Simulation of edge dislocation using Finite Element Method

N. Ramakrishnan[1]

Summary

Understanding the stress fields and energetics of dislocations is of fundamental importance towards comprehending material behaviour at microscopic scale. In this work, a simple sessile edge dislocation is simulated using Finite Element Method (FEM) by feeding in the appropriate stress free Eshelby misfit strain in the model corresponding to the introduction of an extra plane of atoms. The results of the simulation are compared with that of the standard equations of elasticity theory of dislocations and the applicability of the results, near the core of the dislocation, is demonstrated in the light of the published experimental results. It is shown that along special zones of interest, where the standard theory is expected to be valid, the model has an excellent match with the theoretical results up to a distance of about 5 Å. Important features deducible from the experimental results, like asymmetry due to the compressive and the tensile stress fields are also captured in the current model. It is seen that the results of the simulation can provide an accurate prediction of the stress fields of a dislocation much closer to the core of the dislocation than the standard theory. The utility of the Finite Element Method at length-scales of a few nanometers is also demonstrated. The simulated edge dislocation can be used to study interaction between dislocations and also in conjunction with other simulated systems like epitaxial thin films, precipitates in metals etc; hence forms an important step towards building numerical models for dislocation dynamics.

Introduction

The study of stress fields and energetics of dislocations is of great importance in the understanding of material behaviour at microscopic scale. For instance, the study of dislocations in thin films is useful in comprehending the properties of devices affected by dislocations [1]. The recent work of Hytch et al [2] has made it possible to compare analytical models of displacement fields of a dislocation with experimental results at a distance of few nanometers with high accuracy. Benabbas et al [3] had earlier demonstrated the utility of Finite Element Method (FEM) for highly strained materials in nanometer length-scale. In this work an edge dislocation is modeled using FEM. The power of the model is demonstrated by comparing the FEM results with published experimental results as well as theoretical ones and bring out certain interesting observations.

Considerable literature is available on various aspects of dislocations, including their stress fields and energetics [4-6]. The energy of an edge dislocation is [6]:

