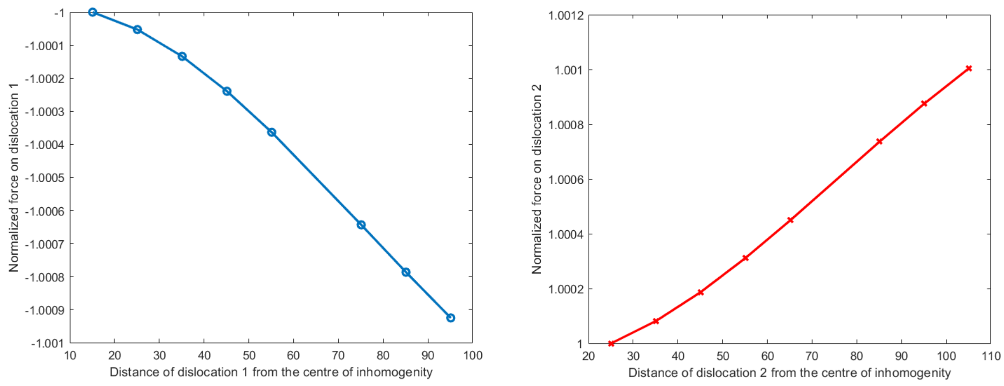

Figure 7. Force on dislocations vs distance

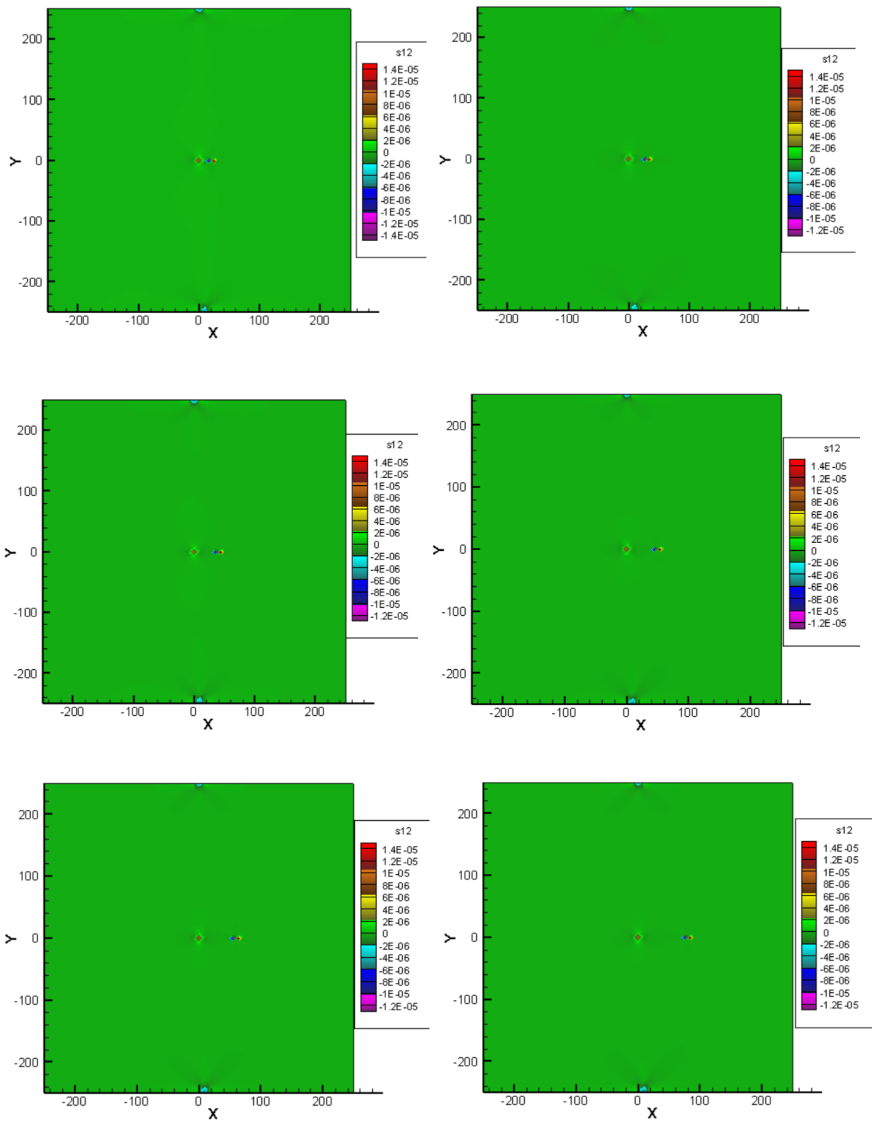

Figure 8. Shear Stress profiles as the dislocation dipole is moved

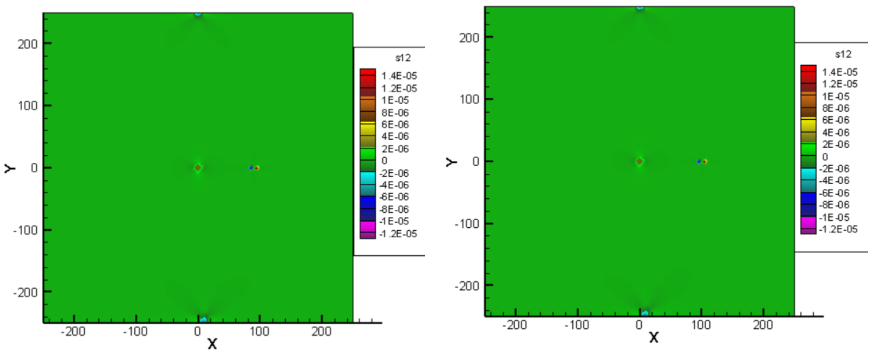

Figure 9. Shear Stress profiles as the dislocation dipole is moved

6. Future work

This work can be extended by incorporating lot of dislocations and letting the system evolve by considering the dynamics of dislocation motion as well. Periodic boundary conditions can also be imposed to model the system better.

7. Conclusion

The effect of an inhomogeneity on the dislocations was studied. The strain in the inclusion seems to affect the dislocations and the nature of the strain also plays a role. The inhomogeneity attracts the positive edge dislocation. The introduction of shear strain attracts the dislocation with a greater force while a normal strain reduces it. The stress due to the inhomogeneity falls off as we move away from it as expected. It is observed that when the dislocation dipole is moved away from the inhomogeneity the dislocations repel each other more than when they were close to the inhomogeneity.

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