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Simulating the evolution of localization based on the diffusion of damage

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Abstract

Based on the failure mechanisms of brittle solids under dynamic loading conditions, a strain-based damage diffusion model is proposed to simulate the evolution of localization due to microcracking. A three-dimensional diffusion equation is formulated with local rate-independent and rate-dependent damage evolution laws, respectively. The diffusion equation governing the evolution of damage is incorporated into the hyperbolic equation governing the wave propagation in a parallel setting. A parametric study is performed to investigate the effects of model parameters on the diffusion of damage. One- and two-dimensional sample problems are considered to illustrate how the dynamic evolution of localization can be simulated without using nonlocal models in the strain–stress space. The relationship between the proposed approach and the existing ones for localization problems is also discussed based on the preliminary results obtained in this paper. It appears that the proposed approach might be an effective numerical procedure to simulate the evolution of localization, with parallel computing, in a single computational domain involving different lower-order governing differential equations.

Keywords: Localization; Diffusion; Multi-physics; Parallel computing

1. Introduction

Much research has been conducted in the world over the last twenty years to model and simulate the initiation and evolution of material failure, and final rupture of engineering structures, as can be found in the open literature and discussed in the Minisymposium (Armero et al., 1999). However, three basic questions still remain:

1. how to identify the relationship among the initiation and evolution of material failure, and final rupture of structural members,
2. how to find a simple mathematical means to describe the failure mechanisms for which the experimental techniques available could be used to determine the model parameters, and

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3. how to design an effective numerical procedure with which the existing computer hardware could be employed to simulate the large-scale failure evolution.

Based on a recent study on failure wave phenomena (Chen and Xin, 1999; Feng and Chen, 1999), an attempt is made in this paper to formulate a strain-based damage diffusion model and to find an effective numerical procedure so that the evolution of dynamic localization can be simulated in a parallel setting.

There exist two different approaches to model the evolution of material failure, i.e., continuous and discontinuous ones, after the onset of failure is identified. Decohesion models and fracture mechanics models are representative of discontinuous approaches in which strong discontinuities are introduced into a continuum body such that the mathematical model is well posed for given boundary and/or initial data. On the other hand, nonlocal (integral or strain gradient) models, Cosserat continuum models and rate-dependent models are among the continuous approaches proposed to regularize the localization problems in which the higher-order terms in space and/or time are introduced into the strain–stress relations so that the mathematical model is well posed in a higher-order sense for given boundary and/or initial data. Usually, only weak discontinuities in the kinematical field variables are allowed in the continuous approaches, i.e., the continuity of displacement field must hold in the continuum during the failure evolution.

As demonstrated for different problems, there are certain kinds of applicability and limitation for different approaches depending on the scale of the problem and the degrees of discontinuity considered (Bazant and Chen, 1997; Pradeilles-Duval and Claude, 1995). Since a complete failure process involves different degrees of discontinuity and every physical phenomenon must obey the conservation laws, the jump forms of conservation laws might provide a useful tool to link continuous approaches with discontinuous approaches. In fact, the transition from continuous to discontinuous failure modes could be identified through the bifurcation analysis of acoustic tensor, as shown with the use of jump conditions (Chen, 1996). If the initiation and orientation of localized failure mode is identified via the bifurcation analysis, either a continuous or a discontinuous approach could be used to model and simulate the evolution of localization depending on the degree of discontinuity and the scale considered.

If a continuous approach is of interest, the use of higher-order terms in space makes it difficult to perform large-scale computer simulation due to the limitation of current computational capabilities. As can be found by reviewing the existing nonlocal models, the nonlocal terms are usually included in the limit surface so that a single higher-order governing equation will appear in the problem domain. Can we find an alternative approach to replace the single higher-order equation with two lower-order equations? If we can, parallel computing might be used for the large-scale simulation of localization problems.

As shown in the previous research (Chen and Sulsky, 1995), the evolution of localization might be equally well characterized by the formation and propagation of a moving material surface of discontinuity. With the use of a moving material surface, a partitioned-modeling approach has been proposed for localization problems. The basic idea of this approach is that local constitutive models are used inside and outside the localized deformation zone with a moving boundary being defined between different material domains. As a result, the extrapolation of material properties beyond the limitations of current experimental techniques might be avoided in modeling the evolution of localization. An attempt has also been made to investigate the use of the jump forms of conservation laws in defining the moving material surface. By taking the initial point of localization as that point where the type of the governing differential equations changes, a moving material surface of discontinuity can be defined through the jump forms of conservation laws across the surface. As the transition from a hyperbolic equation to an elliptic one could be represented by a parabolic one which governs a diffusion process, an analytical solution has been obtained for a dynamic softening bar with the use of a similarity method for the transition involving a weak discontinuity in which the diffusion speed of the moving material surface is assumed to be constant to obtain a closed-form solution (Xin and Chen, 1999). The closed-form solutions obtained by Armero (1997), with the use of a strong discontinuity, also shows that the softening profile propagates at a constant speed along the bar.

In reality, the motion of the material surface depends on the stress state and internal state variables so that the constant diffusion speed can be considered as a special case of diffusion, i.e., the time average of a real diffusion process. Due to the limitation of current experimental facilities, it is still a challenging task to quantitatively determine how the internal energy diffuses in real-time associated with the evolution of localization. However, the problems involving the type change of the governing differential equations, accompanied by certain jumps in field variables during the evolution process, also occur in other areas such as fluid mechanics (Chen and Clark, 1995) and thermal shock wave propagation (Tzou, 1989, 1997). As will be shown in this paper, the use of different governing differential equations, after localization occurs, makes it possible to replace the single higher-order equation with two lower-order equations so that parallel computing might be used for the large-scale simulation of localization problems.

Without the assumption that the diffusion speed is constant, a strain-based damage diffusion model is proposed in this paper to simulate the evolution of localization due to microcracking, based on the dynamic failure mechanisms of brittle solids. A three-dimensional diffusion equation is formulated with local rate-independent and rate-dependent damage evolution laws, respectively. A parametric study is performed to investigate the effects of model parameters on the diffusion of damage. The diffusion equation governing the evolution of damage is then incorporated into the hyperbolic equation governing the wave propagation in a parallel (staggered) setting after localization occurs. One- and two-dimensional sample problems are considered to illustrate how the dynamic evolution of localization can be simulated without using nonlocal models in the strain–stress space. The relationship between the proposed continuous approach and the existing ones for localization problems is also discussed based on the preliminary results obtained here.

