Simulation of crack growth under mixed-mode loading by molecular dynamics method

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Abstract

Atomistic simulations of the central crack growth process in a plane medium using Large-scale Molecular Massively Parallel Simulator (LAMMPS), a classical molecular dynamics code, are performed. The inter-atomic potential used in this investigation is Embedded Atom Method (EAM) potential. The specimens with initial central crack were subjected to Mixed-Mode loadings. The simulation cell contains 400000 atoms. The crack propagation direction angles under different values of the mixity parameter in a wide range of values from pure tensile loading to pure shear loading in a wide diapason of temperatures (from 0.1 K to 800 K) are obtained and analyzed. It is shown that the crack propagation direction angles obtained by molecular dynamics method coincide with the crack propagation direction angles given by the multi-parameter fracture criteria based on the strain energy density and the multi-parameter description of the crack-tip fields.

Keywords: mixed-mode loading; crack propagation direction; molecular dynamics method; LAMMPS; multi-parameter fracture criteria; near-crack-tip fields; Williams series expansion.

1. Introduction

One of the fundamental idea in the fracture assessment of brittle fracture is the local mode I concept [1]. The proposal of mode I dominance was suggested dealing with cracked plates under plane loading and transverse shear, where the crack grows in the direction almost perpendicular to the maximum tangential stress (MTS) in radial direction from its tip [1]. This theory is one of the widely used theories for mixed mode crack growth [2-6]. In more detail the criterion states that the crack propagation starts along the direction on which the tangential stress becomes maximum. The fracture occurs when the maximum tangential stress reaches a critical value for the material equal to the fracture stress in uniaxial tension. For the calculation of the tangential stress a critical distance from the crack tip must be introduced. But the question is what one can use a critical distance from the crack tip? To overcome this difficulty the concept of a core region surrounding the crack tip has been proposed by Sih [2]. The idea is the continuum mechanics solution, as well as experimental measurements, stop at some distance from the crack tip. The distance serves as a scale size of analysis at the continuum level. Together with the MTS criterion the strain energy density (SED) has been used to formulate failure criteria for materials exhibiting both ductile and brittle behavior. Dealing with the strain energy concept it is worth to note that it is necessary to introduce the radius of "core region" surrounding the crack tip [1,2]. The key idea is that the continuum mechanics stops short at a distance from the crack tip. The strain energy density factor (S) was defined as a product of the strain energy density by a critical distance from the point of singularity. Thus it is necessary to introduce the critical distance from the crack tip [3-5]. Nowadays one can possible to estimate the crack propagation direction angle using molecular dynamics simulation [7]. The present study is aimed at the determination of the crack propagation direction angle in a wide range of mixed-mode loading using 1) the multi-parameter maximum tangential stress criterion; 2) the multi-parameter strain energy density criterion; 3) molecular dynamics simulation of the crack propagation behavior under mixed-mode loading.

2. Methods

There are several methods of simulating crack behavior, including molecular mechanics, molecular dynamics, continuous mechanics, finite element method and methods based on DFT theory. Focus of this article is comparison of molecular dynamics and continuum fracture mechanic approach.

2.1. Continuum fracture mechanics approach

In the development of fracture mechanics Williams made a major breakthrough in the analysis of asymptotic stress field at the vicinity of the crack tip in isotropic, linear, elastic plane media. With the eigenfunction expansion method it is possible to establish the separable variable nature of the solution and to obtain asymptotic expressions for the stress field in a plane medium with a traction-free crack submitted to mode I, mode II and mixed-mode loading conditions:

$$\sigma_{ij}(r,\theta) = \sum_{m=1}^{2} \sum_{k=-\infty}^{k=\infty} a_k^m r^{k/2-1} f_{m,ij}^{(k)}(\theta) \qquad (1)$$

with index m associated to the fracture mode; a_k^m coefficients related to the geometric configuration, load and mode; $f_{m,ij}^{(k)}(\theta)$ angular functions depending on stress component and mode. Analytical expressions for angular eigenfunctions are available

$$f_{1,11}^{(k)}(\theta)=\frac{k}{2}\Big[\big(2+k/2+(-1)^k\big)\cos(k/2-1)\theta-(k/2-1)\cos(k/2-3)\theta\Big],$$

$$f_{1,22}^{(k)}(\theta)=\frac{k}{2}\Big[\big(2-k/2-(-1)^k\big)\cos(k/2-1)\theta+(k/2-1)\cos(k/2-3)\theta\Big],$$

