An Intrinsic Dislocation Density – Finite Element Formulation Of Metal Plasticity

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Abstract:
A computational model was developed to simulate elastic and plastic behavior in Body Centered Cubic (BCC) metals and alloys. The model provided for simultaneous simulation of the micro and macro length scales and used periodicity to link the two length scales. The model was implemented in a 3dimensional framework giving rise to a finite element technique incorporating intrinsic dislocation information in the simulation of the material's behavior. The technique was validated by simulating loading over the elastic range and the immediate region beyond yield, of thin steel strips, and comparing the results to those obtained by conventional analysis. Stress-strain curves and slip plane percentage contribution factors were generated. Specifically the stress-strain curves generated upheld Hooke's law and demonstrated a definite yield plateau followed by material recovery after yielding.

Key words: Dislocation density, Multi scale, Percentage slip plane contribution

Notation:

- B - Dislocation mobility (Pa. sec.)
- **b** - Burgers vector
- dl - Length of dislocation segment (m)
- E_e - Young's Modulus for Loading Excluding dislocation information (N/m^2)
- E_p - Young's Modulus for Loading Including dislocation information (N/m^2)
- $E(\beta)$ - Pre-logarithmic energy coefficient (J)
- G - Shear Modulus (N/m^2)
- **R** - Relative position vector for interacting dislocation segments (m)
- T_e - Temperature (deg. K)
- t - Thickness (m)
- V - Representative volume (m^3)
- W - Energy per unit volume (J/m^3)
- ΔW_{pm} - Work done in dislocation motion (J)
- ΔW_{pf} - Work done in net dislocation formation (J)
- ΔW_{pi} - Work done as the dislocations interact (J)
- ΔW_{po} - Work done in overcoming the obstacles to dislocation motion (J)
- α - Constant of proportionality
- β - Dimensionless constant
- β_t - Outer radius of dislocation cylinder (m)
- ΔG - Gibbs free energy (J)
- ε_e - Strain tensor

v - Glide velocity (m/s)
θ - Grain boundary mis-orientation angle (radians)
ρ - Dislocation density (m/m^3)
ρ_o - Density of obstacles to dislocation motion (m^{-3})
σij - Stress tensor (N/m^2)

1. Introduction

Traditional use of numerical techniques for structural analysis applies constitutive relations that are based on average material properties [1]. While being convenient and sufficient for use in elastic deformation problems, they are however at best coarse approximations in their use in large strain problems and problems where size effects are significant [1]. The search for more accurate relations based on a physical and mechanistic foundation has resulted in the micro structural approach. The micro structural approach looks at materials using length scales in the order of 10^{-5}m to 10^{-10}m [2], and involves the monitoring of the movement of atoms and atomic defects that contribute to material deformation and is used to aggregate these contributions to predict macroscopic strain. A fully micro structural approach is however computationally costly due to the large number of degrees of freedom involved. A blend between the micro structural and macro structural analysis has been proposed and involves two or more length scales. The macro structural approach involves the use of length scales in the order of 10^{-3}m and above.

Multi scale material modeling is a modern technique in the field of structural mechanics that is capable of analyzing structures in at least two different length scales [2]. This method has evolved from the field of materials modeling where it was understood that a material's response is profoundly influenced by its microstructure. The need to understand the mechanisms responsible for material behavior and the development of microstructure-property correlations has driven the development of theory and simulation of material behavior. Several techniques have emerged differentiated by their treatment of the micro scale of the problem [2-6].

The commonly used constitutive relations are based on the macro scale approach which ignores the random occurring micro structure to enable the use of averaged material property constants giving reasonable results. The micro structural behavior is based on a phenomenological approach in which the material behavior is modeled along phenomena observed during empirical tests. Alternatively it is based on a mechanistic approach where true material deformation mechanisms are simulated and therefore a more realistic model of the material's micro structural response is obtained. Most previous research work has addressed the use of the phenomenological foundation [2] and opportunity exists to incorporate a mechanistic foundation with the obvious results of negating the need to assume any specific degradation phenomena in the deformation process.

Several researchers have contributed to the development of the so-called discrete dislocation techniques where a continuum finite element model is extended to include individual dislocations [7, 8]. Only their Burgers vectors, and their core locations through stress and displacement fields that they induce, are used to represent these dislocations. The discrete dislocation approach accurately describes the long-range interactions between dislocations but cannot be described as a truly atomic scale phenomenon.