2. Constitutive modeling and solution procedure

The recent research results about the delayed failure wave, as observed in the glass specimens that are shocked to near but below the Hugoniot elastic limit (HEL), suggest that the HEL may not be an elastic limit, but rather, it may be a transition in failure mechanisms. A possible transition is the one from a delayed kinetic-controlled failure process below the HEL to a prompt stress-controlled failure process above the HEL (Grady, 1995a,b). Much research has been done to explore the failure wave phenomenon as reviewed by (Espinosa et al., 1997a,b), but there is currently no consensus on the cause of failure waves.

Based on a recent study on the failure wave phenomenon (Feng and Chen, 1999), it appears that, in the dynamic failure process of certain engineering materials, microfissuring at one location induces local deformation heterogeneity that in turn initiate microfissuring in the adjacent material and so on if a critical state is reached. Hence, a diffusion equation governing the progressive percolation of heterogeneous microdamage appears to capture the essence of the dynamic failure evolution in shocked glasses, as verified with the experimental data available. The use of jump conditions could also result in a diffusion equation governing the failure wave speed through a mathematical argument (Chen and Xin, 1999). To simulate the dynamic failure evolution of a class of brittle solids, a strain-based damage diffusion model is proposed in this paper with focus on the effects of model parameters on the failure responses, the convergence study, and the implementation of the model into commonly used numerical codes.

If the bifurcation analysis of acoustic tensor identifies the onset of localization, a surface of discontinuity will be driven by the heterogeneity and stress concentration with $\boldsymbol{n}$ being the vector normal to the surface. The law of damage diffusion is assumed to be

$$\boldsymbol{J} = -d\frac{\partial C}{\partial \boldsymbol{n}} \tag{1}$$

in which C is the concentration of microcracks (the number of microcracks per unit volume), $\boldsymbol{J}$ the flux of microcracks (the number of microcracks diffusing down the concentration gradient per unit time per unit area), and d the damage diffusivity function. If the damage diffusion is assumed to be isotropic, a shear-induced damage diffusivity function at any location $\boldsymbol{x}$ and time t can be defined as

$$d(\boldsymbol{x}, t) = \lambda_1 \frac{\bar{\varepsilon}_F - \bar{\varepsilon}}{\bar{\varepsilon}_F - \bar{\varepsilon}_L} \tag{2}$$

in which $\bar{\varepsilon}$ is the second invariant of deviatoric strain tensor, with $\bar{\varepsilon} = \bar{\varepsilon}_L$ at the limit state and $\bar{\varepsilon} = \bar{\varepsilon}_F$ at the final state before rupture. As can be seen, the diffusion process will diminish with the evolution of failure, and the model parameter λ_1 controls the rate of diffusion.

To initiate the evolution of damage, an internal damage evolution per unit time must be given here, which takes the form of

$$Q(\boldsymbol{x}, t) = \frac{\bar{\varepsilon} - \bar{\varepsilon}_L}{\bar{\varepsilon}_L t_d} \geqslant 0 \tag{3}$$

for the rate-independent case, and

$$Q(\boldsymbol{x}, t) = \frac{\int_{t_L}^{t} \cdot(\bar{\varepsilon} - \bar{\varepsilon}_L)\mathrm{d}t}{\bar{\varepsilon}_L t_{dr}} \geqslant 0 \tag{4}$$

for the rate-dependent case, with t_d and t_{dr} being the characteristic time of the rate-independent and rate-dependent concentration evolution of microcracks, respectively. The parameter t_L represents the time at which the limit state is reached.

The concentration of microcracks C is related to the damage parameter D which is defined as the volume fraction of material that has lost load-carrying capability (Taylor et al., 1986). For the purpose of simplicity, a linear relationship is assumed between C and D with the material parameter λ_2, namely,

$$D(\boldsymbol{x}, t) = \lambda_2 C(\boldsymbol{x}, t). \tag{5}$$

The equation governing the damage diffusion can then be written as, in a standard form,

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial \boldsymbol{n}}\left(d \frac{\partial C}{\partial \boldsymbol{n}}\right) + Q. \tag{6}$$

The strain-based damage diffusion model is complete if a strain–stress relation is given. For the purpose of illustration, a simple form of isotropic damage is used as below:

$$\sigma = (1 - D)\boldsymbol{E} : \varepsilon \tag{7}$$

with $\boldsymbol{E}$ being the undamaged elasticity tensor.

As can be seen, Eq. (7) does not explicitly involve any higher-order terms in the strain–stress space. However, the gradients of strain appear in Eq. (6) to simulate the evolution of localization due to the assumption that the diffusivity is a function of the second invariant of deviatoric strain tensor, as given by Eq. (2). The key difference between the proposed approach and existing higher-order models is that higher-order terms in space do not explicitly appear in the strain–stress relation so that the diffusion equation and the wave equation can be formulated in a conventional framework and solved in a parallel (staggered) setting. The order of these conventional differential equations is lower than that of existing nonlocal differential equations. If the diffusivity is taken to be a constant, the strain gradients will not appear in the model. As a result, however, the concentration of microcracks would diffuse down the concentration gradient in the same rate whether or not the material is partially or fully damaged, which might not be representative of the physics associated with the failure evolution.

It can be found from Eqs. (3) and (4) that the damage evolution at a given material point (local scale) is standard which satisfies the thermodynamic restrictions. In other words, the damage evolution with time at a given material point is dissipative. The evolution of localized damage in space is governed by diffusion equation (6). Since the damage evolution at each material point within the localization zone is dissipative, the evolution of localized damage in space must be dissipative.

