XIV International Conference on Computational Plasticity. Fundamentals and Applications
COMPLAS XIV
E. Oñate, D.R.J. Owen, D. Peric & M. Chiumenti (Eds)

RESIDUAL STRESS DEVELOPMENT AND EVOLUTION IN TWO-PHASE CRYSTALLINE MATERIAL: A DISCRETE DISLOCATION STUDY

T. N. Tak[*,a], A. Prakash [†], A. Lodh[††], I. Samajdar[†], and P. J. Guruprasad[*]

[*] Department of Aerospace Engineering,
Indian Institute of Technology Bombay,
Mumbai 400076, India
[a]e-mail: tawqeer.nasir@aero.iitb.ac.in

[†]Department of Metallurgical Engineering and Materials Science
Indian Institute of Technology Bombay,
Mumbai 400076, India

[††]IITB-Monash Research Academy,
Indian Institute of Technology Bombay,
Mumbai 400076, India

Key words: Residual Stress, Discrete Dislocation Dynamics, Geometrically Necessary Dislocations

Abstract. Crystalline materials undergo heterogeneous deformation upon the application of external load, which results in the development of incompatible elastic strains in the material as soon as the load is removed. The presence of heterogeneous distribution of elastic strains in the absence of any form of external load results in the building up of stresses referred to as residual stresses. The heterogeneity of strain is attributed either to the presence of multiple phases or to the orientation gradients across the sample volume. This paper is an endeavour to model the presence of second phase in a two-dimensional discrete dislocation dynamics framework, which already contains constitutive rules to include three-dimensional mechanisms, such as line tension and dynamic junction formation. The model is used to investigate residual stress development in single crystals subjected to plane strain loading and then subsequently unloaded to study residual stresses. The dislocation accumulation around the second phase and its effect on the mechanical properties is studied. The orientation dependence of residual stresses as a function of the underlying defect substructure has also been explored. A variety of results are obtained. In particular, the development of stresses as a function of underlying defect substructure is also presented and found to depend upon the orientation of the crystal.

1 INTRODUCTION

Metals and metallic alloys are essentially multiphase materials. The presence of multiple phases in a material completely changes the mechanical behaviour of the system ranging from the macroscopic stress versus strain response to the microscopic defect structure development, which in turn affects the life of a component by accelerating or decelerating failure. Presence of a brittle phase in a crystalline matrix may be detrimental as it tends to be a potential site for failure by giving rise to residual stress, due to the difference in properties between the two phases [1].

Residual stress development in metals and metallic alloys mainly depends upon the manufacturing process. These stresses can be removed by subjecting the material to a wide variety of treatments but cannot be completely nullified, which makes it important to study the development and evolution of the stresses of this type, more so in case of multiphase alloys where they play a crucial role in the failure of a material.

This paper is an endeavour to model residual stresses in a multiphase material using discrete dislocation dynamics (DDD), a framework that models the plastic deformation in crystalline materials as a collective motion of individual dislocations in an imposed displacement field [2], thus exploring a relation between the stress development as a function of defect substructure and establishing a signature of residual stress. Preliminary results that show interesting trends have been presented.

2 DISCRETE DISLOCATION PLASTICITY

The formulation constitutes of a framework for solving quasi-static initial/boundary value problems in which plastic flow is a direct consequence of collective motion of large number of dislocations [3]. The formulation presented here is valid for a material characterised by a linear elastic constitutive relation undergoing small deformation. The formulation is applicable for three-dimensional solids, but the implementation is carried out for plane strain problems.

A linear elastic body of volume V comprising of an elastic inclusion of volume V^* is considered. The matrix material contains a distribution of dislocations, modelled as line defects in elastic continuum. The elastic properties of the matrix and the inclusion are governed by the fourth order tensors $\boldsymbol{\mathcal{L}}$ and $\boldsymbol{\mathcal{L}}^*$ respectively. Each dislocation $\mathbf{i}$ is characterised by its Burgers vector, $\mathbf{b_i}$ and unit normal, $\mathbf{n_i}$ of its slip plane. The body with boundary $S_u \cup S_f$ is now considered to be subject to time dependent traction and displacement boundary conditions $\boldsymbol{T} = \boldsymbol{T_0(t)}$ on S_f and $\boldsymbol{u} = \boldsymbol{u_0(t)}$ on S_u respectively.