The standard discrete dislocation formulation for the inhomogeneous problem of an elastic-plastic body containing an elastic inclusion was derived by Van der Gissen and Needleman [9]. This method models edge dislocations as line defects in an isotropic elastic material constrained to glide on a fixed slip plane. Long-range dislocation interactions occur through their continuum elastic fields while short-range interactions are governed by constitutive rules for dislocation nucleation, motion and annihilation. This method's capacity is limited by the computation of the polarization stress, which corrects for the prescience of the inclusion, which dominates the finite element calculation when the number of dislocations becomes large.

A superposition technique of the discrete dislocation method, as developed by O'day et al. [10] resolved the problem associated with the polarization stress in the standard discrete dislocation method. In this approach the regions of elastic in-homogeneity and the area of the inclusion are handled separately and superimposed onto the fully elastic solution. The technique is therefore advantageous as it may be used in elastically in-homogeneous problems with large numbers of dislocations or many inclusion elements.

The use of 3D discrete dislocation method in the study of small scale plastic phenomena was reported by Zbib et al. [11]. This three dimensional continuum based finite element formulation for elastic-viscous-plasticity incorporates discrete dislocation simulation replacing the usual plasticity constitutive relations. The superposition principle is utilized in order to find the effects of boundaries on the dislocation movement and the multi-scale frame merges the two scales of micro-scale where plasticity is determined, to the continuum scale where the energy transport is based. This technique uses a two stage computation which makes the method computational expensive. The evaluation of the dislocation forces requires very fine mesh particularly when dealing with dislocation-defect interaction [11]. As a result, to capture the effects of small defects, the dislocation segment size must be comparable to the size of the defect. This requirement adds a further computational load to the simulation process by making it necessary to make several simulations before appreciable macro strain is achieved. To achieve 0.3% strain over one

million iterations are required [11]. As a result application is limited to nano-technology. Opportunity exists for researchers to overcome these drawbacks and extend the technique to larger sized structures.

Atomistic to continuum modeling methods are either simultaneous or sequential in their implementation. The Quasi Continuum approach [5] is one method where simultaneous/concurrent solution of the governing equations at multi scales is employed. 'Handshake' algorithms are used to bridge neighboring regions of different resolution. Other such methods include the Three-scale Bridging technique by Broughton et al [12] and the Dynamic Bridging Scale method by Park el al [13]. These methods have been applied successfully in the solution of problems where the bulk material remains relatively homogeneous and the micro scale is confined to a relatively small volume. Sequential/decoupled methods do not involve direct matching of boundary conditions at multiple length scales. Instead lower length scale simulations generate information that is used as input data in higher length scales. Atomistic simulations of motion of a representative number of atoms were used by Hao et al [14] to generate bulk elastic and plastic properties while Spearot et al [15] used them to generate interfacial properties. Clayton et al [16] used atomistic simulations to generate displacement gradients which were transferred across length scales. These methods can be used where a small group of defect types are considered under periodic conditions which enable the micro scale simulation to as reasonably small as possible.

Several methods have been presented for the development of variational principles for materials with microstructure. Svendsen [17,18] presented a thermodynamic model for materials with internal degrees of freedom. The model is cast in a variational formulation founded upon a dissipation rate density based on a dissipation potential. Cermelli et al [19] presented a formulation of a variational principle consisting of an energy functional for a body containing isolated defects in terms of a regular function of the defect configuration. The method avails a basis for the study of a finite set of dislocations and is illustrated in the study a finite number of Volterra dislocations in a plane domain. Groma et al [20-22] proposed a variational method to calculate the stress field generated by a system of dislocations. The principle is restricted to the small deformation limit theory and the functional is sum of the elastic Gibbs free energy and a term representing the interaction of the defects and the stress field. The method allows for the study of a wide range of problems as illustrated in the study of core regularization problems and dislocation-solute interaction.

In all these approaches the variational methods provide systematic and compact technique to study the problems at hand while allowing relatively simple accounting of the physical interactions. These methods however focus on a global thermodynamic evolution based on small strain theory and do not differentiate various dislocation constitutive behaviour. A formulation for large strains and the capacity to account for different dislocation evolution phenomena needs to be developed. In addition a formalization that captures the interactions at the dislocation core and its integration into a meso scale dislocation density variational principle is required. An extended review of dislocation dynamics applied to multi scale techniques is found in [23].

2. Materials and Methods

2.1. Model Development

This work developed a framework that incorporated the dislocation information in a continuum finite element model, under quasi static conditions. The underlying objective was to formulate a finite element technique capable of single cycle micro-macro evaluation of elasto-plastic deformation of structures. It formed the basis of a dislocation density continuum approach that could be extended to a variety of materials based boundary value problems.