Because of the simplicity of the strain-based damage diffusion model, there are only two model parameters, λ_1 and t_d (t_{dr}), which are directly related to the damage diffusion process, while the other model parameters can be determined from either the pre-limit or limit responses (including the final rupture). In addition, the strain-based model can be easily implemented into the displacement-based finite element programs. It should be pointed out that the existing experimental data do not warrant the formulation of a more advanced damage diffusion model. Hence, the focus of this paper is to demonstrate how an effective solution procedure can be designed to simulate the essential feature of the evolution of localization without using nonlocal models in the strain–stress space.

The numerical procedures for conventional diffusion and wave equations can be found in the standard books (Belytschko and Hughes, 1983; Reddy and Gartling, 1994; among others). For the one- and two-dimensional sample problems considered in Section 3, central difference in space and forward integration in time will be used to solve the diffusion equation, while constant stress elements in space and forward integration in time will be employed to solve the wave equation. When the diffusion equation and the wave equation are solved in a parallel (staggered) setting, the time step satisfying both stability conditions is used to solve the whole problem at the same time. The solution procedure for the response after the limit state is reached ($\bar{\varepsilon} \geqslant \bar{\varepsilon}_L$) can be summarized as follows:

1. Solve Eq. (6) with Eqs. (3) or (4) being active only at those materials points where the limit state is reached.
2. Find the current damage value from Eq. (5).
3. Find the current value of stress from Eq. (7) for the given values of damage and strain.
4. Solve the wave equation for the given value of stress, and go to Step 1 with the new value of strain.

3. Parametric study and illustrations

Consider a tensile bar of length L with mass density ρ, that is fixed at the left end $x = 0$ and loaded at the right end $x = L$. If a diffusion equation governs the evolution of localization after a limit state is reached at $x = 0$, a closed-form solution has been obtained with the use of local rate-independent elastoplastic models, and a moving material surface with a constant diffusion speed (Xin and Chen, 1999). To verify the proposed procedure for localization problems, the rate-independent damage diffusion model with the use of Eq. (3) is first used to simulate the evolution of localization without assuming a constant diffusion speed for the moving material surface between localization and elastic zones. In other words, the moving surface will come out as a result of the solution process instead of that determined prior to the solution. As shown later, the numerical solutions qualitatively replicate the closed-form solutions.

To illustrate the effects of model parameters on the damage diffusion process, let

$$\bar{\varepsilon}_L = 0.002, \qquad \bar{\varepsilon}_F = 0.01, \qquad \lambda_2 = 1\ \text{m}^3,$$

$$E = 50\ \text{GPa}, \qquad \rho = 2500\ \text{kg/m}^3, \qquad L = 1\ \text{m}.$$

The limit state is reached at $x = 0$ and $t = t_L = L/\sqrt{E/\rho}$ for the following boundary and initial conditions:

$$u(0,\text{t}) = 0, \qquad \varepsilon(L,t) = \frac{\sigma}{E} = 0.0015, \qquad C_{,x}(L,t) = 0,$$

$$u(x,0) = 0, \qquad u_{,t}(x,0) = 0, \qquad C(x,0) = 0,$$

respectively.

The evolution of strain after the limit state is reached is shown in Fig. 1, and the corresponding damage and stress fields are given in Figs. 2 and 3. As can be seen from these three figures, the evolution of localization predicted by the proposed procedure qualitatively replicate the closed-form solution (Xin and Chen, 1999), but the diffusion speed is not constant any more. The effect of λ_1 on the diffusion of damage is demonstrated in Fig. 4, and the effects of t_d on the diffusion of damage and the damage evolution history are shown in Fig. 5a and b, respectively. As can be found from Figs. 4 and 5, both the parameter λ_1 and t_d can control the rate of diffusion. However, the parameter t_d controls the rate of diffusion (locally) at a given material point, while the parameter λ_1 influences the rate of diffusion globally. In other words, the damage evolution history at a given material point cannot be controlled by λ_1 . If a rate-dependent damage model with the use of Eq. (4) is employed, the shape of the solution curves looks smoother due to the gradual increase of damage through the integral in addition to some minor differences in the effects of model pa-

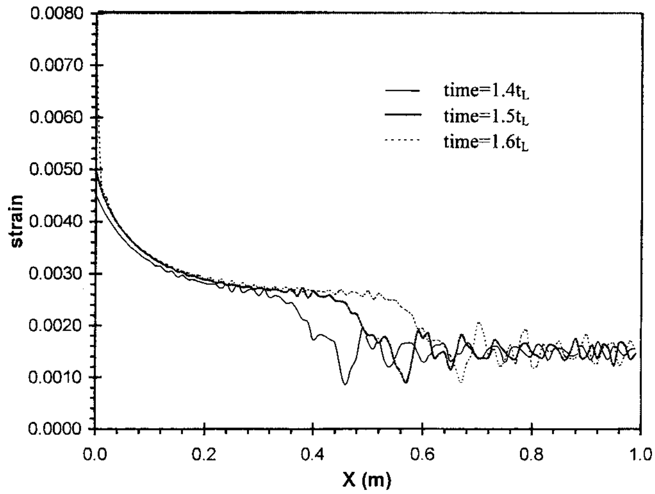

Fig. 1. The evolution of strain after the limit point is reached ($\lambda_1 = 150.0$ m^2/s, $t_d = 0.0015$ s).

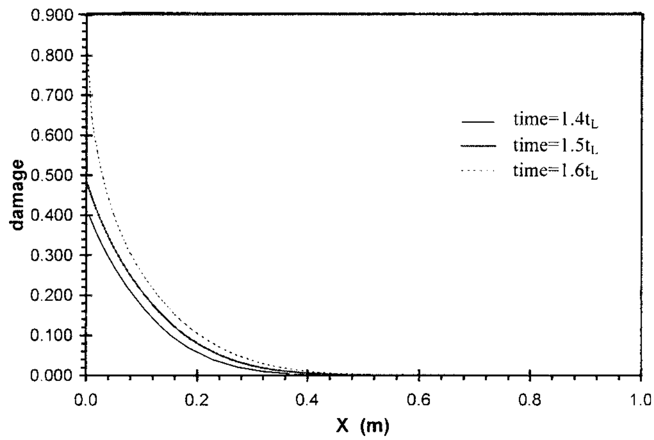

Fig. 2. The evolution of damage corresponding to Fig. 1.