$$f_{1,12}^{(k)}(\theta)=\frac{k}{2}\Big[-\big(k/2+(-1)^k\big)\sin(k/2-1)\theta+(k/2-1)\sin(k/2-3)\theta\Big],$$

$$f_{2,11}^{(k)}(\theta)=-\frac{k}{2}\Big[\big(2+k/2-(-1)^k\big)\sin(k/2-1)\theta-(k/2-1)\sin(k/2-3)\theta\Big],$$

$$f_{2,22}^{(k)}(\theta)=-\frac{k}{2}\Big[\big(2-k/2+(-1)^k\big)\sin(k/2-1)\theta+(k/2-1)\sin(k/2-3)\theta\Big],$$

$$f_{2,12}^{(k)}(\theta)=\frac{k}{2}\Big[-\big(k/2-(-1)^k\big)\cos(k/2-1)\theta+(k/2-1)\cos(k/2-3)\theta\Big].$$

The multi-parameter fracture mechanics concept consists in the idea that the crack-tip stress field is described by means of the Williams expansion (1). In this work the central crack in an infinite plane medium is considered. Analytical determination of coefficients in crack-tip expansion for a finite crack in an infinite plane medium is given in [3]. Since all the coefficients in the Williams asymptotic series expansion for the geometry considered are known it is possible to estimate the crack propagation direction angle by means of the multi-parameter fracture mechanics concept. For research in this contribution, two fracture criteria were chosen for the estimation of the initial crack growth direction: maximum tangential stress (MTS) criterion and strain energy density (SED) criterion [2]. The most well-known criterion for the estimation of the crack propagation direction is MTS (maximum tangential stress). This criterion is strictly stress-based and its analysis does not depend on the conditions of plane stress and plane strain. It assumes that a crack extends in the direction of the maximum tangential stress. Mathematically written:

$$\frac{\partial\sigma_{\theta\theta}}{\partial\theta}=0,\quad \frac{\partial^2\sigma_{\theta\theta}}{\partial\theta^2}<0 \qquad .$$

In this work, the multi-parameter form of the MTS criterion is tested while considering various numbers of the initial terms of the Williams expansion (1). Therefore, the tangential stress has to be expressed via the power series and then its maximum is sought numerically. The criterion based on the minimum of the strain energy density deals with strain energy and therefore the conditions for predicting crack growth direction depend on whether or not the specimen is subjected to plane strain or plane stress conditions. Specifically, the minimum strain energy density criterion states that a crack will grow in the direction where the strain energy density reaches its minimum. This condition can be written as:

$$\frac{\partial S}{\partial\theta}=0,\quad \frac{\partial^2 S}{\partial\theta^2}>0,\quad S=\frac{1}{2\mu}\left[\frac{\kappa+1}{8}\big(\sigma_{rr}+\sigma_{\theta\theta}\big)^2-\sigma_{rr}\sigma_{\theta\theta}+\sigma_{r\theta}^2\right]$$

The Williams series expansion (1) is used for approximation of the stress tensor components and the minimum is sought through numerical methods. A procedure for searching the extreme of the function is programmed in Waterloo Maple code. The relevant quantities are expressed by means of the Williams series expansion considering both various terms numbers in Williams series expansion and various distances from the crack tip. The results of the calculations are shown in Tables 1-4. N is the number of terms keeping in the Williams series expansion, $r_c=r/a$ is the dimensionless distance from the crack tip.

2.2. Atomistic modeling for mixed-mode loading of the plane medium with the central crack

To model copper plate under mixed loading we used large-scale atomic/molecular massively parallel simulator (LAMMPS) [8] in combination with embedded atom method (EAM) [9]. EAM potentials are widely used in variety of different simulations, focusing mainly on mechanical properties. Potentials for copper were proposed by Foiles et al. [10] and shown decent results in elastic limit, therefore, all the displacements considered in this work are elastic.

Periodic boundary conditions were implemented in all three directions of the cell. To neglect the effect of neighboring cells we choose the size of the central crack to be relatively small (1:10 ratio) to the size of the simulation cell. Furthermore, we added small non-interacting boundaries to the edge of the plane. Total number of atoms in the cell is 300000.

Before mixed loading is applied, plate is optimized to the minimal energy with conjugated gradient method. When minimum energy state is achieved, we apply mixed strain. During all 50000 steps of simulation, we collect data of the state of all atoms in the cell. Results are shown on pictures below, color coding is obtained by OVITO [11] tool. Brighter colors correspond to higher stress.