From the principle of conservation of energy, work done by external loads in plastic deformation at room temperature, W_P, is dissipated in the evolution of the micro structure consisting of dislocation fields in material matrix [24]. Consequently, W_P equals [24]

$$W_p = \int_V \Delta W_m \, dV \quad \ldots (1)$$

The work done in the evolution of the microstructure ΔW_m is a sum of the contributions of dislocation motion, dislocation formation and annihilation, dislocation interactions and work done against obstacles to dislocation motion as shown in Fig. 1, and may be summarized in the relation

$$\Delta W_m = \Delta W_{pm} + \Delta W_{pf} + \Delta W_{pi} + \Delta W_{po} \quad \ldots (2)$$

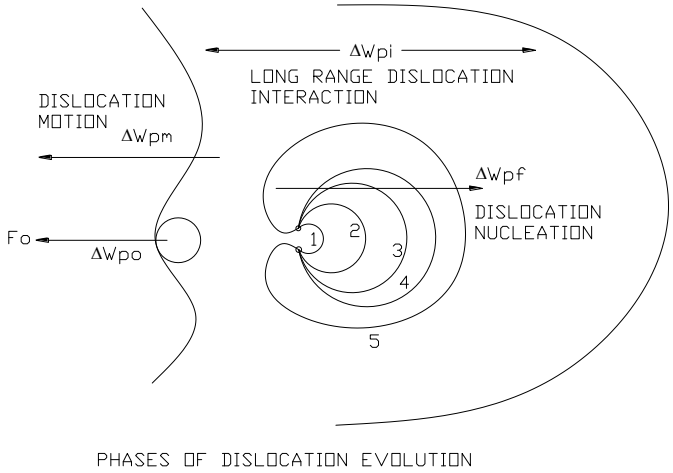

Fig. 1: Work done in dislocation evolution

Under adiabatic conditions, work is done at the expense of the strain energy of the total system. The above various contributions are developed as follows:

Work done in dislocation motion ΔW_{pm} is given by the relation [24]

$$\Delta W_{pm} = \int_u \int_l \left[\left(b_p . \sigma_{ij} \right) x dl_p \right] du \quad \ldots\ldots(3)$$

where

b_p is the burgers vector for segment 'p'

dl_p is the length of segment 'p'

du is the displacement of segment 'p'

Work done in net dislocation formation, ΔW_{pf} includes work in total dislocation formation less the work done in dislocation annihilation. This work is equal to the net change in elastic strain energy of the elemental volume with change in total length of dislocations contained and is given by the relation [24]

$$\Delta W_{pf} = \int_u \int_l E(\beta) \ln \left(\frac{\alpha |\beta_t|}{|b_t|} \right) d(dl_t) \quad \ldots\ldots(4)$$

Consider two dislocation segments denoted "p" and "q" and separated by a vector **R**. Work done as the dislocations interact ΔW_{pi} is given by [24]

$$\Delta W_{pi} = -\frac{G}{2\pi} \int_u \int_l \left(\frac{(b_p x b_q).(dl_p x dl_q)}{R} \right) + \frac{G}{4\pi} \int_u \int_l \left(\frac{(b_p . dl_p).(b_q . dl_q)}{R} \right) + \frac{G}{4\pi(1-\upsilon)} \int_u \int_l \left\{ (b_p x dl_p).T.(b_q x dl_q) \right\} \quad \ldots\ldots(5)$$

where $T = \dfrac{\partial^2 R}{\partial x_i \partial y_j}$

Work done in overcoming the obstacles to dislocation movement is ΔW_{po}. This work, done by slow moving dislocations, is modeled as a varying body force over the elemental volume acting normal to the dislocation line. The body force is determined by obtaining the activation energy for dislocation motion against these effects as a function of the number of discrete obstacles and summing over an elemental volume to give [24]

$$\Delta W_{po} = \iint_{ul} \Delta G . \rho_o . dl . du . t + \iint_{ul} B . v . dl_p . du \quad \ldots\ldots\ldots(6)$$

The work allows for invariance of the micro structural properties of the material hence $\Delta G, \rho_0$ *and* t are constant. The physical interpretation of this constraint is that dislocation obstacle's dissipative strength and density, and the slip plane spacing are maintained constant. Having provided for slow moving dislocations, dislocation mobility and velocity are also assumed constant.