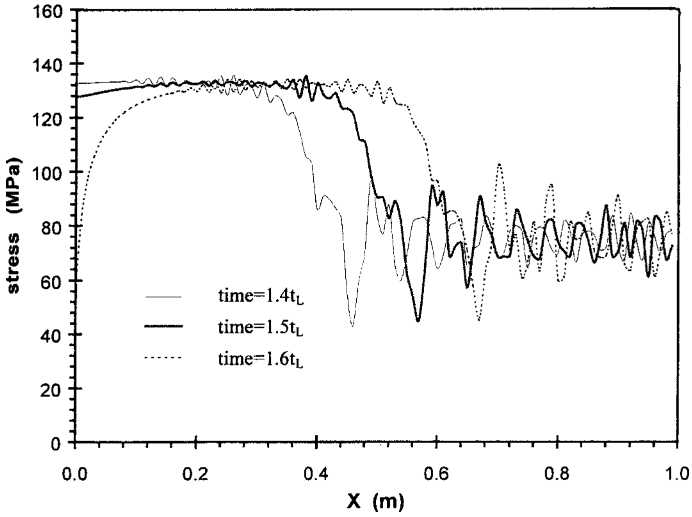

Fig. 3. The decrease of stress corresponding to Fig. 1.

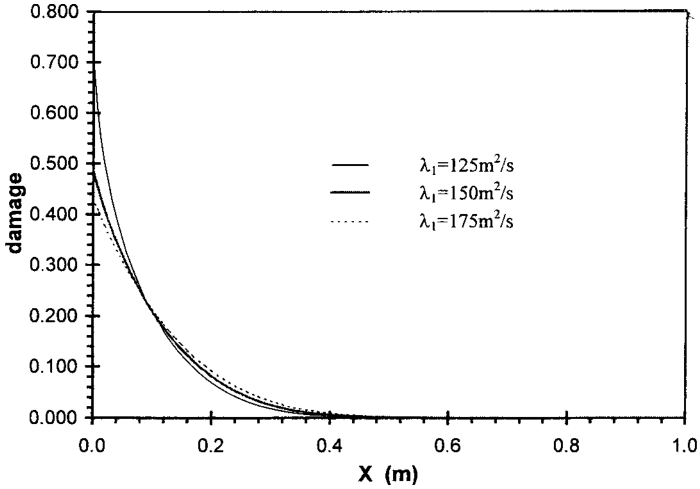

Fig. 4. The effect of λ_l on the damage profile ($t_d = 0.0015$ s, time $= 1.5t_L$).

rameters. However, both the rate-independent and rate-dependent models predict the same essential features of the evolution of localization, and a finite zone of localization with mesh refinement, as shown in Figs. 6 and 7.

A two-dimensional problem, as depicted in Fig. 8, is considered here to further demonstrate the proposed procedure. Two types of finite element meshes, with rectangles consisting of four triangular elements, are adopted as shown in Fig. 9. The same values of model parameters as in the one-dimensional case are employed in the two-dimensional case with Poisson's ratio being 0.3. A tensile force is applied at the top of the specimen so that the value of $\bar{\varepsilon}$ in the incoming wave is about three-quarters of $\bar{\varepsilon}_L$. A weak element is located at the origin. A bifurcation analysis is not performed here so that the isotropic damage diffusion

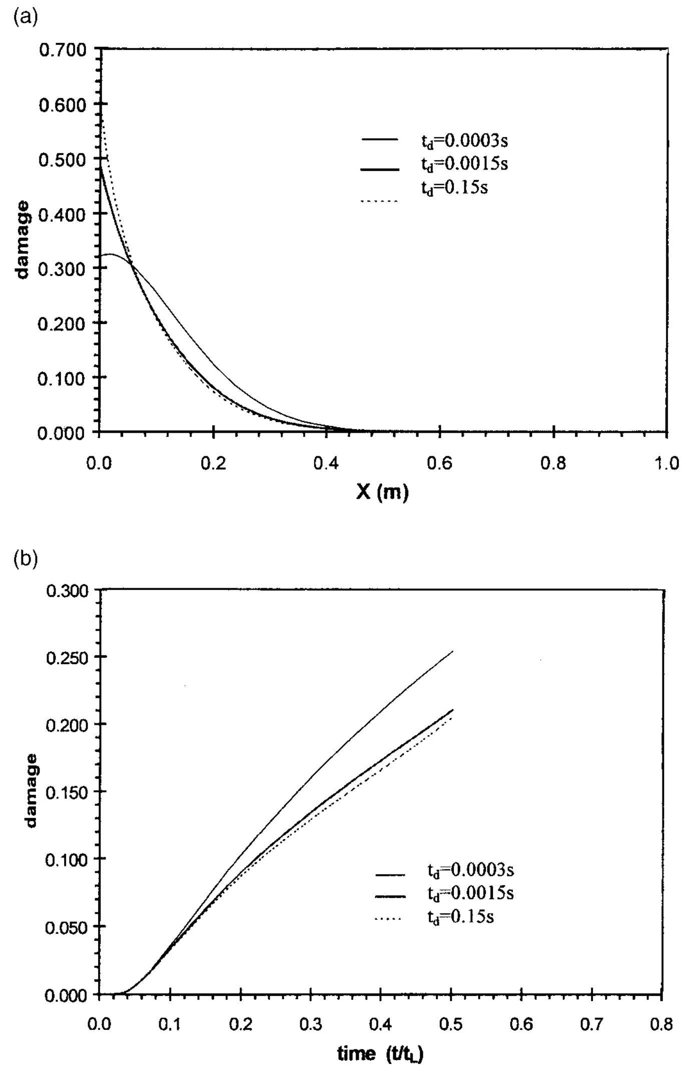

Fig. 5. (a) The effect of t_d on the damage profile ($\lambda_l = 150.0\ m^2/s$, time $= 1.5t_L$) and (b) the effect of t_d on the damage history corresponding to Fig. 5a.

model will predict a circular damage contour. However, the use of a shear-induced damage diffusivity function, as given by Eq. (2), should yield localized deformations of mode II.