$$E_{dl} = \frac{Gb^2}{4\pi(1-\upsilon)}[2+\ln(\gamma_0/b)] \quad (1)$$

[1]Regional Research Laboratory, Bhopal-26, India

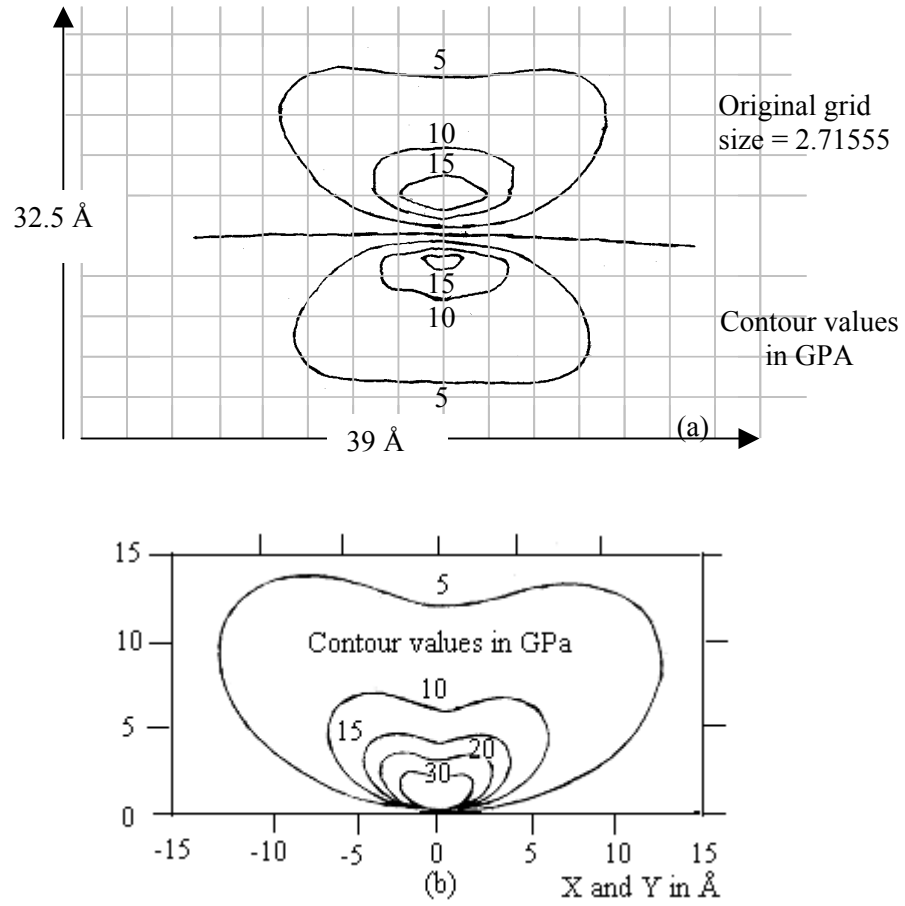

Fig. 1. Plot of σ_x (contours in Gpa) on the introduction of an edge dislocation (a) FEM simulated values (b) plot of the theoretical equation

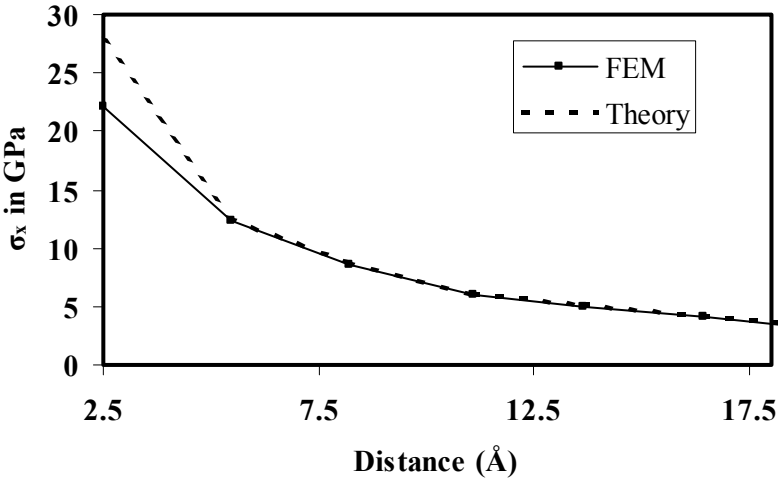

Fig.2. Comparison of the theoretical and FEM plots of σ_x values along the y-axis

Where, E_{dl} is the energy per unit length of the dislocation, G is the shear modulus, b is the Burgers vector, υ is the Poisson's ratio and γ_0 is the size of the domain which is usually taken ~100b. The σ_x component of the stress of an edge dislocation with the dislocation line along z-axis and the extra half plane along negative-y axis is given by [6]:

$$\sigma_x = \frac{Gb}{2\pi(1-\upsilon)} \quad \frac{y(3x^2+y^2)}{(x^2+y^2)^2} \tag{2}$$

Finite Element Method

To illustrate the Finite Element Method and to compare the results with available analytical results, the introduction of a simple edge dislocation with Burgers vector along [100] is considered. The initial mesh configuration consists of bi-linear quadrilateral elements with material properties corresponding to Si as an illustrative case. For defining the boundary conditions, using the symmetry of the domain, half the length of the system is considered and plane strain condition is assumed. Anisotropic conditions are incorporated by feeding the three independent moduli of the cubic lattice as input. The edge dislocation is modeled by feeding the strain (Stress free Eshelby strain [7]) corresponding to the introduction of an extra plane of atoms. This strain is:

$$\varepsilon_T = b / (a + b) \approx 1/2 \tag{3}$$

Where, ε_T is the strain imposed on a column of elements representing the extra half plane of atoms and 'a' is the spacing of atoms along the [100] direction. In this simplified illustration 'b' is taken to be equal to 'a'. It is to be noted that the assumed direction of the Burgers vector is for a simplified illustration although the energetically preferred dislocation in Si is along the close packed [110] direction on the (111) plane.