A dislocation length function

$$l = f(u) \quad \ldots (7)$$

is adopted and as a first approximation, the dislocation is modeled as a near circular boundary between the slipped and un-slipped portions of the crystal about the slip plane. Consequently, the dislocation function is written as

$$l = 2\pi u \quad \ldots (8)$$

Using equations (3), (4), (5), (6) and (8) in (2), expanding the cross products in terms of the alternating tensor, using $(\mathbf{b}_{p}.\sigma_{ij}) = S_j$, and rewriting gives

$$\Delta W_m = \frac{1}{2\pi}\int_u\int_l \left[S_j dl_p \varepsilon_{jpk}\right] dl_k + \int_u\int_l E(\beta)\ln\left(\frac{\alpha|\beta_t|}{|b_t|}\right) n_t d(dl_t) - \frac{11G}{4\pi}\int_u\int_l \left(\frac{b_p b_q dl_p dl_q}{R}\right) + \frac{1}{2\pi}(\Delta G.\rho_o.t + B.v)\int_u\int_l dl_p dl_p \Big\} \ldots (9)$$

Equation (9) is the dislocation evolution energy functional for a micro element 'm', with the dislocation displacement expressed in terms of the dislocation segment length. This expression is integrated over the meso scale into the macro scale and combined with the elastic strain energy of a macro scale element to yield the following expression

$$\Pi_{pe} = \int_V \left(\varepsilon_e^T \sigma_e + u_e^T X_e\right) dV + \int_\zeta \left(u_e^T P_e\right) d\zeta + \int_V \Delta W_m \ldots (10)$$

Equation (10) is the total energy functional for a macro element incorporating two variables, the macro scale displacement u_e and the micro scale dislocation segment length dl. Applying variational techniques in minimizing this relation with respect to the macro scale displacement and the dislocation length yields an equilibrium equation governing the evolution of elasto-plastic behavior of the material. This formulation employs the simultaneous form of multi scale technique as the solution of the micro scale and macro scale are handled simultaneously with periodicity used to couple the two length scales.

2.2. Implementation

Thin strips were subjected to loading cycles with loads varied from 0.04 to 3.0 times the estimated yield stress with equal load increments. The maximum induced stress and its corresponding induced strain over the length of the sample for each loading cycle were recorded. A constant obstacle density of $1\text{x}10^{11}$ /m^3 and a constant stored dislocation density of $5\text{x}10^{12}$ m/m^2 were used. Mobile dislocation densities were generated by a stress based function [25]

$$\rho = (\sigma_{max}/(0.4 * G * b))^2 \ldots (11)$$

where the generated stress from the aprior loading cycle was used as an input. Dislocation nucleation was intrinsically accounted for in the increments to dislocation densities across the simulation cycles. Grain boundary dislocation density was generated by a quadratic function [25]

$$\rho_m = (\theta/b)^2 \ldots (12)$$

dependant on the angular mis-orientation across the grain boundary which in turn was related to the generated stress.

$$\theta = \theta_{min} + \left((\theta_{max} - \theta_{min}) * \left(\frac{\sigma_{max}}{G}\right)\right) \ldots (13)$$

Single dislocation density values were used for each micro scale cell and the interaction between the various dislocation families was expressly captured in the dislocation evolution energy functional. Grain boundaries were naturally generated as the boundaries of the micro structural cells with a wavelength of 50nm.

3. Results And Discussion

Simulations were carried out to evaluate the contribution of the {110}, {112} and {123} slip planes. A percentage slip plane contribution 'a-b-c' was defined where 'a' was the contribution of the {110} plane, 'b' was the contribution of the {112} plane and 'c' was the contribution of the {123} plane. These simulations were used to investigate the performance of the model in three areas. The first was where the {110} slip plane provided low percentage slip plane contribution contrary to observations from crystal geometry studies [24]. The second was where the {112} and {123} slip planes provided equal contributions again contrary to observations from crystal geometry studies [24]. The results obtained from these simulations showed that the

simulation resulted in scattered data leading to the inference that this model correctly demonstrated that low percentage contributions by the {110} plane and equal contribution by the {112} and {123} planes did not occur. The third was where the {110} slip plane was the main plane of activity and hence had the highest percentage slip plane contribution consistent with observations from crystal geometry studies [24].

The second validation criterion was generation of acceptable deformation curves. Fig. 2 shows curves incorporating dislocation information simulations for percentage slip plane contribution 70-25-5, 75-20-5, 80-15-5, 75-25-0, 80-20-0, 90-10-0 and 95-5-0.