With the use of the rate-independent damage diffusion model, the profile of the second invariant of deviatoric stress tensor in the post-limit regime ($t = 1.3t_L$) is shown in Fig. 10, and the corresponding profile of the second invariant of deviatoric strain tensor is given in Fig. 11. The damage contours with different meshes are demonstrated in Fig. 12. If a rate-dependent damage diffusion model is used, the stress and strain profiles in the post-limit regime ($t = 1.3t_L$) are shown in Figs. 13 and 14, and the damage contours with different meshes are given in Fig. 15. Because of the gradual increase of damage through the integral, the maximum value of damage in Fig. 15 is less than that in Fig. 12. The stress and strain profiles in the deep post-limit regime ($t = 1.6t_L$) are demonstrated in Figs. 16 and 17 for the rate-dependent model. As can

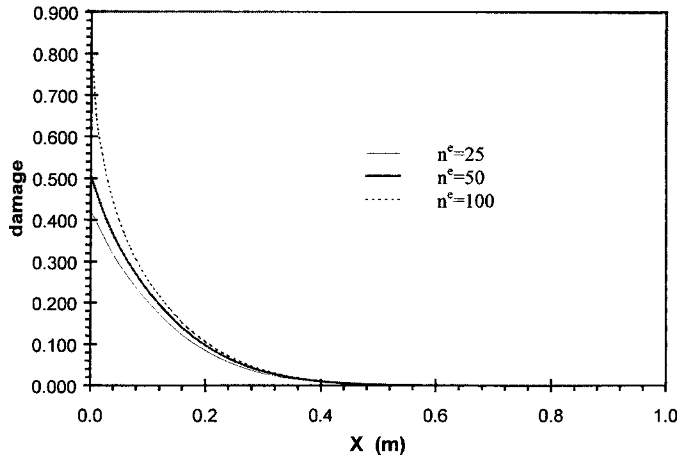

Fig. 6. The convergence study with different meshes for the rate-independent model ($\lambda_l = 150.0$ m^2/s, $t_d = 0.0015$ s, time $= 1.6t_L$).

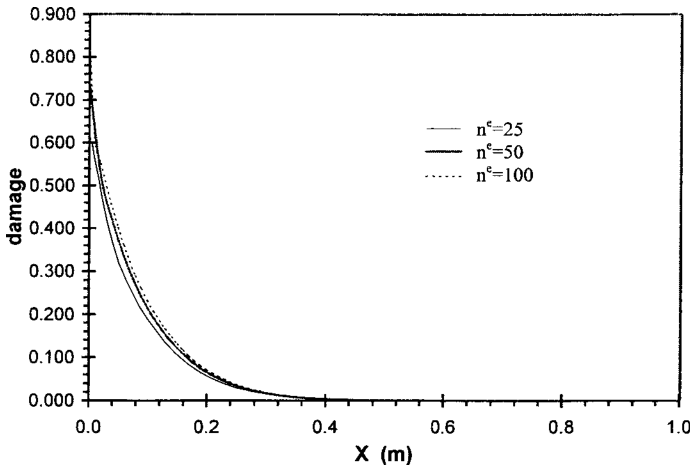

Fig. 7. The convergence study with different meshes for the rate-dependent model ($\lambda_l = 150.0$ m^2/s, $t_{dr} = 8 \times 10^{-8}$ s^2, time $= 1.6t_L$).

be seen, a clear shear band appears in the strain profile. It is interesting to note that the convergent behavior of the rate-independent model in the two-dimensional case looks better than that in the one-dimensional case while the convergent behavior of the rate-dependent model looks in the opposite way.

4. Concluding remarks

Based on the dynamic failure mechanisms of brittle solids, a strain-based damage diffusion model is proposed to simulate the evolution of localization due to microcracking. A three-dimensional diffusion equation is formulated with local rate-independent and rate-dependent damage evolution laws, respectively. As a result, a single higher-order governing equation can be replaced with two lower-order governing

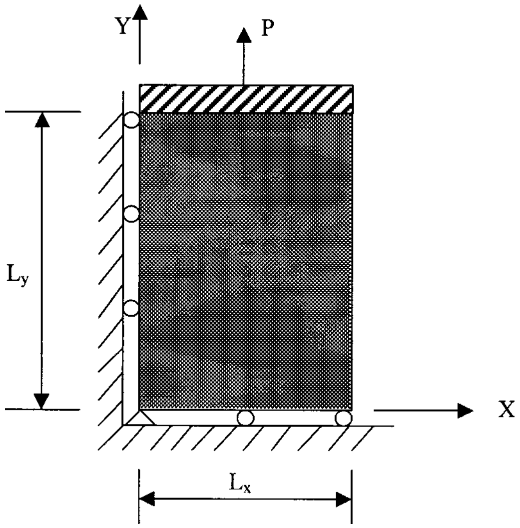

Fig. 8. The problem geometry and boundary conditions for two-dimensional simulation.

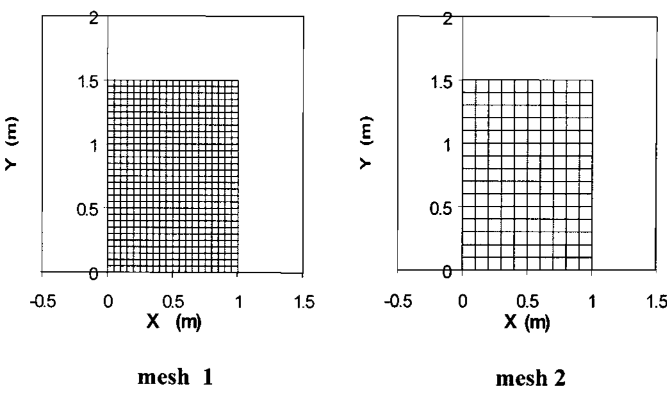

Fig. 9. Finite element meshes used for two-dimensional simulation.

equations in a single computational domain for localization problems. A parametric study is performed to investigate the effects of model parameters on the diffusion of damage. One- and two-dimensional sample problems are considered to illustrate how the dynamic evolution of localization can be simulated without using nonlocal models in the strain–stress space. As can be found from the numerical solutions, the essential features of the evolution of localization, and a localization zone of finite width can be predicted with the proposed procedure.