The ensuing deformation is assumed to be quasi-static and is limited only to small strains. The deformation process will lead to motion of dislocations, generation of new dislocations by nucleation and mutual annihilation, and their pinning at obstacles. The analysis of the deformation process is performed in an incremental manner in time where the incremental step at any time step involves three main computational stages. The first of them involving the computation of the current dislocation configuration and the associated stress and strain values for current configuration; the second step comprises of determining the Peach-Koehler force, driving force for change in dislocation structure, and the third being the determination of instantaneous rate of change of dislocation structure, computed on the basis of a set of constitutive equations for motion, annihilation and generation of dislocations.

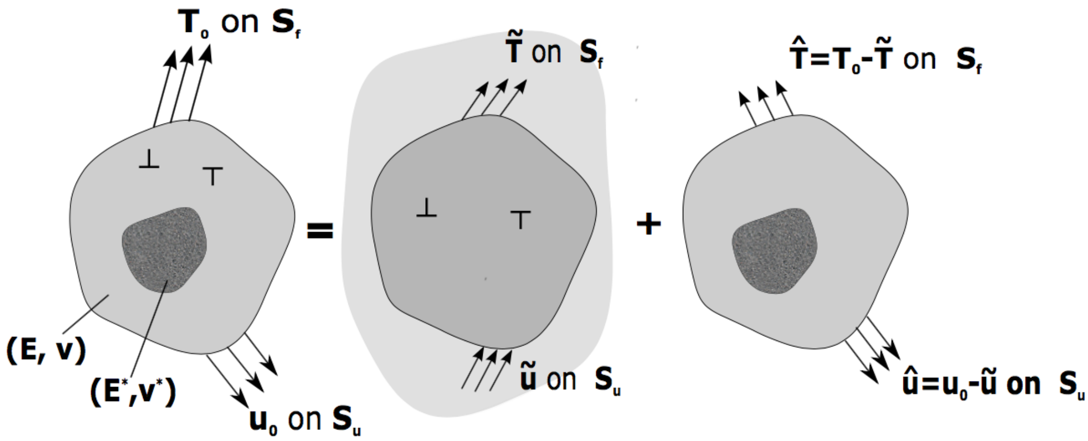

Figure 1: Decomposition of a problem for a body with dislocations and an inclusion into a problem of interacting dislocations in the infinite solid and a complementary field for the non-homogenous body without dislocations.

The formulation is based on decomposing the problem into two equivalent problems as shown in figure 1, one solving for the fields due to individual dislocations ($\sim$) and the other for the fields ($\wedge$) due to the external boundary conditions. After solving for the individual fields, the solutions are superposed. The first step, determining the instantaneous state of the body, involves determination of the current state of the body, which follows the formulation of [4] to determine the present dislocation structure and compute the current state of the body in terms of the displacement, strain and stress fields corresponding to the underlying dislocation substructure, and is written as the superposition of two fields,

$$\boldsymbol{u} = \tilde{\boldsymbol{u}} + \hat{\boldsymbol{u}} \qquad \boldsymbol{\epsilon} = \tilde{\boldsymbol{\epsilon}} + \hat{\boldsymbol{\epsilon}} \qquad \boldsymbol{\sigma} = \tilde{\boldsymbol{\sigma}} + \hat{\boldsymbol{\sigma}} \tag{1}$$

where ($\sim$) fields are associated with n dislocations in their current configuration but in an infinitely large medium of homogenous matrix material, and are obtained by superposition of fields of individual dislocations. Standard equations of linear elasticity are supposed to be valid outside the dislocation core area. These fields are obtained by superposition of fields $(\boldsymbol{u^i}, \boldsymbol{\epsilon^i}, \boldsymbol{\sigma^i})$ associated with each individual dislocation,

$$\tilde{\boldsymbol{u}} = \Sigma \boldsymbol{u}^i \qquad \tilde{\boldsymbol{\epsilon}} = \Sigma \boldsymbol{\epsilon}^i \qquad \tilde{\boldsymbol{\sigma}} = \Sigma \boldsymbol{\sigma}^i \tag{2}$$

