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A lattice Boltzmann model of statistical evolution of microvoids

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Abstract

A lattice Boltzmann model is proposed for the simulation of the statistical evolution of numerous microvoids under high stress triaxiality subjected to dynamic loadings. It considers the size distribution of microvoids during ductile fracture based on the balance law of microvoids' number. A series of lattice Boltzmann equations governing the statistical evolution of microvoids are derived by using distribution function and multi-scale technique. Numerical results show that after a given time of evolution, microvoids in rate-sensitive materials are small and compact, whereas microvoids in rate-insensitive materials appear to be big and sparse, and the porosity in rate-insensitive material increases faster than that in rate-sensitive material. These numerical results might put insight into the mechanism of ductile fracture.

Keywords: Lattice Boltzmann method; Microvoids; Statistical evolution

1. Introduction

Understanding the fracture process of materials is crucial to the development of new materials with high strength and toughness. Cracks and dislocations are the two major defects determining these mechanical properties in metals. Ductile fracture of metals may result from nucleation, growth and coalescence of microvoids. There are millions of microvoids within a material element during the fracture processes. It is certainly a formidable task to deal with each one of these voids individually, and in most cases is unnecessary. The existence of numerous microvoids makes it possible to describe their behavior in a statistical average sense. Curran et al. [1] proposed the model to describe the statistical evolution of microscopic cracks or voids on the basis of experimental observations. Xing [2,3] gave a set of equations governing the statistical evolution of microcracks based on the balance law of microcracks' number and the dislocation mechanism of plastic deformation. Based on the expression for void growth rate and the balance law of microvoids' number, Li and Huang [4] investigated the statistical evolution of microvoids under high stress triaxiality. Bai et al. [5] studied the statistical evolution of ideal microcracks system. Due to their complexity, it is worth seeking a new approach to further study on statistical evolution of microvoids.

Recently the lattice Boltzmann method (LBM) has been developed as an alternative method for computational fluid dynamics (CFD). This method originated from a Boolean fluid model known as the lattice gas automata (LGA) that simulates the motion of the fluids by particles moving and colliding on a regular lattice. Although these particles are more mesoscopic than truly microscopic, the level of description used in LBM is closer to physical reality than the standard numerical schemes of CFD. The kinetic nature brings certain advantages over conventional numerical methods, such as their algorithmic simplicity, flexibility, intrinsic parallelism and simple meshes. During the past few years much progress has been made that extend the LBM becoming a tool for simulating many complex fluid dynamics problems that are quite difficult to simulate by conventional methods [6–11]. A recent study showed that the LBM could be further used to simulate other kinetic equation besides CFD [12].

The statistical evolution of numerous microvoids under high stress triaxiality subjected to dynamic loadings will be investigated by LBM in this paper. We propose a simple LBM model for simulation of the size distribution of microvoids and the porosity effect of strain rate-sensitivity in materials based on the balance law of microcracks' number. A series of lattice Boltzmann equations governing the statistical evolution of microvoids are derived by using distribution function and multi-scale technique. The evolution curves of the number density of microvoids in materials are calculated and compared with each other. The numerical experiments could lead to an

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improved understanding of microscopic mechanism of fracture process.

2. The equations of microvoid evolution

2.1. Basic definitions

Given the different effects induced by external stress, temperature, etc., the fractures of solid materials include brittle fracture, fatigue, delayed fracture and environmental fracture. The basic concepts of non-equilibrium statistical mechanics in the description of material fracture by the non-equilibrium statistical theory and the evolution of microscopic cracks or voids can be generalized as the following [2]:

(i) The fracture is a non-equilibrium irreversible dynamic process. It is determined by the nucleation, growth and coalescence of the microscopic voids.
(ii) The fracture processes consist of two states, one is the nucleation and growth of numerous microvoids, the other is the propagation of the single main crack.
(iii) The nucleation and growth of the microvoids are based on dislocation, migration and their interaction microscopically.
(iv) The evolution of the microvoids is stochastic and undetermined, thus its principle is statistical.
(v) The macroscopic mechanical factors describing the fracture should be ensemble statistical average.