Future research is required to better understand the convergent behavior, to perform the bifurcation analysis for the diffusion equation, and to apply the proposed procedure to general cases. Based on the preliminary results obtained in this paper, however, it appears that the proposed approach might be effective in simulating the evolution of localization with parallel computing. The research results for localization problems might also be useful for those engineering problems involving the transition among different governing differential equations in a single computational domain.

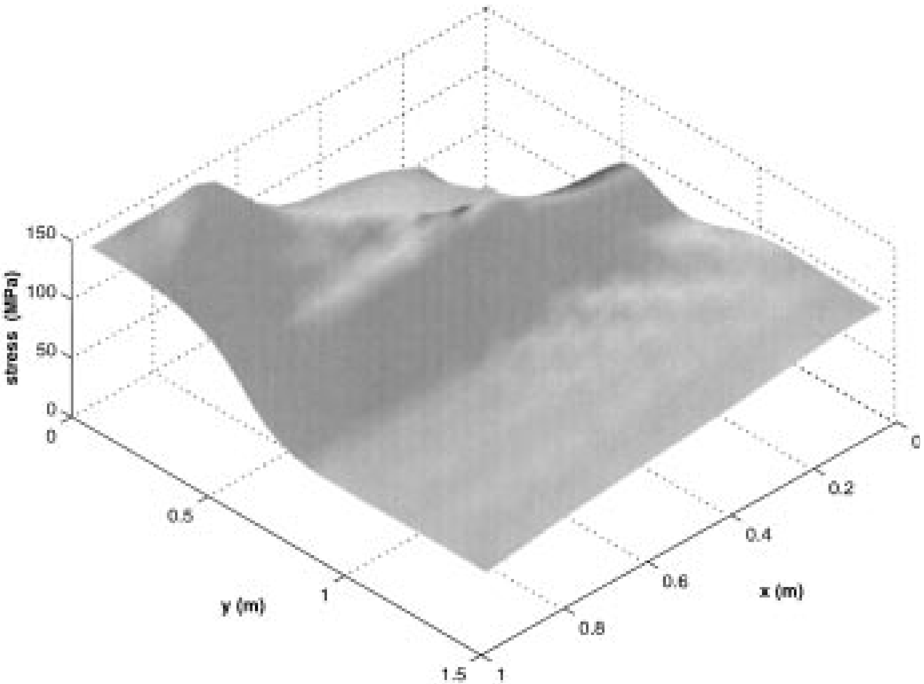

Fig. 10. The stress profile in the post-limit regime for the rate-independent model.

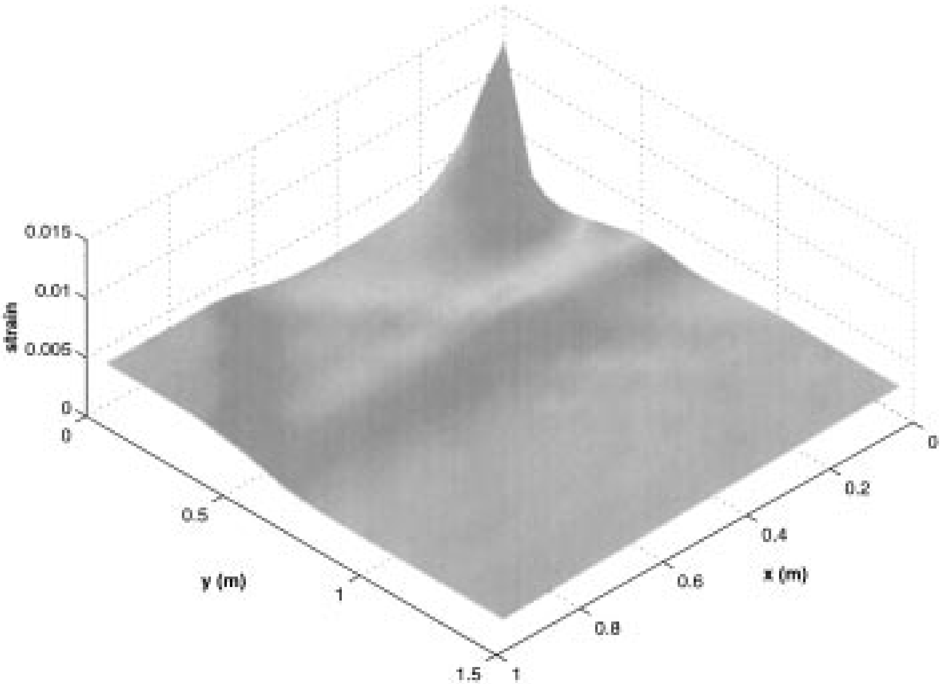

Fig. 11. The strain profile corresponding to Fig. 10.

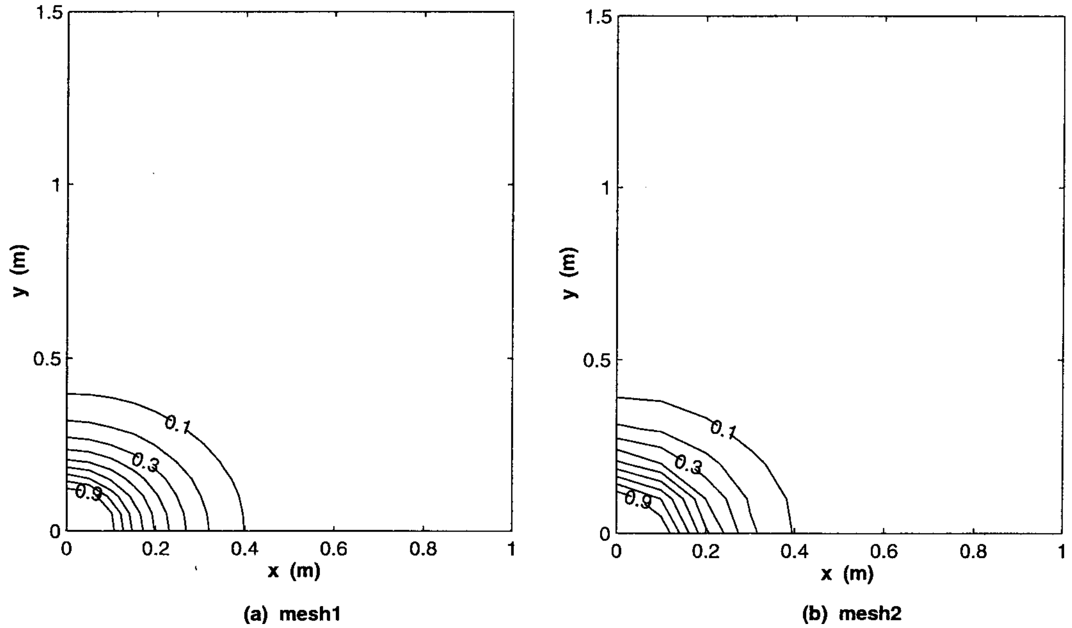

Fig. 12. Damage contours with different meshes.