The governing equations for $(\sim)$ fields can therefore be summarised as:

$$\nabla \cdot \tilde{\boldsymbol{\sigma}} = \mathbf{0} \qquad \tilde{\boldsymbol{\epsilon}} = \nabla \tilde{\boldsymbol{u}} \qquad \tilde{\boldsymbol{\sigma}} = \boldsymbol{\mathcal{L}} \colon \tilde{\boldsymbol{\epsilon}} \qquad \text{in} \quad V^M \cup V^* \tag{3}$$

with following boundary conditions on S,

$$\boldsymbol{\nu} \cdot \tilde{\boldsymbol{\sigma}} = \tilde{\boldsymbol{T}} \quad \text{on} \quad S_f \quad \text{and} \tag{4}$$

$$\boldsymbol{u} = \tilde{\boldsymbol{u}} \quad \text{on} \quad S_u \tag{5}$$

where ν is the outer unit normal to S. The absence of boundary conditions facilitates the finding of solution of the $(\sim)$ fields. Since the formulation has been restricted to the modelling of edge dislocations alone, the solutions are available in textbooks [5]. The $(\wedge)$ fields take care of the actual boundary conditions as well as the presence of inclusion. The governing equations may be written as follows:

$$\nabla \cdot \hat{\boldsymbol{\sigma}} = \mathbf{0} \qquad \hat{\boldsymbol{\epsilon}} = \nabla \hat{\boldsymbol{u}} \qquad \text{in} \quad V^M \cup V^* \tag{6}$$

$$\hat{\boldsymbol{\sigma}} = \boldsymbol{\mathcal{L}} \colon \hat{\boldsymbol{\epsilon}} \quad \text{in} \quad V^M \tag{7}$$

$$\hat{\boldsymbol{\sigma}} = \boldsymbol{\mathcal{L}}^* \colon \hat{\boldsymbol{\epsilon}} + (\boldsymbol{\mathcal{L}}^* - \boldsymbol{\mathcal{L}}) \colon \tilde{\boldsymbol{\epsilon}} \tag{8}$$

It is important to notice the contribution of polar stresses to the $(\sim)$ fields in the inclusion, which results due to the dislocation strain fields and the difference in the elastic properties between matrix and inclusion.

$$\boldsymbol{\nu} \cdot \hat{\boldsymbol{\sigma}} = \hat{\boldsymbol{T}} = \boldsymbol{T_0} - \tilde{\boldsymbol{T}} \quad \text{on} \quad S_f \tag{9}$$

$$\boldsymbol{u} = \hat{\boldsymbol{U}} = \boldsymbol{u_0} - \tilde{\boldsymbol{U}} \quad \text{on} \quad S_u \tag{10}$$

μ and B are used to denote the shear and bulk moduli of the matrix material where as μ^* and B^* represent the respective moduli for the second phase. The displacement fields due to the presence of dislocations in the matrix are assumed to remain smooth across the interface of the matrix and second phase, which makes the problem a well posed one and can be solved by using Finite Element Method.

For any dislocation configuration to be stable in a deformed body, it has to fulfil the conditions for thermodynamic equilibrium, which makes the rearrangement of dislocations a vital activity in a deformation process. The dislocations will time and again have to reorganise themselves to minimise the energy of the system. The rearrangement takes place under the action of a gliding force, referred to as Peach-Koehler force, which essentially can be described as the change of the potential energy of the body associated with an infinitesimal variation of the dislocation position in the glide plane. The expression for the Peach-Koehler force, f^i may be written as:

$$f^i = \boldsymbol{m^i} \cdot \{\hat{\boldsymbol{\sigma}} + \sum_{j \neq i} \boldsymbol{\sigma^j}\} \cdot \boldsymbol{b^i} \tag{11}$$

Short range interactions are accounted for by a set of constitutive rules for (i) dislocation nucleation, (ii) dislocation annihilation, (iii) dislocation obstacles, (iv) dislocation glide, (v) junction formation and (vi) dynamic sources. The three-dimensional interactions are modelled through constitutive rules.