2.2. Evolution equations

The internal and surface microvoids grow under external force. The microscopic structure can be seen as a series of discontinuous fluctuation on the background of the mean structure for the microscopic cracks of the matrix and the discontinuity of the phase structure. Suppose t is the time of loading, r is the size of microcracks or the radius of microvoids, $\dot{r}$ is the growth rate of microvoids, according to general law of Langevin, we have

$$\dot{r} = K(r) + F(r, t) = K(r) + \beta(r) f(t) \tag{1}$$

where $K(r)$ is migration growth rate, which is determined by the background of mean structure of the matrix and the external force; $F(r,t)$ determined by the discontinuous fluctuation of the matrix and the external force; $f(t)$ the fluctuation function; $\beta(r)$ is the fluctuation coefficient of amplification. Suppose $f(t)$ satisfies Gaussian distribution, we have

$$< f(t) >= 0, \qquad < f(t) f(t') >= Q\delta(t - t') \tag{2}$$

where Q is the fluctuation coefficient, and δ is the Dirac function.

Suppose $M(r,t)\,\mathrm{d}r$ is the number of microvoids with size between r and $r+\mathrm{d}r$ per unit volume at time t. The growth rate of M is attributed to the migration growth rate, fluctuation growth rate and the nucleation rate. Based on the balance law of microvoids' number and dynamics of microvoids, the differential equation that governs the evolution process can be written as [2]:

$$\frac{\partial M(r,t)}{\partial t} = -\frac{\partial}{\partial r}\left[\left(K(r) + \frac{Q\beta(r)}{2}\frac{\partial \beta(r)}{\partial r}\right) M(r,t)\right] + \frac{Q}{2}\frac{\partial^2}{\partial r^2}[\beta^2(r) M(r,t)] + q(t)\delta(r - r_0) \tag{3}$$

where $q(t)$ is the nucleation rate per unit volume at t.

When the fluctuation is ignored, the evolution equation of microvoids' number density may be expressed as

$$\frac{\partial M(r,t)}{\partial t} = -\frac{\partial}{\partial r}[K(r)M(r)] + q(t)\delta(r - r_0) \tag{4}$$

Because of the time reversal asymmetry of Eqs. (3) and (4) above, the irreversibility of the evolution of microvoids is revealed.

The initial condition and the boundary condition, respectively, can be written as

$$M(r, t = 0) = 0, \qquad M(r \to \infty, t) = 0 \tag{5}$$

Eq. (5) means all the microvoids or microcracks are produced by the external force, and there are no unlimited cracks before the matrix is broken.

Based on the knowledge of growth and nucleation of microvoids, the Griffith critical size or radius of microvoids is

$$c_k = \frac{\gamma E}{\pi(1 - \nu^2)\sigma^2} \tag{6}$$

where σ denotes the vertical stress imposed on the microvoid, γ the surface energy, E the Young modulus and ν is the Poisson's ratio.

The case of high stress triaxiality is studied in the paper. Suppose macroscopic mean stress applied on material element increases suddenly from zero to Σ_m at time $t=0$, and keeps constantly afterwards. The effect of the nucleation rate will not appear on the right-hand side of Eq. (4) because the size of nucleating voids c_k is always smaller than that of growing voids r in the high stress triaxiality in which the density of nucleating voids will be small. Hence, the evolution equation of microvoids' number density can be rewritten as [4]:

$$\frac{\partial M(r,t)}{\partial t} + \frac{\partial(\dot{r} M(r,t))}{\partial r} = 0, \qquad [\dot{r} M(r,t)]_{r=c_k} = q(t),$$
$$M(\infty, t) = 0, \qquad M(r, 0) = 0, \quad (r > c_k) \tag{7}$$

where second part of Eq. (7) is based on the following fact that the nucleating voids are equivalent to voids which grow from $r \le c_k$ to $r > c_k$, and the nucleation rate $q(t)$ can be taken approximately as a constant value q under constant temperature and macroscopic stress.

The growth rate of microvoids under spherically symmetric loading condition is [4]:

$$\dot{r} = G(\Sigma_m, p)\dot{\varepsilon}_0 r \tag{8}$$

where

$$G(\Sigma_m, p) = \frac{1}{2}\left[\frac{3m}{2}\frac{\Sigma_m/\sigma_0}{1 - p^m}\right]^{1/m} \tag{9}$$