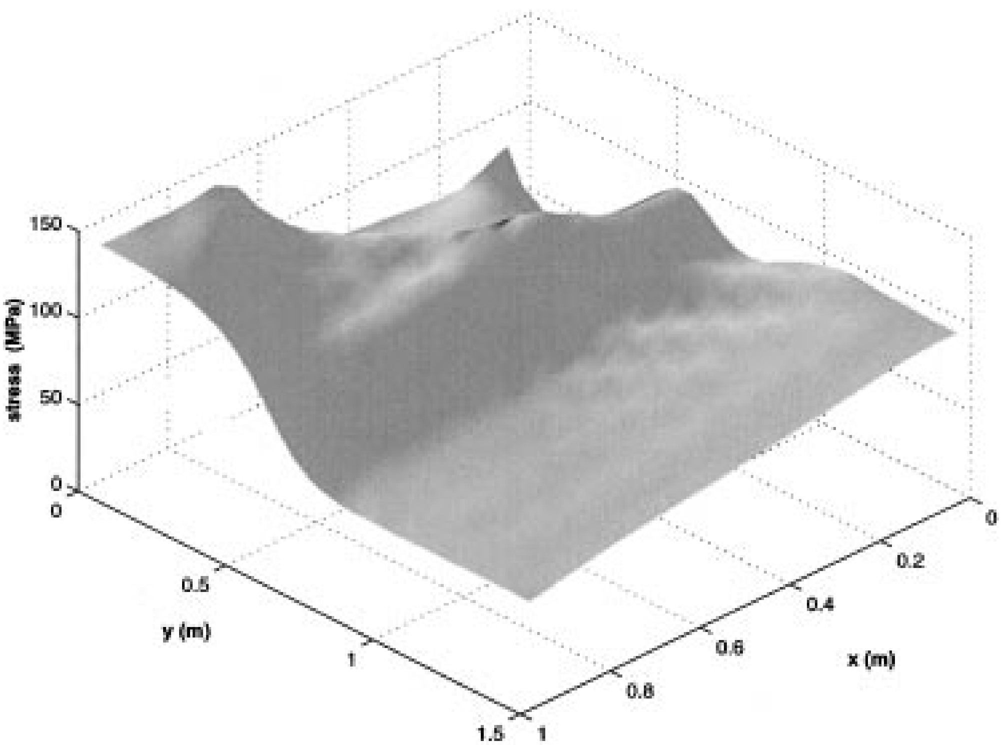

Fig. 13. The stress profile in the post-limit regime for the rate-dependent model.

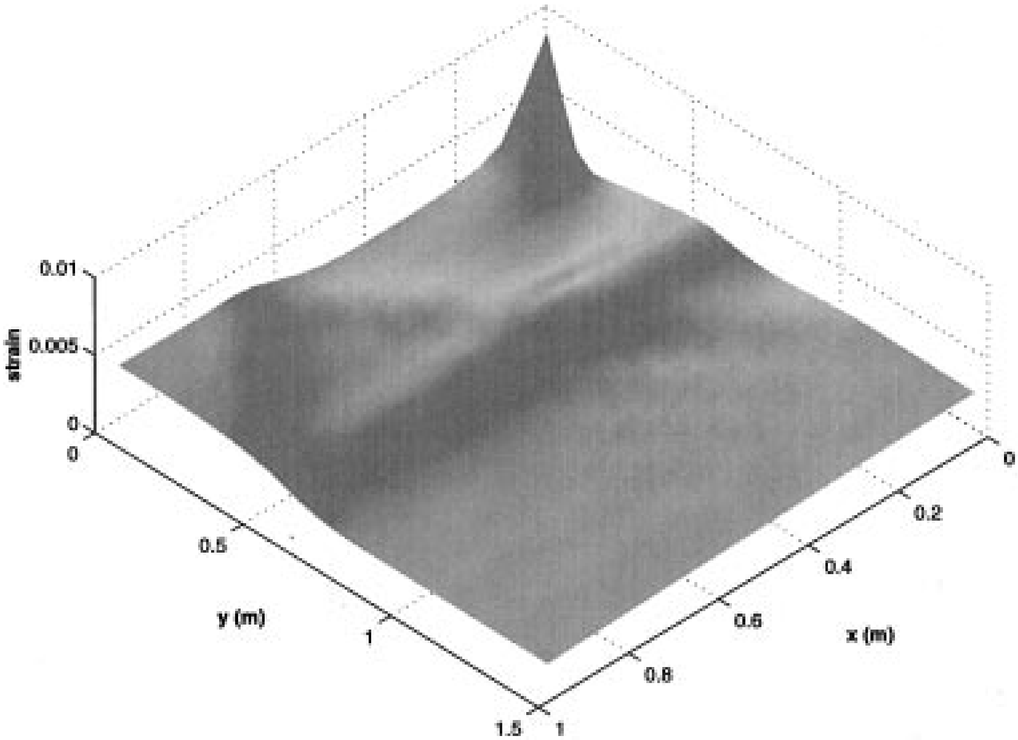

Fig. 14. The strain profile corresponding to Fig. 13.