In case of a two dimensional analysis, performed here, an initial density of sources and obstacles is specified a priori, each of them being a point source on a slip plane. Dislocations are nucleated in the form of dipoles when the magnitude of Peach-Koehler force at the location of the source i exceeds a critical value, for a prescribed time t_0. During the deformation, dislocations get pinned at these locations and are released only when the Peach-Koehler force exceeds $\tau_{obs} b_i$. While the number of sources remain constant throughout the entire deformation, the case is different in actual conditions, i.e., (i) the density of sources and obstacles increases as the dislocation density increases and (ii) line tension acts to restrict dislocation multiplication. These mechanisms are captured in two dimensions following the approach given in [6], wherein they have successfully been able to include key features of these interactions into two dimensional simulations to enable the dislocation source and obstacle population to evolve dynamically. This is achieved by modelling the formation of junctions upon the interaction of dislocations on intersecting planes. A junction, once formed, can act as a source or an obstacle to dislocations gliding on the slip plane, thus increasing the density of sources and obstacles with ensuing deformation.

3 RESULTS

To implement the framework discussed above using finite element method, a boundary value problem to simulate the uniaxial deformation of a planar crystal is formulated. A crystal of FCC type with dimensions, L x H with a second phase with dimensions w x h, as shown in figure 2, is subjected to compression followed by unloading along x_1-axis. Plane strain condition is invoked. A uniform displacement of $u_1 = \pm U/2$ and vanishing shear stress at $x_1 = \pm L/2$ is prescribed while a traction free condition is maintained at surfaces, $x_2 = \pm H/2$.

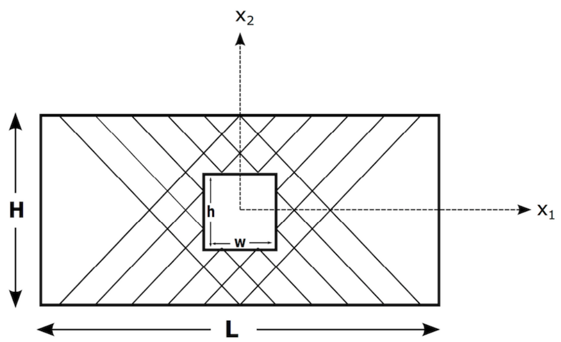

Figure 2: Geometry of the compression problem analysed for an FCC crystal with an inclusion oriented for double slip.

For the present simulations, a sample of dimensions 8μm x 4μm with a precipitate volume fraction $v_f^p = 0.03$ and dimensions 1μm x 1μm was used. The simulations were initially carried out for a single orientation with two slip systems oriented at $\phi = \pm 54.75^o$ to the loading x_1 axis. The slip planes are such that they extend from one free surface to another without intersecting the surfaces where the displacement boundary conditions are prescribed. The material was initially assumed to be dislocation free with initial source and obstacle density, $\rho_s = \rho_o = 1.56$ x 10^{13}m^{-2}. The static obstacles were assigned a constant strength $\tau_{obs} = 150$ MPa. The mean nucleation strength was taken to be $\tau_{nuc} = 17$ MPa. Standard values for other material parameters like Young's modulus $E = 70$ GPa, Poisson's ratio $\nu = 0.3$, drag factor $B = 10^{-4}$ Pa s, Burger's vector, $b = 0.25$nm, were used. For the second phase, the values for Young's Modulus and Poisson's ratio were taken to be $E = 500$ GPa and $\nu = 0.17$ respectively. Nucleation time remains fixed at t$_{nuc} = 10ns$.

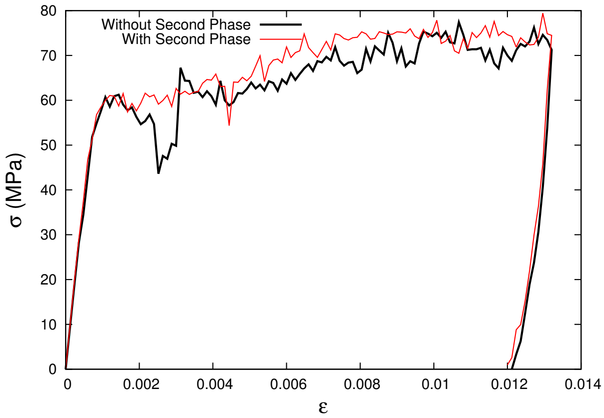

Figure 3: Representative stress versus strain response for an FCC crystal, with and without second phase, during loading and unloading.

