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AN INTEGRATED MULTISCALE COMPUTATION MODEL TO LINK ATOMIC AND CONTINUUM APPROACHES

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ABSTRACT

Materials fracture often involves various length scales from dislocation evolution at the atomic scale level to crack propagation at the continuum levels. In this study, an integrated multi-scale model is proposed by concurrent coupling an atomic region, a meso-scale region and traditional continuum region. The meso-scale region is defined as a region with subcracks in comparison with a main large crack. The atomic region is solved by the molecular dynamics method and the meso-scale region is a finite element region where potentials in various forms may be introduced as fracture criteria. Cohesive-zone model with the cohesive law being the potential was used in the meso-scale region. This model has the advantage to simulate the complete process of a crack growth from the micro-, to meso- and then to the continuum regions. Unified description of the computation algorithm is presented. Simulation examples using a model with a primary crack and a subcrack located in front of the primary crack in bcc alpha-iron are given.

Key words: Multi-scale computation, Length Scale, Molecular Dynamics, Finite Element Method.

INTRODUCTION

Materials fracture often involves various length scales from dislocation evolution at the atomic scale level to crack propagation at the continuum levels. The current capabilities of atomic simulations are still restricted to nanoscale length of around 100nm order and are far from meeting practical demands of simulating various defects in solids, so a compromise between physical precision and computational feasibility is needed. In the large-scale atomic models, control of computation conditions and interpretation of the obtained results are difficult. Models by coupling

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various length scales and methods provide a means to solve such problems. Attempt in this direction has begun since 1970s. In the flexible-border or multi-region techniques, a fully atomic region is embedded into one or more outer regions and fully coupled atomistic [1] and finite element techniques to consider problems with complex nonlinearities were proposed [2-4]. An advantage of these models is natural inclusion of atomic potentials as a fracture criterion. Such models successfully explained some brittle microscopic fracture behavior of pure single crystals. More recently, the quasicontinuum method with a spatial mesh adaptively refined around highly energetic regions appears to be more promising [5]. Multiscale computation has been extended to include mean-field quantum mechanics in order to implement semiempirical tight-binding and molecular dynamics and finite element methods within one system [6].

The difficulty inherent in multiscale modeling is the treatment of mesoscale microstructure and how it is integrated and connected to micro (or nano)-scale and macro-scale microstructures. Computation at the mesoscale level itself involves multiple physical phenomena. For example, for pure materials of single crystals, dislocation nucleation and subsequent interaction and evolution are dominant factors, while void or micro-crack formation of various length dimensions and evolution are important in more engineering structural materials. In the case of composites, the interface between the reinforcement and matrix represents another microstructure and fracture length scales. The fracture behavior of brittle solids often involves the coalescence of many small cracks before linking with a main crack [see the review of Ref. (7) and references therein]. This subject has been studied extensively within the scope of continuum elasticity [7]. The interaction between individual cracks and the effective elastic properties with many cracks is of primary concern. These problems have not been treated on the atomic scale. Viewed from multiscale computation, the volume average quantities with regards to the problem having many cracks can be readily taken into account in the continuum region within the traditional treatment of coupling atomic and continuum models. This study is concerned with the interaction of individual cracks: a primary large crack and a small void-like crack. The primary crack tip region is deemed atomic, while a meso-scale region is introduced to describe the area with the sub-crack and this zone is based on the cohesive-zone concept where a fracture criterion is embedded automatically. This model has the advantage to consider crack growth interaction at different length scales while still maintaining atomic resolution in the most important region. Unified description of the computation algorithm is presented and simulation examples using bcc a iron are given.

MODEL AND FORMULATION

Fig.1 shows a central crack model used in the computation; only half of the model is plotted with the center of the main crack being a symmetrical axis. $a/l = 2.167$ is assumed as an initial geometrical condition. The details of the atomic crack tip region embedded within the continuum are shown later. The atomic region notch was created by removing three layers of atoms. The sub-crack region is called a meso-scale region where the cohesive zone theory is applied. The total energy of the system, E,

$$E[\mathbf{u}] = E(\text{atom}) + \int_{\Omega} W(\nabla \mathbf{u}) dV + \int_{\Sigma} \Phi(d) ds, \qquad (1)$$

where $E(\text{atom})$ is the total energy of the atomic region, $\mathbf{u}$ the displacement field, Ω the continuum domain, $W(\nabla \mathbf{u})$ the potential energy of the continuum; $\Phi(d)$ the cohesive-zone potential.

