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Multiscale Analysis of the Mechanical Properties of the Crack Tip Region

S. Zhufeng[a], M.A.A. Mohd Salleh[b,*], B. Jeż[c] and N. Yusoff[a]

[a]*School of Mechanical Engineering, Engineering Campus, Universiti Sains Malaysia, 14300 Nibong Tebal, Penang, Malaysia*
[b]*Faculty of Chemical Engineering and Technology, Universiti Malaysia Perlis, 02600 Arau, Perlis, Malaysia*
[c]*Department of Technology and Automation, Faculty of Mechanical Engineering and Computer Science, Czestochowa University of Technology, al. Armii Krajowej 19c, 42-200 Częstochowa, Poland*

Doi: 10.12693/APhysPolA.144.399 *e-mail: menorwahida@usm.my

This paper attempts to find the possibility of describing the supplementary parameters of the macroscopic crack strength field based on the variation at the microscopic level. The analysis focuses on the development of cracks in the vicinity of the crack tip of a central crack panel made from iron material with a cubic crystal structure under tensile loading. We use the combination of finite element and molecular dynamics simulation methods. Molecular dynamics simulation analysis shows that the motion velocity of molecules near the crack tip region is less than the Rayleigh wave velocity, V_R, which is about 0.22 V_R. The average velocity is smaller in other directions that are not parallel to the crack. The velocity of the molecular near the crack tip indicates the ductile phenomenon of the crack tip region because it comes from the potential energy, which means that on the crack extension line, the kinetic energy of the molecular motion is greater than that in the other directions but is close to that in the 45° direction. It shows that the crack expansion direction is still mainly along the crack extension line under the load.

topics: multiscale analysis, molecular dynamics simulation, finite element modeling, lattice constant

1. Introduction

Due to the singularity of the crack tip, the definite condition of stress fields at the crack tip and the crack tip extension are difficult to characterize through finite element methods (FEM). Researchers have tried to find the intrinsic reason for the dynamic extension of the crack tip by using multiscale modeling, which is an alternative approach to studying local physical phenomena in a large structure with microstructural features. Many multiscale analyses of the crack tip region from orders of centimeters to orders of nanometers have been conducted [1–5], focusing on explaining the change in crack extension from the microscopic level.

Recently, finite element and molecular dynamics techniques have been introduced in this aspect to model the material nonlinearity of the crack tip region. However, the common difficulty in creating such cross-scale models is determining how to properly handle the transition relationship between the lattice model and the continuum solid model. The cause of this problem arises from the essence of the internal force at different scales.

Because of the difficulty of accurately describing the crack tip stress field with the parameter J-integral, the present study proposes a combination of finite element and molecular dynamics simulation of the extension of the crack tip region, aiming to find a fittable parameter associated with the microscopic crack extension, along with the macroscopic parameter to describe the crack tip stress field. The analysis framework relies on the common nodes of the FEM area and the molecular dynamics (MD) zone, in combination with the stress field of the MD region obtained through finite elements. Through this, the applied load is transmitted to the MD area for relaxation, so that the internal atoms are fully relaxed and the movement of the atoms in the MD area at the crack tip can be observed at each time step.

2. Materials and method

2.1. Finite element modeling and analysis

To explore the development of the crack under load, the MD simulation of the crack tip region of the central crack panel under tension was conducted using open-source software, XMD. The central crack panel (CCP) specimen with $a/W = 0.5$, $W = H = 20$ mm, which is subjected to a uniform tensile load, is shown in Fig. 1a. Considering the

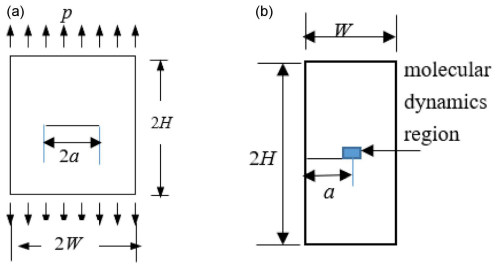

Fig. 1. (a) Central crack panel model. (b) The molecular dynamics region of central crack panel model.