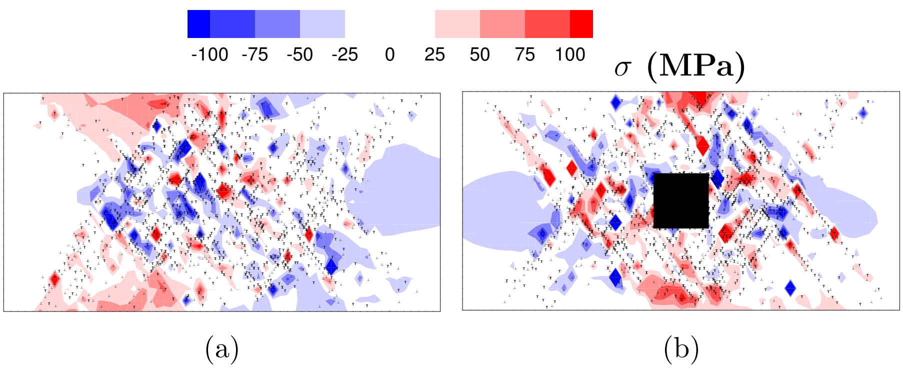

Figure 4: Contours showing residual stress distribution in a deformed sample after unloading for (a) without a second phase (b) with second phase

A nominal strain rate of the order of $10^4 s^{-1}$ was applied. The sample was loaded in simple uniaxial compression. With the nucleation of first dislocation loop, the material begins to yield. In order to demonstrate the effect of presence of a second phase particle in a material, two cases (i) a sample without a second phase and (ii) a sample with a second phase present in it, were simulated. Both the samples were loaded in compression up to a strain, $\epsilon = 0.012$ followed by unloading to a zero value of macroscopic stress, by reversing the direction of the applied load. Representative stress versus strain response was plotted, as given in figure 3.

From the results given in figure 3, it can be seen that the presence of a second phase in an otherwise homogenous matrix changes the mechanical response of the material; the sample with a second phase hardens more than the one without a second phase. This happens as a result of the obstruction to the flow of dislocations in the matrix caused by the presence of the second phase. It was observed that unloading to a zero value of finite body stresses doesn't make the material completely stress free. The average value of stress present in the sample in presence of a second phase, after unloading, was found to be σ = 2.67 MPa, which is more than σ = 1.968 MPa, the value obtained for the sample without a second phase. In order to relate the presence of these stresses with the underlying defect substructure, the geometrically necessary dislocation (GND) density was computed for both the cases. The GND density values for the sample with a second phase was found to be ρ_{GND} = 2.67 x 10^{12} m^{-2}, which is more than ρ_{GND} = 1.96 x 10^{12} m^{-2} observed in the sample without a precipitate, which suggests a correlation between the residual stress development and the GND density. This has also been illustrated by representing the dislocation configuration superimposed upon the stresses contours as shown in figure 4. It can be seen that in a material with second phase, the dislocation pile ups around the second phase lead to the accumulation of more residual stresses.

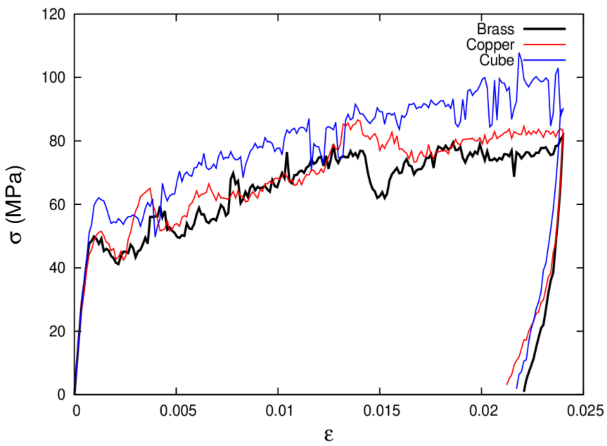

Figure 5: Representative stress versus strain response for an FCC single crystal with a second phase under compressive load for three different matrix orientations.

Additional simulations were carried out to study the orientation dependence of residual stress development in a material. Uniaxial compression tests, for three different matrix orientations, viz., Cube ({100} < 001 >), Brass ({011} < 211 >), and Copper ({112} < 111 >) were carried out. The samples were deformed upto a strain, $\epsilon = 0.023$ and were subsequently unloaded to a zero value of macroscopic stress as shown in figure 5. It was observed that the samples, after unloading, show a different distribution of residual stresses depending on their orientation, which is illustrated in the contours given in figure 6. The average values of residual stresses for the three different orientations were computed. It was found that Cube orientation develops the maximum residual stress, $\sigma_{Cube} = 4.93$ MPa, and Copper develops the least, $\sigma_{Copper} = 3.97$ MPa, while the residual stress value in the Brass orientation, $\sigma_{Brass} = 4.24$ MPa was found to lie midway between the two, which establishes the hypothesis that residual stress development in a two phase alloy is orientation dependent. A similar behaviour was observed for Bauschinger effect as well.

