MODELING THE BRITTLE-DUCTILE TRANSITION IN FERRITIC STEELS—S. J. Noronha and N. M. Ghoniem (University of California, Los Angeles)

OBJECTIVE

To model the brittle-ductile transition in terms of basic dislocation mechanisms; so that a) the effect of irradiation and consequent microstructural change on DBTT can be predicted, b) to estimate the plastic work done theoretically from the dynamics of dislocations around the crack-tip and c) to the explain the physical basis of master-curve hypothesis.

SUMMARY

The crack tip plastic zone is represented using an array of dislocations emitted from the crack-tip plasticity on loading. The dislocations emitted shield the crack-tip, thereby enhancing the applied stress intensity for fracture from the Griffith value. The stress intensity at fracture is thus a function of the dislocation distribution around the crack tip. This distribution in effect is controlled by the mobility and nucleation energy of dislocations. The method is used to simulate the case where microcracks in the plastic zone of the macrocrack initiate cleavage fracture.

PROGRESS AND STATUS

Introduction

It is now a well-accepted fact that cleavage in ferritic steels in the lower shelf and near the transition temperature is controlled by the microcracks originated in the precipitates. We model the system using a microcrock in the field of macrocrack, both emitting dislocations and generating plastic zone. We outline the details of the model and the calculation procedure in the next section. The results obtained are described in the following section. We also compare our predictions with experimental results reported in the literature. Finally we discuss possible improvements to our model.

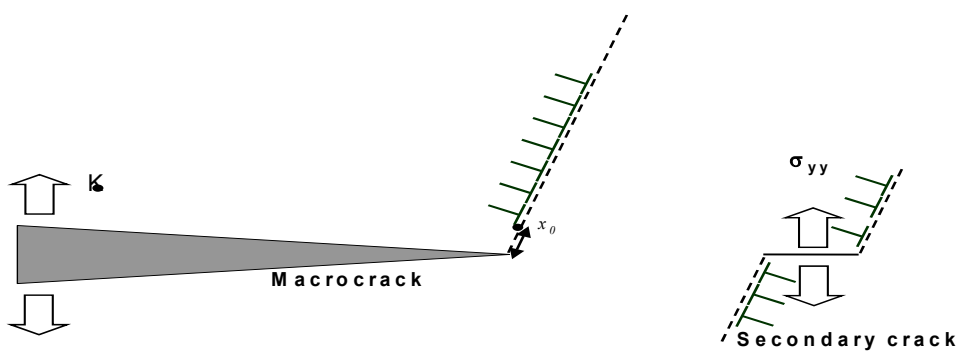

Fig. 1. The geometry of crack and dislocations used in the 2D coupled macrocrack-microcrack simulation model.

Model and Method of Calculation

The geometry of the 2-d model used is shown in Fig. 1. A semi-infinite crack (macrocrack) with a finite crack (microcrack) situated ahead of it in its crack plane is loaded. A dislocation

source is assumed to exist at a distance x_0 from, and situated on the slip plane passing through, each crack tip. The value of x_0 used in simulation is *10b*, where *b* is the burgers vector; the slip plane is oriented at an angle of 70.5^0 to the crack plane. A dislocation is emitted when the resolved shear stress on a dislocation at x_0 is greater than τ_f. Where τ_f is the friction stress used and is chosen to be equal to $\sigma_y/\sqrt{3}$, where σ_y corresponds to the uniaxial yield stress at a given temperature. The temperature dependence of fracture toughness is then obtained by inputting the corresponding friction stress value. The resolved shear stresses are obtained using expressions based on derivations for semi-infinite crack [0] and finite crack [0]. The emitted dislocations move along the slip plane away from the crack tip, and the stress at the source increases until another dislocation is emitted. (For each positive dislocation emitted, a negative one is assumed to move into the crack.) In the case of microcrack, the sources on opposite sides of the crack are at equivalent positions x_o and operate simultaneously. (This ensures that no net Burgers vector remains in the crack). Dislocations are assumed to move with a velocity v given by