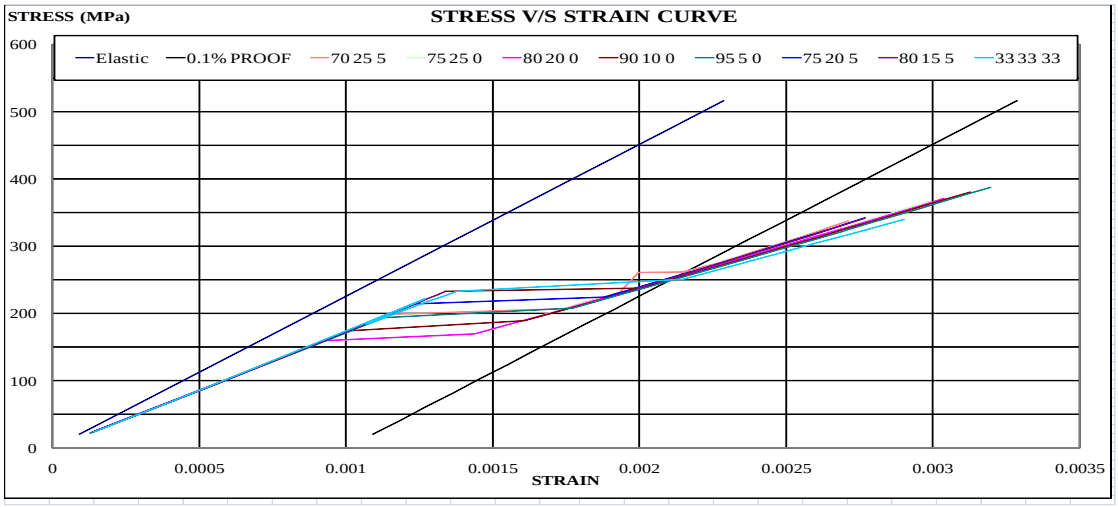

Fig 2: Stress/Strain curves for coarse mesh simulation for various slip plane percentage contribution

The elastic range of these curves consisted of straight lines. This indicated that the stress was proportional to the strain despite the incorporation of dislocation information, and Hooke's law was upheld. Elastic constants C_{11}=24.2, C_{12}=14.65, C_{44}=11.2, G =8.6, poisons ratio of 0.291 [24] were used as input data. Young's Modulus obtained for these curves lay between 171-174 GPa which was 17% below the value of 206 GPa obtained from conventional analysis for low carbon steels [26]. This was attributed to the fact that crystal material properties used in the dislocation data were for perfect, stress free iron crystals grown in controlled conditions. These did not incorporate the effects induced by carbon content and other alloy constituents that strengthen typical steel materials at the macro level. The model therefore conformed to the expected behavior in the elastic region of loading with dissonance occurring only in the value of the Young's Modulus.

In addition the curves showed a "plateau" yield at near constant stress as dislocation contribution become significant. The ability of the formulation to predict yield was considered a major achievement and this was consistent with existing knowledge that dislocation evolution was the principal contributor to plastic flow.

These results also showed that as the percentage contribution of the {110} slip plane was increased, the yield stress increased. This indicated that the existence of the {112} slip plane resulted in a weaker material matrix. This was consistent with the fact that the {112} slip plane is a twinning plane consisting of a material defect with lower slip activation energy levels [24]. In addition, the two-slip plane systems exhibited lower yield values than the 3-slip plane system. This suggested that the {123} slip plane required larger amounts of energy for activation of slip than the other two slip planes. This again was consistent with empirical evidence as the {123} slip plane is active only at elevated material temperatures which provide the additional slip activation energy required.

The post yield behavior for all the cases studied showed material recovery and a straight line post yield behavior of gradient 117-124 GPa. The recovery was attributed to the countering of the dissipative effects of the dislocations by the strengthening effects of the increased dislocation density. The simulations generated an almost constant gradient post yield curve. This was contrary to experimental observation and was attributed to the use of a constant stored dislocation density and a stress based dislocation density algorithm. It is proposed that future work focus on the development of dislocation density evolution algorithms.

Key to this formulation was the notion of the "percentage slip plane contribution". Drawing from minimization concepts a plot of the Yield stress versus the {110} percentage slip plane contribution for 2 plane systems were prepared and is shown in Fig. 3. The results presented show a minimum yield stress of 159MPa at 75% {110} percentage slip plane contribution for the 2 slip plane system for all obstacles densities equal to or less than $10x10^{21}$. At $10x10^{24}$ the yield stress dropped to 137MPa but at

the same slip plane contribution. This common minimum suggested that the representative Yield Stress was in the order of 137MPa to 159MPa at a {110} percentage slip plane contribution of the order of 75%.

