Simulation of the Crack Growth Under Mixed-mode Loading: Fracture Criteria and Molecular Dynamics Approach

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Abstract. The crack propagation direction angle is investigated by the use of two approaches. The first one is based on the classical mathematical theory of brittle fracture and the Williams series expansion of the stress field at the vicinity of the crack tip. The second approach is based on the molecular dynamics method. 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: molecular dynamics method, crack propagetion direction angle, mixed mode loading, LAMMPS, specimen with initial central crack.

1. Introduction

In recent years the development of molecular dynamics (MD) provides a more effective method for investigating the crack propagation. Many researchers have devoted themselves to investigating crack propagation in various materials [1-6]. Plenty of studies have shown that the direction of the crack propagation and dislocation transmission is related closely to the orientation of preset crack. fracture mechanics is a useful tool for the design of mechanical and material properties of mechanical components. The propagation and growth of cracks in materials are the most important factors in fracture mechanics. The fracture process usually includes two steps, namely crack formation and crack propagation. The propagation of a crack in a material depends on defects such as impurities, vacancies, dislocations, slip bands, and twins. Crack growth or propagation in polycrystalline metal may be either transgranular or intergranular, whereas that in singlecrystal metal may be either slip or dislocation. In view of these facts, the importance of understanding the crack growth process has created interest in the mechanical properties near a crack tip in single-crystal metals. 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. Approaches

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.

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.

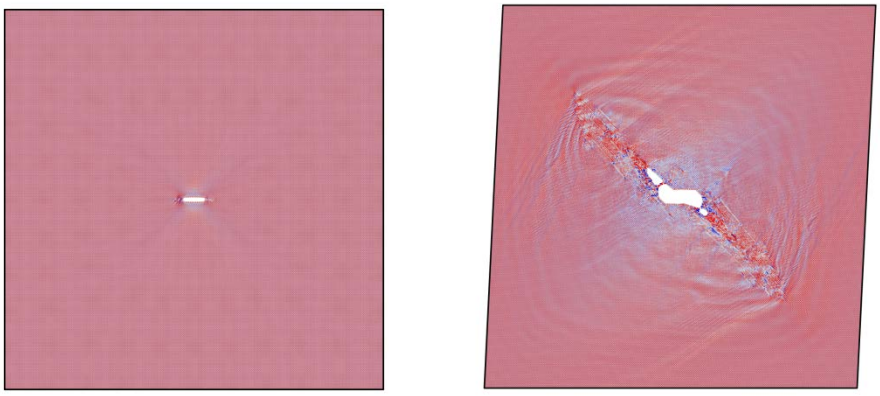

Figure 1. Copper plate just arter energy minimization and after 25000 steps with stress tensor component σ_{11} shown.

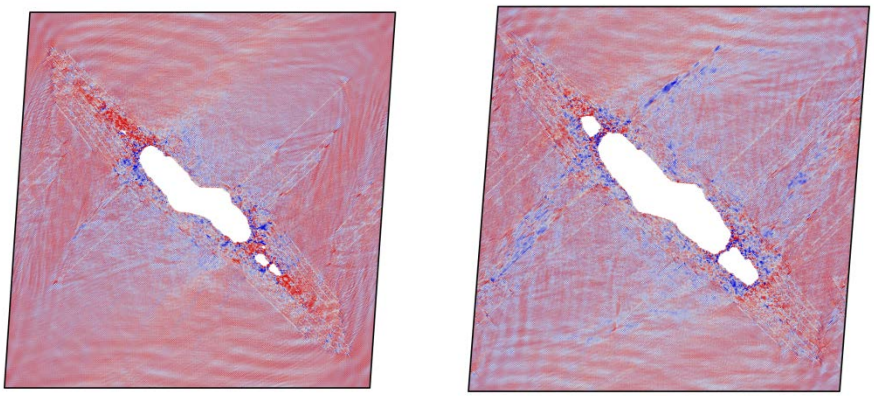

Figure 2. Copper plate after 35000 and 45000 steps.

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.

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 (mode I and mode II) loading conditions:

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

with index m associated to the fracture mode; a_k^m amplitude 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 [3,4]. 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]. In this paper two fracture criteria were chosen for the estimation of the initial crack growth direction: MTS criterion and SED criterion [1]. The most well-known criterion for the estimation of the crack propagation direction is MTS. It assumes that a crack extends in the direction of the maximum tangential stress. In this work, the multi-parameter form of the MTS criterion is tested while considering various numbers of terms of the Williams expansion (1).