The model is implemented using a large deformation algorithm developed by Ramakrishnan et al [8] which can handle large rotations as well as strains accurately that was essentially developed for metal forming applications involving very large deformation. The energy per unit length of the system, on the introduction of a dislocation, obtained from the simulation is 6.72×10^{-9} J/m. The corresponding value obtained from equation (1) is 8.84×10^{-9} J/m. It is seen that the simulated result is in reasonable agreement with the one calculated from the theory. The marginal difference in the values could be due to the difference in the core energy values and the shape of the domain in the simulation. To reduce the end effects, a geometry that is about ten times larger than the zone of interest was considered.

Results and Discussion

Fig. 1a shows the plot of σ_x on the introduction of an FEM simulated edge dislocation and Fig. 1b shows the plot of the theoretical equation [4]. A close correspondence is seen in the shape as well as the stress values of the contours between the analytical and the simulated plots. Similarly a good fit is seen between the theoretical and simulated plots of σ_y as well.

In order to make a critical comparison of the current model with that of the experimental results [2] the following important points are noted from their paper: i) the comparison of numerical results with theory that is developed for the sinusoidal displacement component at a distance of 74 Å ii) experimental results showing curved displacement contour lines which is not captured by the theoretical result. Curved lines imply a top-down asymmetry in the displacement field, which in turn is due to the compressive and tensile stress fields of the dislocation as in Fig 1a.

Further, to compare the current model with the theory and with that of the experimental results [2] of the plot of σ_x along y-axis are considered in Fig.2. To interpret these plots the material rotation field [9] around the simulated dislocation is plotted in (Fig.3) which provides a better idea about the asymmetry. It is seen from Fig.2 that there is an excellent match between the simulated and theoretical results of σ_x except upto a distance of about 5 Å .On the other hand, a comparison of the theoretical values, which is zero along x-axis, with the model for σ_x shows a matching to 0.13 GPa at a distance of 75 Å starting with a difference of 4.5 GPa at a distance of 3.75 Å. This discrepancy can be understood by taking into account the material rotation field around a dislocation (Fig.3). Along the y-axis the material rotation is zero, which can be easily deduced from symmetry considerations and hence the standard theory (which does not take into account material rotation) is in excellent match with the simulated result. On the other hand along the x-axis there is significant material rotation near the core of dislocation, leading to deviation from the theory. This aspect is also is reflected in the curved displacement contours in the experimental results [2]. Another point, which can be noted from the comparison, is that the displacement contours of the experimental results are highly curved to a distance of 5 Å from the centre of the dislocation. This feature is also captured in the plot of the FEM calculated material rotation along the x-axis (Fig.4), wherein, the maximum value of the material rotation (~7 degrees) occurs at about 6 Å. It is important to point out that the small strain theory of elasticity is not valid in the core region of the dislocation. Hytch et al [2] have made numerical comparisons of the sinusoidal component of the displacement field with the theoretical expressions at a distance of 75 Å to an accuracy of 0.03 Å. Their choice of this distance can be better understood in the light of the above discussions.

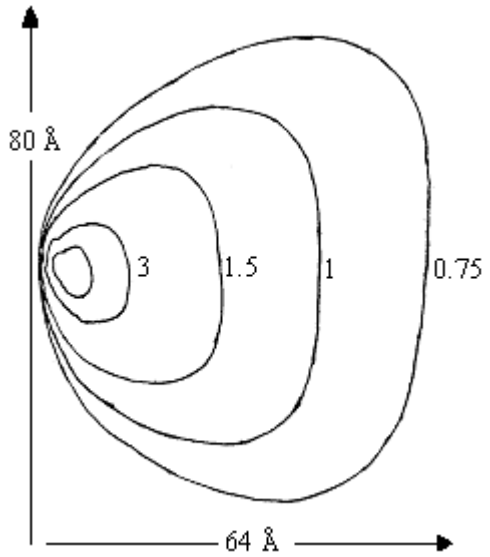

Fig.3.Material rotation in degrees contours in the symmetrical half of the domain around an FEM simulated edge dislocation