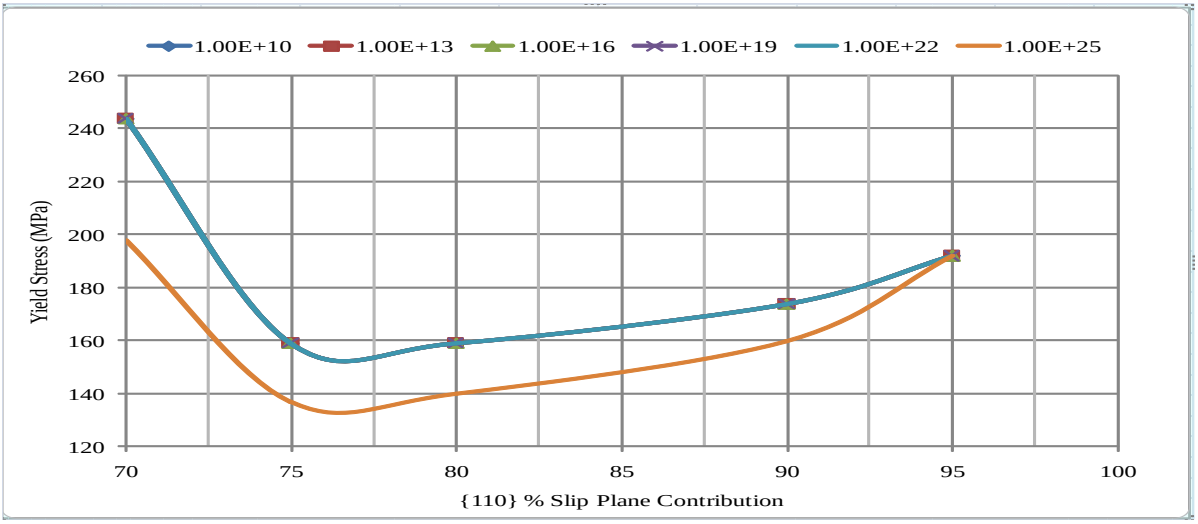

Fig 3: Yield Stress v/s {110} Slip plane percentage contribution For 2 Plane Slip System for Various obstacle densities

The formulation utilized a black box technique to superimpose dislocation information onto an elastic matrix thereby precluding the need to monitor individual dislocation segments. This was one of the principal advantages of the method as the simulation's demand for computational power approached that of standard elastic analysis with the only additional load existing in the micro element's material property computation. The 3D discrete dislocation formulation [11], executed a variable time step and simulation cycles were in the order of one million to achieve a strain of 0.3% for nano-scale samples. The method presented in this paper achieved similar strains in 25 cycles which took approximately 2 seconds for "coarse mesh" of 40 finite elements and 76 seconds for "fine mesh" of 240 finite elements.

It was found that the method was not constrained by large increases of dislocation segments which posed a computational challenge during the evaluation of the polarization stress for the standard discrete dislocation method. In addition, the method was not limited to nano-technology, again due to the computational challenge encountered as was 3D discrete dislocation method. The method did require the differentiation of the levels of initial plasticity across the specimen as did the superposition discrete dislocation method and this was conveniently achieved by specifying initial dislocation densities values at the macro scale. Traction boundary conditions were also handled at the macro scale.

4. Conclusion

This work detailed the development and evaluation of a variational technique that utilized a discrete dislocation formulation in a black box finite element technique. The dislocation information was contained in a scalar density function. The results confirmed that this minimization of total energy involving two length scales, and the correlation of dislocation segment lengths and dislocation densities was acceptable.

The results agreed with existing literature and it was observed that slip plane activity was shared between a {110} slip plane and the {112} slip plane. In addition the results were consistent with empirical findings that indicated that the {110} slip plane had higher slip activation energy than the {112} slip plane, and the {123} plane required the highest slip activation energy normally provided in high temperature loading.

The model correctly simulated elastic behavior and upheld Hooke's law. The model also correctly simulated material yielding and post yield material recovery. However the choice of dislocation density evolution algorithm was considered to be a critical component in the model's inability to simulate post yield strengthening.

The method successfully demonstrated the direct use of dislocation evolution information in an elastic finite element simulation to generate elastic behavior and elastic-plastic transition.

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