The results obtained by the MTS criterion are shown in Table 1 where N is the number of terms keeping in the Williams series expansion, $r_c = r/a$ is the dimensionless distance from the crack tip. The first column gives the crack propagation direction angles obtained by the MTS criterion when the leading term of the Williams asymptotic expansion is taken into account. While the following columns show the crack propagation direction angles given by the multi-parametric asymptotic expansion of the stress field in the vicinity of the crack tip. Here the multi-parameter crack tip expansion of the stress field contains 100 terms. One can see that the values of the crack propagation direction angle obtained by the one-parameter fracture criterion are close to the values of the second column especially for Mode II loading. It can be seen the influence of T-stresses at the crack tip. As the distance from the crack tip increases the difference between results given by the one-parameter fracture criterion and the multi-parameter fracture criterion enhances. The SED criterion states that a crack will grow in the direction where the strain energy density reaches its minimum:

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

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.

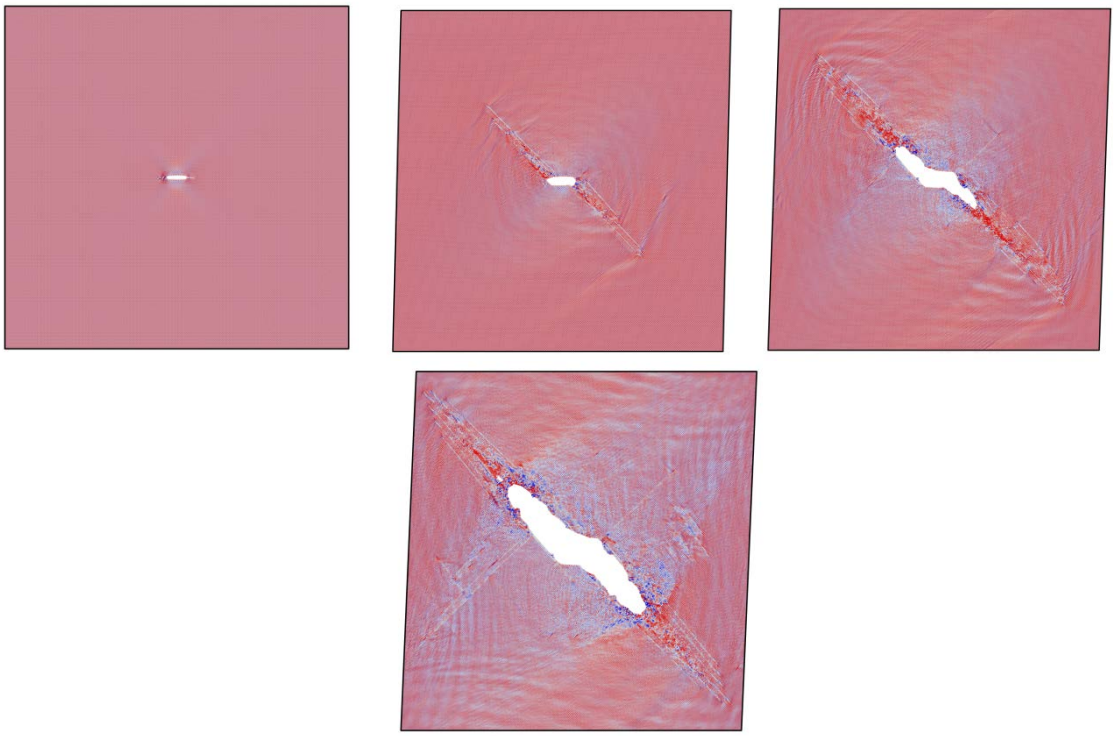

Figure 3. Plate with different value of mixity at 0, 25000, 35000 and 45000 steps.

3. Conclusions

The paper is focused on the application of the different approaches for the determination of the initial crack propagation angle. Copper plate with the central crack under complex mechanical stresses (Mode I and Mode II loading) is studied by extensive molecular dynamics simulations based on the EAM potential. On the other hand, the complete Williams expansion for the crack tip fields containing the higher-order terms is used. 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. 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. 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. Thus one can conclude that the criteria of classical continuum mechanics MTS and SED can give satisfactory predictions for crack initiation direction. The crack propagation direction angles given by the conventional fracture mechanics reasonably agree with the angles obtained from molecular dynamics simulations. 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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