$$\mathrm{v}_{x_i} = \left(\frac{\left|\tau_{x_i}\right|}{\tau_0}\right)^m \mathrm{v}_0 \left(\frac{\left|\tau_{x_i}\right| - \tau_f}{\tau_{x_i}}\right) \qquad (1)$$

for $\left|\tau_{x_i}\right| > \tau_y$ and v = 0 for $\left|\tau_{x_i}\right| < \tau_f$. The computations were carried out with m = 2.67 and v_0 = 4.5 x 10^{-10} ms^{-1}, appropriate to the velocities of screw dislocations in iron at 273K [0]. During the simulation, the applied stress intensity is increased in small increments and the positions of dislocations are determined. It is found that the dislocations reach near equilibrium positions. It should be noted that with the dislocations in near-equilibrium positions, the temperature and strain-rate dependence of K_F, the numbers of dislocations emitted at fracture, and the plastic zone size are determined only by the temperature and strain-rate dependence of the yield stress, σ_y.

The emitted dislocations shield the crack from external load by compressive stresses they exert at the crack tip. The shielding stress intensity factor for each dislocation (K_D) is calculated at each crack tip. The expressions for semi-infinite were used from [0] and that for finite crack from [0] and the total net shielding stress intensity factor is obtained by summation. The fracture criterion for this model is a critical crack-tip stress intensity of the microcrack. Thus, when $k = K_{IC}$, cleavage fracture of the matrix is assumed to occur; the applied load at the macrocrack, K_A then gives the critical loading for fracture propagation K_F and the microscopic cleavage fracture stress (σ_F) is the net stress due to the macrocrack field and the array of dislocations emitted from it.

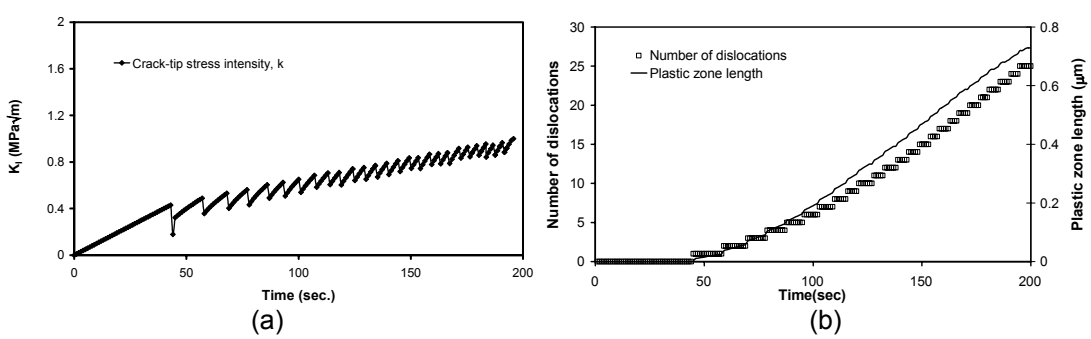

Fig. 2(a). The stress intensity at the micocrack tip and as a function of simulation time; crack size=1μm, yield stress=800 MPa; (b) The number of dislocations and the plastic zone length as a function of simulation time; crack size=1μm, yield stress=800 Mpa.

Results and Discussion

A typical behavior of the crack tip stress intensity at the microcrack(k) while it is loaded is shown in Fig. 2a. The fracture criterion in this case is k reaching a critical value (chosen as 1 MPa√m, an approximate value for pure cleavage to occur in Fe). Each drop in the curve corresponds to the dislocation emission at the crack-tips. The emitted dislocations shield the crack and enhance the stress required for cleavage. The amount of shielding (K_D) can be interpreted as the *plastic work during crack propagation*. In this case, the microcrack size is 1μm, the yield stress is 800 MPa and the rate of loading, dK/dt = 0.01 MPa√m s^{-1}. Fig.2b shows the number of dislocations and length of the plastic zone developed at the microcrack tip with the progress in simulation.