From Fig. 1-3 one can see that the crack propagation direction angle is approximately 45°. For better comparison we measured crack propagation angles at different stages of crack growth using J-Mol tool. We compared our observations with results of classical linear fracture mechanics, given in Tables above. For all cases of mixity parameter studied in molecular dynamics calculations our measurements of crack propagation directions are close to the theoretical results obtained for multi-parameter fracture criteria (column 2 of Tables 1-4).

From our simulations we can get crack propagation directions and crack angles. Calculations were run for three different values of M^e: 0.4, 0.5 and 0.6. Calculated values of crack angles were -51.5°, -46.6° and -42.2° accordingly.

Table 1. Crack propagation direction angles obtained from the MTS fracture criterion at various radial distances from the crack tip

N	$r_c = 0.05$	$r_c = 0.1$	$r_c = 0.25$	$r_c = 0.5$	$r_c = 0.75$	$r_c = 1.25$	$r_c = 1.5$	$r_c = 1.75$	M^e
-70.53	-66.21	-62.49	-55.08	-49.65	-47.39	-45.72	-45.40	-45.29	0
-67.53	-67.53	-62.20	-58.34	-51.34	-46.55	-44.63	-42.99	-42.70	0.1
-64.47	-58.01	-54.10	-47.60	-43.44	-41.83	-40.72	-40.52	-40.67	0.2
-62.86	-55.83	-51.91	-45.69	-41.84	-40.38	-39.39	-39.23	-39.06	0.25
-61.18	-53.53	-49.64	-43.72	-40.18	-38.87	-38.01	-37.87	-37.56	0.3
-57.48	-48.60	-44.83	-39.58	-36.65	-35.63	-35.01	-34.93	-34.14	0.4
-53.13	-43.03	-39.50	-35.00	-32.62	-31.95	-31.56	-31.52	-31.37	0.5
-47.72	-36.61	-33.46	-29.80	-28.11	-27.63	-27.44	-27.45	-27.35	0.6
-40.61	-29.12	-26.52	-23.77	-22.66	-22.42	-22.40	-22.44	-22.61	0.7
-36.12	-24.93	-22.68	-20.40	-19.54	-19.39	-19.44	-19.49	-19.47	0.75
-30.81	-20.42	-18.55	-16.75	-16.13	-16.06	-16.14	-16.20	-16.26	0.8
-17.19	-10.57	-9.59	-8.71	-8.60	-8.46	-8.55	-8.59	-8.53	0.9

Table 2. Crack propagation direction angles obtained from the SED fracture criterion at various radial distances from the crack tip (plane strain conditions), $\nu = 0.3$

N	$r_c = 0.05$	$r_c = 0.1$	$r_c = 0.25$	$r_c = 0.5$	$r_c = 0.75$	$r_c = 1.25$	$r_c = 1.5$	$r_c = 1.75$	M^e
-82.34	-82.36	-82.33	-81.74	-79.05	-75.27	-68.55	-66.02	-63.70	0
-76.19	-75.98	-75.84	-74.94	-72.04	-68.56	-62.68	-60.68	-57.95	0.1
-70.14	-69.52	-69.20	-67.94	-64.95	-61.81	-56.72	-54.81	-52.18	0.2
-67.14	-66.24	-65.81	-64.35	-61.37	-58.40	-53.69	-51.93	-51.36	0.25
-64.13	-62.90	-62.34	-60.72	-57.76	-54.97	-50.63	-49.00	-46.38	0.3
-58.10	-55.99	-55.17	-53.26	-50.45	-48.03	-44.38	-43.01	-40.55	0.4
-51.91	-48.65	-47.59	-45.52	-42.97	-40.93	-37.92	-36.81	-34.64	0.5
-45.35	-40.71	-39.47	-37.43	-35.24	-33.58	-31.20	-30.33	-28.63	0.6
-38.01	-31.95	-30.69	-28.88	-27.15	-25.90	-24.13	-23.48	-22.46	0.7
-33.82	-27.21	-26.01	-24.40	-22.93	-21.89	-20.42	-19.88	-20.53	0.75
-29.04	-22.20	-21.14	-19.77	-18.58	-17.74	-16.58	-16.15	-15.99	0.8
-16.75	-11.44	-10.82	-10.08	-9.48	-9.06	-8.49	-8.28	-8.56	0.9

Table 3. Crack propagation direction angles obtained from the SED fracture criterion at various radial distances from the crack tip (plane strain conditions), $\nu = 0.5$