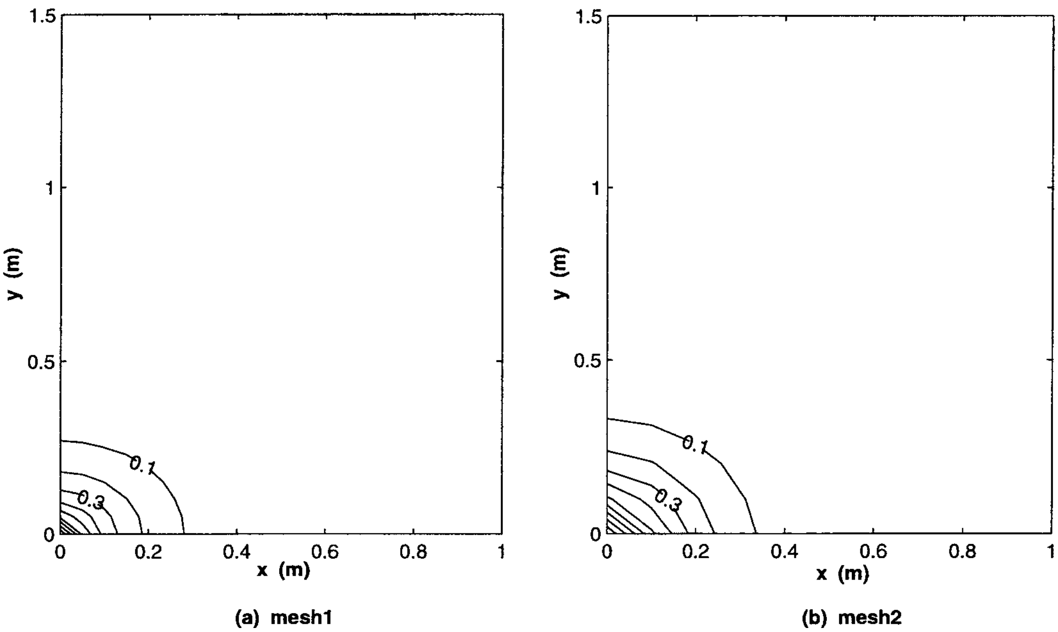

Fig. 15. Damage contours with different meshes.

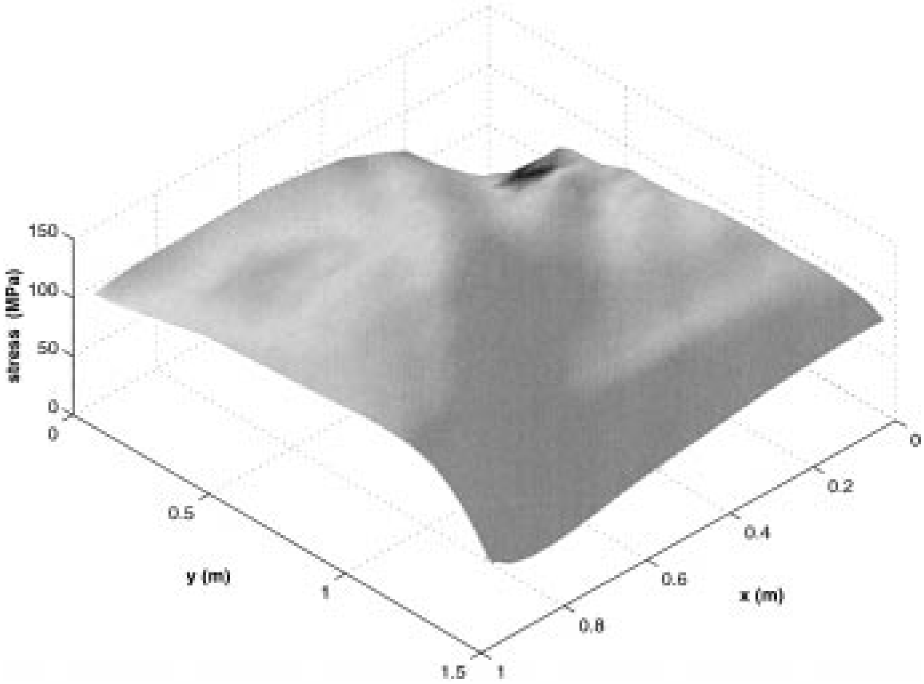

Fig. 16. The stress profile in the deep post-limit regime for the rate-dependent model.

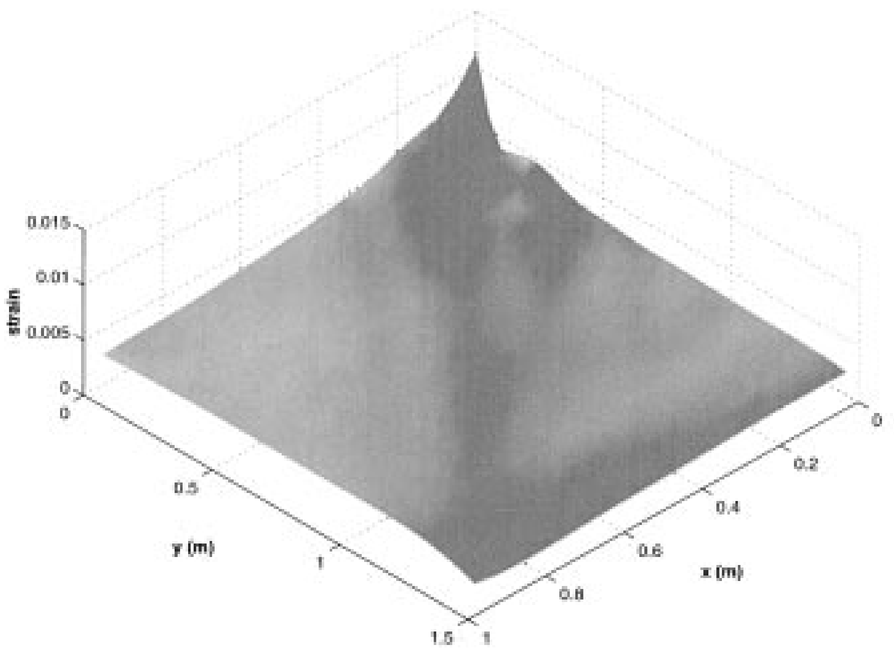

Fig. 17. The strain profile corresponding to Fig. 16.

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