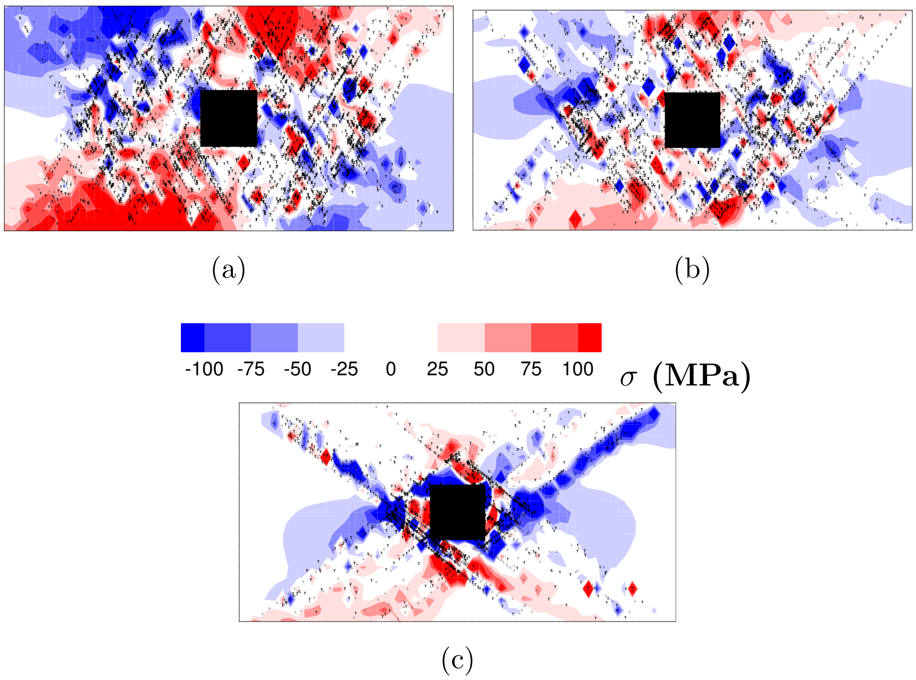

Figure 6: Contours showing residual stress distribution in a deformed sample after unloading for three different orientations (a) Cube (b) Brass (c) Copper

4 SUMMARY

A mechanism based discrete dislocation dynamics model was used to simulate the development of residual stresses in a two phase face centred cubic (FCC) material. It was observed that the presence of a harder phase in the matrix changes the mechanical behaviour of the material, which can be observed from a representative stress versus strain response, and leads to the hardening of material and development of residual stresses in a material. Moreover, it was also observed that the residual stress development in a two phase crystalline material not only depends upon the mechanical properties of the second phase but also the orientation of the matrix. A trend between the development of residual stress and defect substructure was observed.

REFERENCES

[1] Withers, P.J. and Bhadeshia, H.K.D.K. Residual Stress Part 1- Measurement techniques. *Mater. Sci. Technol.* (2001) **17**:355–365.

[2] Cleveringa, H.H.M., Van der Giessen, Erik, Needleman, A. A discrete dislocation analysis of residual stresses in a composite material. *Phil. Mag.* (1999) **79**(4): 893-920

[3] Van der Giessen, E. and Needleman, A. Discrete dislocation plasticity: a simple planar model. *Modelling Simul. Mater. Sci. Eng.* (1995) **3**(5):689

[4] Lubarda, V.A., Blume, J.A. and Needleman, A. An analysis of equilibrium dislocation distributions. *Acta Mater* (1993) **41**:625 - 642

[5] Dieter, G. E. *Mechanical Metallurgy.* McGraw-Hill Book Co. Newyork, Vol. I., (1986).

[6] Benzerga, A. A., Brèchet, Y., Needleman, A. and Van der Giessen, E. Incorporating three-dimensional mechanisms into two-dimensional dislocation dynamics *Modelling Simul. Mater. Sci. Eng.* (2004) **12**(3):557