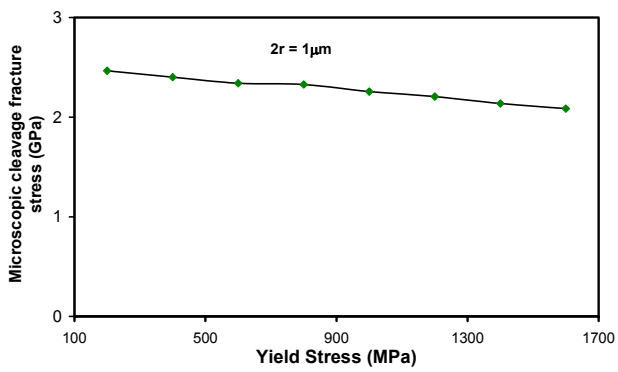

Fig. 3a. The stress at the particle at fracture as a function of yield stress.

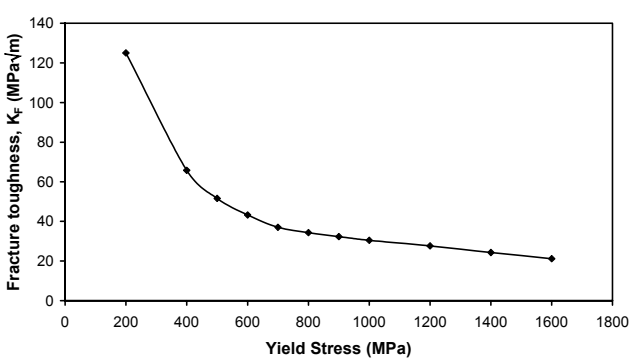

Fig. 3b. The fracture toughness as a function of yield stress, the criterion of fracture is the critical crack-tip stress intensity of the microcrack.

A microcack of size 1μm is placed at a distance of 10μm from the macro crack tip (10μm is the average distance obtained in [4] with which we compare our results). Fig. 3a shows the variation of microscopic cleavage fracture stress (σ_F) (that is the net stress due to the macrocrack stress field and the dislocation array developed at the macrocrack at fracture) as a function of yield stress is less than 10% consistent with the experimental observations. Fig. 3b shows the macroscopic fracture toughness, K_F as a function of yield stress. There is sharp increase in the fracture toughness at low yield stresses, which correspond to the transition from brittle to ductile behavior. However this sharp upturn is not captured when we map the fracture toughness as a function of temperature, since the variation of yield stress at or near the transition-temperature region is found to be weak. In Fig.3c portion of the fracture toughness curve in Fig.3b is mapped to temperature using experimental yield stress [4] to obtain the brittle-ductile transition curve. We can see that model fits well to experim-

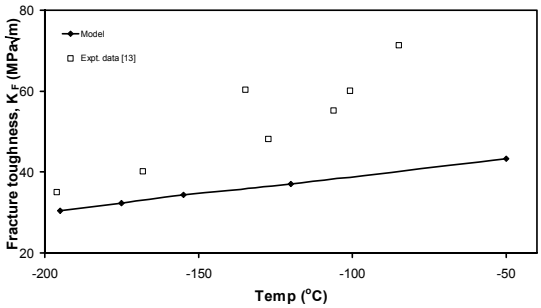

Fig. 3c. The fracture toughness values from above Fig. (5a) mapped to temperature and the experimental fracture toughness.

ental results at lower shelf fracture toughness; however it does not predict the sharp upturn at the transition. Note, the yield stress range to which we could map the data is very narrow (600-100MPa), due to the unavailability of data for a broader temperature range. Also our model does not consider dislocation multiplication, which will have significant effect at lower yield stress or high temperature regime.

Conclusions and Outlook

The, 2-d dislocation dynamics is used to study the crack system involved in the fracture of ferritic steels; a macrocrack with microcracks ahead of it. The dynamic interaction between dislocations emitted from both macrocrack and microcrack has been included. The crack-tip behavior and the predicted brittle to ductile transition have good agreement with experiment at the low temperature region. However the model does not predict the sharp upturn near the transition temperature. It should be noted that our simulations do not involve dislocation multiplication processes, which become significant at higher temperatures near the transition temperature. This draw back could be overcome by carefully devising local rules using 3D dislocation simulations, which is now in progress.

Acknowledgements

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References

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