Theoretical and Applied Fracture Mechanics 79 (2015) 84–90

Contents lists available at ScienceDirect

Theoretical and Applied Fracture Mechanics

journal homepage: www.elsevier.com/locate/tafmec

Lattice structure: Scaling of strain related energy density

Jiafeng Ding [a], Zhennan Zhang [a,b,*], Xiurun Ge [a]

[a] School of Naval Architecture, Ocean and Civil Engineering, Shanghai Jiao Tong University, Shanghai 200240, China
[b] State Key Laboratory for GeoMechanics and Deep Underground Engineering, China University of Mining & Technology, Xuzhou 221008, China

ARTICLE INFO

Article history:
Available online 11 August 2015

Keywords:
Discretized lattice
Strain energy density
Fracture
Scaling
Numerical simulation

ABSTRACT

The strain energy density (SED) was used as the criterion to characterize stable and unstable crack growth in the fracture mechanics of linear and non-linear constitutive relations. It applies equally well for continuum mechanics problems in general. It is free from the restrictions of theories that implicate linear superposition. The energy density combines strain and stress and is not exclusive to strain alone nor stress alone. "Energy" and "density" for a point like element are the basic ingredients. The element can be microscopic and visualized as atoms or molecules. In this sense, the energy density criterion can be applied to the lattice structure and can also predict macro fracture. In this work, material is modeled with a lattice bond structure. Through the SED-based scaling law, the discrete form of SED criterion, which is specially used to lattice structure, is derived. The fracture mechanism of the lattice structure is analyzed. It is shown that the limit strain of the micro bond is related to the lattice size. The smaller the lattice size is, the larger the limit bond strain. It presents the same singularity order as the macro strain field near crack. The manifestation of scaling of strain is that micro bond strain is always much higher than the macro strain. Bond rupture is associated with the bond strain and the SED factor. The simulation results by the lattice structure with the SED criterion are almost free of lattice size dependency. It is suggested that the lattice structure can be modeled by the energy density and scaling of strain. The strain energy density approach can be applied to develop scale shifting laws in general.

1. Introduction

Linear elastic fracture mechanics has had a long standing success to predict macro fracture behavior of high strength materials. Although a variety of modified fracture criteria have advanced, they are all derivatives and/or variations of the stress intensity factors, based on the energy release concept. The energy release rate is a theory system based on the macro continuum mechanics, which does not consider the microstructures of material and the energy mechanisms on different scales. When it is applied to the piezoelectric material with crack, which involves with the multi-scale mechanical processes, the energy release rate becomes negative under certain boundary conditions [1]. This contradicts with the reality. Different from the energy release rate concept, the strain energy density (SED) criterion proposed in the earlier works [2–6] reveals the fracture mechanism from the standpoint of strain energy density. It is not exclusive to strain along nor stress along, but combines them together. Considering the same fracture problem of piezoelectric material aforementioned with the SED criterion, it is found the surface energy density factor is always positive-definite [1]. Thus, the SED criterion presents some advantages in fracture prediction.

The SED criterion was originally proposed to deal with the line crack, but its philosophy can be extended to other crack cases. With the SED conception, Lazzarin et al. [7,8] developed the local strain energy density approach to the sharp V-shaped notch. The local SED criterion states that when the average strain energy density over a controlled volume at the V-notch vertex exceeds a critical value, a failure process occurs. The value of the average strain energy density depends on the size of the controlled volume for a given crack case. Thus, the determination of the controlled volume size is the crucial issue of the local strain energy density approach. By recovering the V-shaped notch to a line crack, the radius of the controlled volume surrounding V-notch vertex, which determines the size of the controlled volume, is associated with the fracture toughness of material in [7]. Later, Lazzarin and Berto [9] and Berto et al. [10,11] extended the local strain energy density

* Corresponding author at: School of Naval Architecture, Ocean and Civil Engineering, Shanghai Jiao Tong University, Shanghai 200240, China. Tel./fax: +86 21 34204346.
E-mail address: zhennanzhang@sjtu.edu.cn (Z. Zhang).

http://dx.doi.org/10.1016/j.tafmec.2015.05.009
0167-8442/

approach to the blunt U- and V-notches under Mode I loading. The local SED criterion is different from the original SED fracture criterion in that the original one is a point-related criterion while the local one is a volume-related criterion. The local strain energy density approach has been extensively applied to the blunt fracture cases. Berto and Lazzarin [12] have made a comprehensive review on this approach.

A fracture phenomenon does not result from the monoscale mechanical process, but the multiscale. So, to characterize the fracture with the multiscale concept, a scaling law is needed to bridge different scales. According to the original SED criterion, the critical surface energy density does not vary with scales. This suggests that the original SED criterion contains a certain multiscale shifting law. As expected, a scaling law [13–18] has been drawn out from the SED theory in recent years. Through this scaling law, the strain energy densities on different scales are associated together, which provides an approach for the cross-scale analysis.