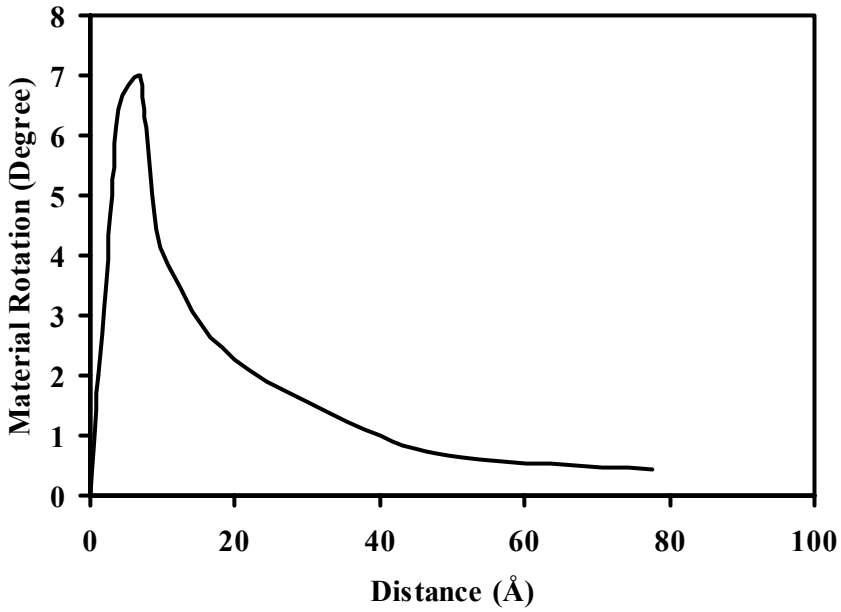

Fig.4.FEM calculated material rotation values for an edge dislocation along the X axis showing a peak value of 7˚ at a distance of about 6 Å.

In general, this simulated dislocation model can be used in various other-systems with complexity, like precipitates in metals, epitaxial superlattices and epitaxial islands. Calculations like critical thickness for dislocation nucleation in strained layer systems can also be performed. One such work for predicting the critical thickness of epitaxially built thin film is presented in [11]

Reference

1. Jain, S.C., Harker, A.H. and Cowley, R.A. (1997): " Misfit Strain and Misfit Dislocation in Lattice Mismatch Expitaxial Layers and Other Systems", *Phil. Mag.* Vol. A 75, pp.1461-1515.
2. Hytch, M.J., Putaux J .L. and Penisson, J .M. (2003): " Measurement of the Displacement Field of Dislocations to 0.03 Å by Electron Microscopy", *Nature,* Vol. 423, pp.270-273.
3. Benebbas, T., Francois, P., Androussi, Y. and Lefebvre, A. (1996): "Modelling of Iridium Rich Clusters in MOCVD", *J. Appl. Phys.* Vol. 80, pp.2763.
4. Hirth, J.P. and Lothe, J. (1968): *Theory of Dislocations,* McGraw-Hill, New York.
5. Weertman, J. and Weertman, J. (1964): *Elementary Dislocation Theory,* McMillan, New York.
6. Bollmann, W. (1970): *Crystel Defects and Crystalline Interface*, Springer-Verlag,Berlin.
7. Mura, T. (1987): *Micromechanics of Defects in Solids,* Martinus Nijhoff, the Netherlands.
8. Ramakrishnan, N., Singh, K.M., Suresh R. K. V. and Srinivasan, N. (1998): " An Algorithm Based on Total-Elastic-Incremental-Plastic Strain for Large Deformation Plasticity", *J.Mater.Proc.Tech,* Vol. *86*, pp.190-199.
9. Malvem, L. E. (1969): *Introduction to the Mechanics of Continuous Medium*, Englewood cliffs: Prentice-Hall, Chap.4.
10. Hull, D. and Bacon, D.J. (1984): *Introduction to Dislocations*, Pergamon Press: Oxford.
11. Subramaniam, A. and Ramakrishnan, N. (2003): " Analysis of Thin Film Growth using Finite Element Method ", *Surface and Coating Technology* Vol. 167, pp.249-254.