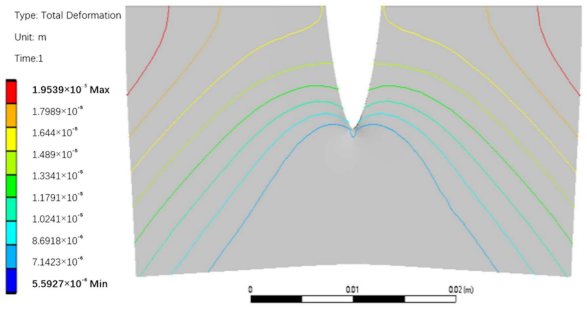

Fig. 2. The total deformation under tensile load of 100 MPa.

symmetry of the geometry and the load, only half of the specimen is taken for finite element modeling. The material is assumed to be 304 stainless steel with a yield stress, σ_0, of 205 MPa. For molecular dynamics simulations, the MD region of the central crack panel model is shown in Fig. 1b, which is the lattice constant of the material.

For a body-centered cubic (BCC) lattice ferrite material, its lattice size is about 10^{-7} mm, so it needs the tension load to make the MD region easily reachable in a yield state. It is necessary to make the yield crack region big enough for the MD calculation. The displacement for the MD calculation is the average displacement field of the grid nodes in the MD region, which is obtained through finite element calculations. For this purpose, a uniform tensile load $p = 100$ MPa was applied to generate a ductile state at the crack tip, with a maximum equivalent von Mises stress being 871.29 MPa, which is higher than the yield stress of the material. The generated total deformation is 0.0056 mm, as shown in Fig. 2, which is fit for the MD simulation.

2.2. Kinetic analysis of the cross-scale crack tip zone

Figure 3a shows the crack tip of the molecular dynamics region obtained through the finite element calculations, which is 44 lattices up, 22 latices left, and 23 latices right from the lattice node of the displacement field. Considering the difference between

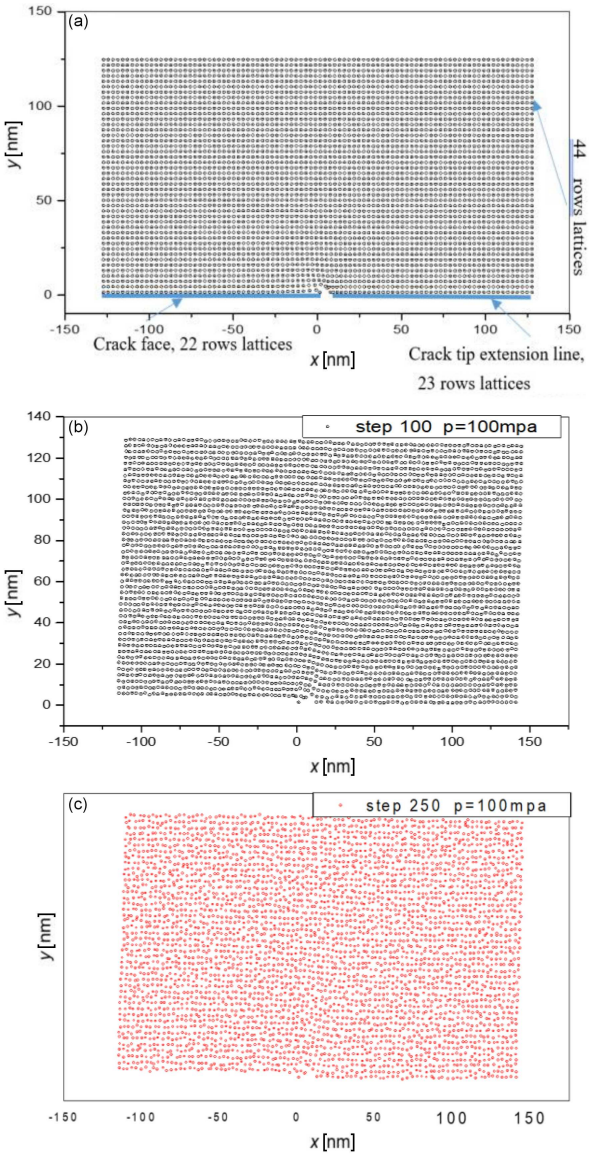

Fig. 3. (a) Molecular dynamics zone at (b) 100th step, and (c) 250th step.

the continuum and the discretized models, the displacement field obtained by the finite elements is appropriately modified by the means of multiplication of the flexibility coefficient as an applied displacement field for the molecular dynamic simulation. The empirical many-body embedded atom method (EAM) potential function is used to relax the molecules and obtain the motion velocity and kinetic energy of the atoms under the applied displacement field and the potential function.