The material considered is *a* iron represented by Johnson's pair potential [8]. Molecular dynamics technique of the velocity Verlet algorithm is used to calculate atom movement with a time step of 1fs and the velocity scaling law to control temperature at 300K. The cohesive surface separation model [9] is used in the meso-scale region. The model relates cohesive tractions **T** to displacements by $\mathbf{T}=-\P f/\P\mathrm{D}$, where f is the potential and D is the displacement of cohesive points. f may be in various forms [9, 10] and a form giving linear cohesive relationship between **T** and D is introduced here for the brittle materials system, namely, $T_t = K_t\Delta_t$ and $T_n = K_n\Delta_n$, where the subscripts t and n represent quantities at the tangent and normal directions, respectively, and K_n and K_t are spring constant-like parameters. Such cohesive laws are then embedded into cohesive finite elements [5]. The cohesive elements are interspersed throughout the material of interest; here, the finite element region between the main crack tip and sub-crack tip is such a region to see how the main crack and sub-crack interact. In the atomic region, the crack plane is assumed to lie on {100} planes, the cleavage plane of BCC *a* iron.

Additional boundary conditions between the atomic region and meso-scale region are needed, i.e., the continuity of force and displacement of the atoms and finite element nodes at the boundary [4]. The atomic and continuum regions share a common boundary at the neighbor array of atoms and finite element nodes. Based on the virtual work principal, the continuum part in Eq (1) is discritized into finite elements. Quasi-static mode I loading, K_I, was applied in terms of the mode I main crack .

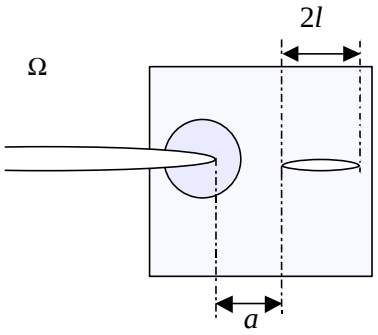
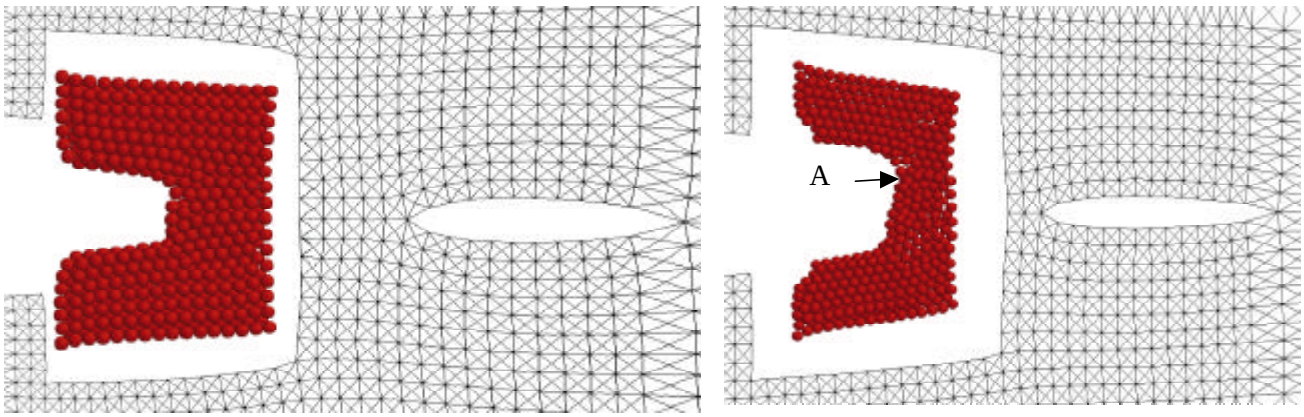


Figure 1 Central crack model with one sub-crack located in front of the main crack tip.