N	$r_c = 0.05$	$r_c = 0.1$	$r_c = 0.25$	$r_c = 0.5$	$r_c = 0.75$	$r_c = 1.25$	$r_c = 1.5$	$r_c = 1.75$	M^e
-90.00	-89.28	-88.54	-86.07	-81.11	-76.21	-68.81	-66.17	-63.74	0
-83.99	-82.82	-81.85	-78.90	-73.92	-69.49	-63.00	-60.69	-58.01	0.1
-77.91	-76.14	-74.88	-71.50	-66.65	-62.70	-57.07	-55.05	-52.26	0.2
-74.82	-72.68	-71.26	-67.02	-62.97	-59.27	-54.03	-52.17	-51.41	0.25
-71.68	-69.12	-67.55	-63.86	-59.28	-55.88	-50.97	-49.24	-46.47	0.3
-65.19	-61.66	-59.80	-55.98	-51.78	-48.78	-44.68	-43.22	-40.65	0.4
-58.28	-53.60	-51.55	-47.80	-44.10	-41.57	-38.17	-36.97	-34.73	0.5
-50.68	-44.80	-42.70	-39.28	-36.16	-34.10	-31.38	-30.42	-28.69	0.6
-41.90	-35.06	-33.13	-30.28	-27.84	-26.27	-24.22	-23.50	-22.47	0.7
-36.84	-29.80	-28.05	-25.57	-23.50	-22.18	-20.47	-19.87	-20.27	0.75
-31.13	-24.27	-22.77	-20.70	-19.03	-17.97	-16.60	-16.11	-15.95	0.8
-17.21	-12.46	-11.63	-10.54	-9.70	-9.16	-8.47	-8.23	-8.38	0.9

Table 4. Crack propagation direction angles obtained from the SED fracture criterion at various radial distances from the crack tip (plane stress conditions), $\nu = 0.3$

N	$r_c = 0.05$	$r_c = 0.1$	$r_c = 0.25$	$r_c = 0.5$	$r_c = 0.75$	$r_c = 1.25$	$r_c = 1.5$	$r_c = 1.75$	M^e
-79.66	-80.01	-80.26	-80.33	-78.36	-74.95	-68.48	-65.96	-63.70	0
-73.35	-73.59	-73.78	-73.60	-71.39	-68.24	-62.58	-60.40	-57.94	0.1
-67.19	-67.14	-67.20	-66.69	-64.35	-61.50	-56.60	-54.73	-52.16	0.2
-64.16	-63.88	-63.85	-63.16	-60.79	-59.09	-53.57	-51.84	-51.34	0.25
-61.14	-60.58	-60.44	-59.58	-57.21	-54.67	-50.51	-48.92	-46.36	0.3
-55.14	-53.80	-53.41	-52.25	-49.96	-47.76	-44.26	-42.94	-40.52	0.4
-49.09	-46.66	-46.03	-44.64	-42.54	-40.69	-37.83	-36.75	-34.62	0.5
-42.83	-39.00	-38.16	-36.70	-34.88	-33.39	-31.14	-30.30	-28.61	0.6
-36.00	-30.60	-29.67	-28.32	-26.88	-25.76	-24.10	-23.48	-22.45	0.7
-32.17	-26/06	-25.15	-23.93	-22.70	-21.77	-20.40	-19.89	-20.62	0.75
-27.82	-21.27	-30.44	-19.39	-18.40	-17.66	-16.57	-16.17	-16.02	0.8
-16.44	-10.97	-10.47	-9.89	-9.39	-9.02	-8.49	-8.30	-8.63	0.9

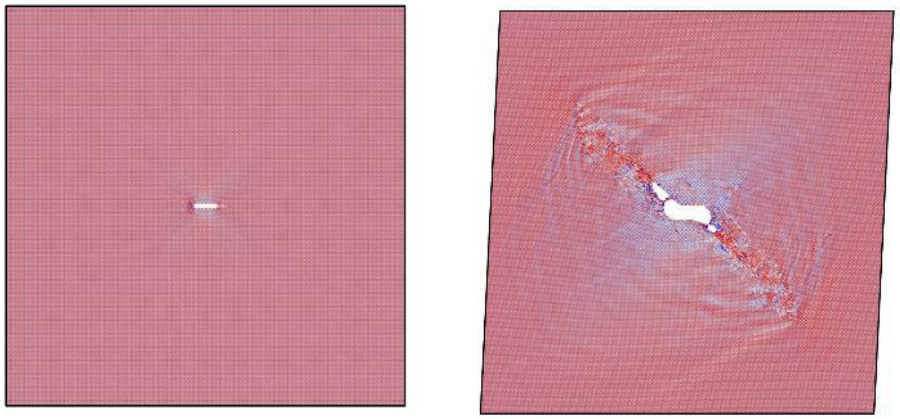

Fig. 1. Stress tensor component σ_{11} in copper plate just arter energy minimization (left) and after 25000 steps (right).