In this study, the tracking analysis of the atomic motion in front of the crack tip under external loading was conducted. The mechanism of the crack expansion was configured by increasing the external load, repeating one or two steps until the crack begins to expand, and then observing the movement of the atoms in the MD area. The initial position of the atoms in the MD region is shown in Fig. 3a.

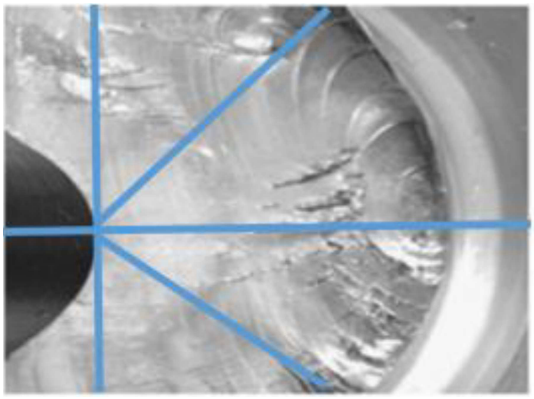

Fig. 4. The three characteristic lines clearly appearing in a part-through surface crack profile [6].

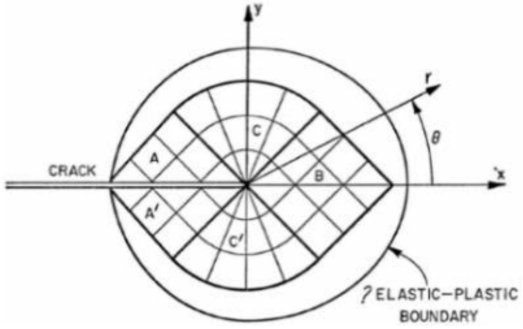

Fig. 5. Prandtl slip line field.

TABLE I

Atomic motion and kinetic energy in different directions in the crack tip region.

	Angle [°]		
	0	45	90
Average speed [nm/s]	300.88	266.8	257.3
Kinetic energy ($\times 10^{-9}$) [J]	1.413	1.172	1.095

The crack tip region was analyzed with MD software, and the positions of the atomic relaxation at the 100th and 250th steps are shown in Fig. 3b and Fig. 3c, respectively.

3. Results and discussion

The molecular dynamics simulation shows that there are nanoscale slip lines at the crack tip, which are also seen in a part-through surface crack profile shown in Fig. 4 [6]. The simulated average velocity and kinetic energy of the atoms at the crack development line at angles 0°, 45°, and 90° under loadings are summarized in Table I.

The data show that the kinetic energy of the lattice is lowest in the direction perpendicular to the crack line, and as compared to this direction, the kinetic energy of the lattice at the 45° line is about 7% higher and about 29% higher in the crack extension line. This kinetic energy variation indicates that the residual strength of the crack tip is different in different regions. The three characteristic lines suggest that the material is no longer isotropic in the crack tip region, which explains why the passivation of the crack tip region strengthens the extension of the crack and affects the extension direction of the crack in the microstructure perspective.

The MD simulation results also agree well with the Prandtl slip line field (Fig. 5), which assumes plasticity surrounds the crack tip completely. The consistency of these findings ensures that joining the characteristic-line-related parameter and the J-integral parameter to describe the crack strength field is feasible.

4. Conclusions

The molecule along the crack path ahead of the crack tip is shown to have higher energy than the other directions. It is the energy aggregation band under the external load, which is in a relatively unstable state and is the most likely direction for the crack to grow.

Due to the stress concentration at the crack tip, the plastic yield zone will appear in the crack tip zone in response to the external load. By then, the material in this zone is anisotropic, and the deformation in this area is no longer elastic. Therefore, the characterization of the stress intensity factor becomes difficult.

As molecular kinetic energy changes with line angles related to the direction of the crack extension, a fittable parameter related to the changes of characteristic lines can be considered as an alternative parameter describing the microstructural changes. Therefore, together with the macro stress field, the crack tip stress fields can be described more accurately.

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