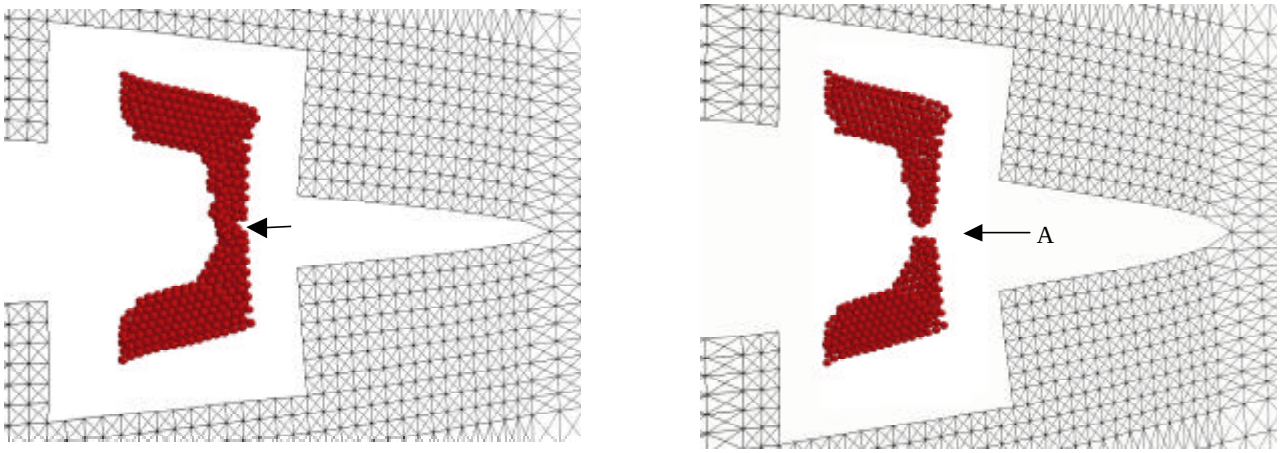
RESULTS, DISCUSSION AND SUMMARY

Figure 2 (a)-(d) shows a series of typical snapshots obtained in the simulation. Fig. 2 (a) demonstrates that both the atomic region and sub-crack region still undergo elastic deformation at an applied loading level of $K_I = 1.53\mathrm{MPam}^{1/2}$; it also indicates atom and finite element arrangement in these regions. Figs2. (b)-(d) are the results during subsequent loading for the case of $K_I = 2.37,\ 2.65$ and $2.7\ \mathrm{MPam}^{1/2}$, respectively. In Fig. 2 (b), atom movement to form crack-like extension, as indicated at Point A, within the atomic region is observed; the point A is slightly away from the initial notch plane. Meanwhile, the sub-crack also propagates towards the atomic region but is then stopped at a distance of about 2 lattice parameters in front of the atomic region. The loading level for this configuration of Fig. 2(b) is smaller than that reported in the literature [2]. This is may be due to the blunted initial notch tip, compared to the atomic sharpness crack tip in the literature. In Fig. 2(c), on further loading increase, the sub-crack propagates

completely across the continuum region to reach the atomic region and initiates a new crack in the atomic region as shown at Point A of Fig. 2(c). It is this new crack that governs the final failure path (Fig.2 (d)). Note that the system grows into unstable growth with additional small loading increment from the state shown in Fig.2(c). This clearly demonstrates the importance of the initial sub-crack. Further investigation regarding effects of lattice trapping and various parameters involved in the model is under way. In summary, the present study provides an effective method for simulating crack growth and crack interaction at different length scales.



(a) $K_I = 1.53 \text{MPam}^{1/2}$ (b) $K_I = 2.37 \text{MPam}^{1/2}$



(c) $K_I = 2.65 \text{MPam}^{1/2}$ (d) $K_I = 2.7 \text{MPam}^{1/2}$

Figure 2 Simulation results for 4 loading levels (a) $K_I = 1.53 \text{MPam}^{1/2}$,(b) $K_I = 2.37 \text{MPam}^{1/2}$, (c) $K_I = 2.65 \text{MPam}^{1/2}$ (d) $K_I = 2.7 \text{MPam}^{1/2}$. Note that the deformation magnifications for the atomic region and continuum region are different.

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