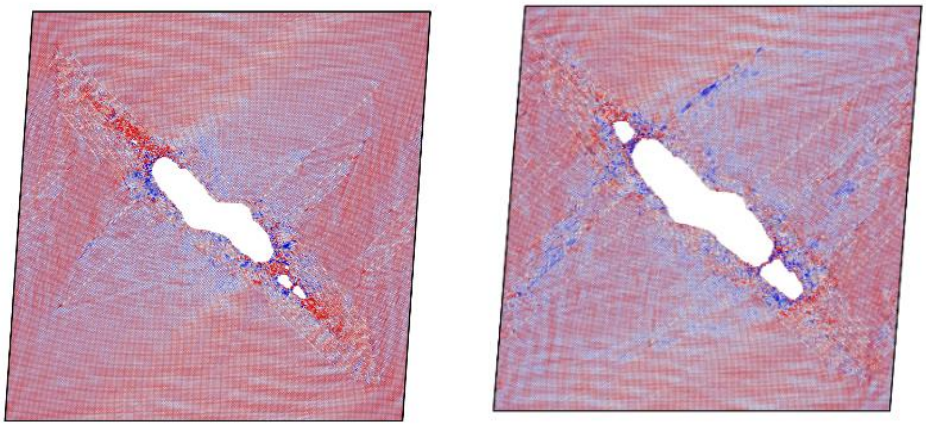

Fig. 2. Copper plate after 35000 and 45000 steps.

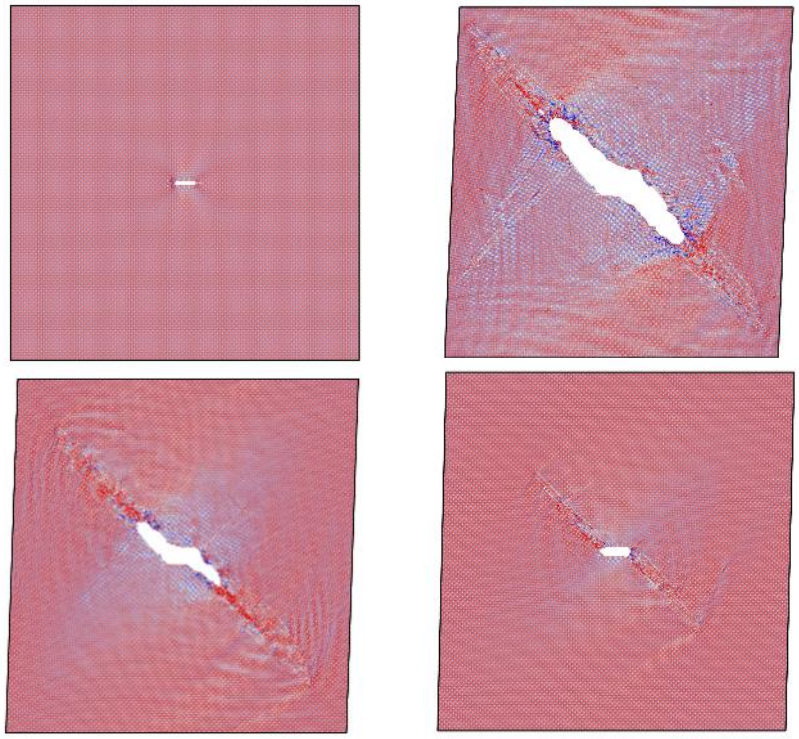

Fig. 3. Plate with different value of mixity at 0, 25000, 35000 and 45000 steps.

3. Conclusion

The paper is focused on the application of the different approaches for the determination of the initial crack propagation angle. The crack propagation angle is obtained by 1) the multi-parameter fracture mechanics approach based on two fracture mechanics criteria, MTS and SED; 2) atomistic modeling for the mixed-mode loading of the plane medium with the central

crack. It is shown that the initial crack propagation angles given by the both approaches are very close especially for the case when the higher order terms in the Williams series expansion are kept.

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