The SED theory was originally developed in the framework of continuum mechanics. It was formulated in terms of continuum quantities. However, material is intrinsically discrete since it consists of atoms on the micro scale. The SED criterion in its current form cannot be used to analyze the micro discrete structure. What is the micro fracture mechanism that leads to the macro fracture behaviors? How should we characterize the fracture mechanism of the discrete structure from the standpoint of SED? To answer these questions, we will consider the fracture mechanism on the micro scale through the SED theory and the according scaling law [13–18]. To reach this target, we describe material with a lattice model at first. Then a discrete form of SED criterion, which is specially used for the micro discrete structure, is derived through the scaling law. Based on this discrete form of SED criterion, the micro fracture mechanism is analyzed. With this SED criterion, the discrete lattice structure can reproduce the macro fracture behaviors. As suggested in [19], although the macro and micro approaches are different, they must agree in the end. As a bond rupture criterion, the discrete form of SED criterion can make the lattice model free of the lattice size-dependency problem [20,21].

2. Lattice bond modeling of material

The micro structure of material can be represented by a lattice structure. So far there are many kinds of lattice models. The newly-developed discretized virtual internal bond (DVIB) [22] is different from the classical lattice method in that its discrete structure is composed of unit bond cells. Each unit cell can take any geometry with any number of bonds. It can capture the characteristics of the grain-composed microstructure. In this study, we choose the DVIB as the lattice model. Its modeling method can be depicted by Fig. 1. The interaction between particles is characterized by an interatomic potential. The force–displacement relation of unit bond cell is derived as

$$F_i = \frac{\partial}{\partial u_i}\left(\sum_{I<J}\Phi_{IJ}(\ell)\right) = \sum_{I<J}\frac{\partial \Phi_{IJ}(\ell)}{\partial u_i} = \sum_{I<J}\left(\Phi'_{IJ}(\ell)\cdot\frac{\partial \ell}{\partial u_i}\right) \tag{1}$$

and its stiffness matrix is

$$K_{ij} = \frac{\partial^2}{\partial u_i \partial u_j}\left(\sum_{I<J}\Phi_{IJ}(\ell)\right) = \sum_{I<J}\frac{\partial^2 \Phi_{IJ}(\ell)}{\partial u_i \partial u_j} = \sum_{I<J}\left(\Phi''_{IJ}(\ell)\cdot\frac{\partial \ell}{\partial u_i}\cdot\frac{\partial \ell}{\partial u_j} + \Phi'_{IJ}(\ell)\cdot\frac{\partial^2 \ell}{\partial u_i \partial u_j}\right) \tag{2}$$

where ℓ is the bond length; u_i is the component of the particle displacement array; $\Phi_{IJ}(\ell)$ stands for the interatomic potential between particle I and J.

In [22,23], the initial micro bond stiffness coefficient is related to the macro material constants, i.e.,

$$\Phi''_{IJ}(\ell_0) = \gamma\cdot\frac{EV}{\Omega\ell_0^2} \tag{3}$$

where V is the volume of unit cell; Ω is the bond number of unit cell; ℓ_0 is the undeformed bond length, $\Phi'_{IJ}(\ell_0)=0$; γ is a coefficient, $\gamma=6$ for 3D cases, $\gamma=3$ for in-plane stress cases and $\gamma=16/5$ for in-plane strain cases; E is the macro Young's modulus of material.

3. Scaling from macro continuum to micro discrete structure

Consider a unit bond cell immediately near crack tip, shown as Fig. 2a. The micro volume energy density of a unit cell is identified as

$$W_{mi} = \frac{U}{V} = \frac{1}{V}\sum_{I<J}\Phi_{IJ}(\ell) \tag{4}$$

where U is the total strain energy stored in a unit cell.

According to [13,14], the shifting law of strain energy density between the micro and macro scale can be written as

$$m_{mi/ma}W_{mi}r_{mi} = W_{ma}r_{ma} \tag{5}$$

where r_{mi} and r_{ma} stands for the characteristic size of micro and macro scale, respectively; $m_{mi/ma}$ the shifting coefficient of strain energy density from the micro to the macro scale, for homogenous material $m_{mi/ma}=1.0$. However, the homogeneity is only a postulation. It omits some important mechanical mechanisms that contribute to the fatigue crack growth [24]. In the non-homogeneity case, the determination of the shifting coefficient is still an open issue.

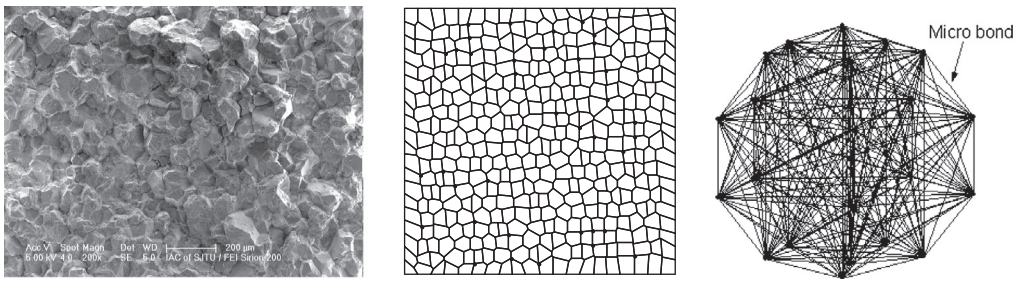

Fig. 1. Modeling method of discretized virtual internal bond for material (a) mesostructure of material (SEM image of Marble); (b) discrete bond system and (c) unit lattice bond cell.