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The Simulations of the Void Initiation from the multiple seeds by Molecular Dynamics and the FEM

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ABSTRACT

We have been studied the void formation from the single seed by using MD. Moreover, the same model has been simulated by using FEM. In this paper, as the next step, which will connected to the mezzo-scopic and the macroscopic fracture, we study the void initiation from multiple seeds. A square unit cell with some atom defects is constructed with nickel atoms and is subjected to the tensile load by using Molecular Dynamics. A same configured model with some small voids is simulated by using FEM. In this simulation, the mechanical properties, which are given by the potential function of the Molecular Dynamics, are used. When there is only one seed, one void grows simply from the seed. If there are multiple seeds, we observe the void growth and the void vanishing by the influence from the other voids. The behaviors of the voids initiation by the two methods, which are microscopic and macroscopic method, are compared to each other.

KEYWORDS

Molecular Dynamics, void initiation, FEM, computational simulation, Ni.

INTRODUCTION

Formation of a void is a considerable feature for a number of engineering materials, because failure by coalescence of the voids is an important fracture mechanism in ductile solids. There are some theoretical solutions of the void formation for nonlinear elastic solid. On the other hand, it is important to study microscopic void formation, in order to consider the initiation of the void. We have been studied the void formation from the single seed by using Molecular Dynamics (MD) [1-3]. There are many studies about crack simulations by MD. But, we think that the atom order crack can not grow and exists as steady state. If

an atomic order crack exists, it will immediately close by the inter-atomic power. Moreover the optimum configuration of the very small defect should be sphere by surface tension. By our void growth simulation, the atom order void can exist in steady state by reducing the load. On the other hand, the atom order void can not grow to the macroscopic void, although the void in the liquid can grow to very huge. Thus, we think that the following scenario to the destruction of a solid.

1) The atom order void initiation and growth.
2) The mezzo-scopic crack initiation by chaining the atom order voids.
3) The macroscopic destruction by the crack growth.

The step 2) might be denoted as phase changing from simple voids to a complex crack. We have been studied the step 1) [1-3]. In this paper, as the next step, which will connected to the mezzo-scopic and the macroscopic fracture, we study the void initiation from multiple seeds. A square unit cell with some atom defects is constructed with nickel atoms and is subjected to the hydrostatic tensile load by using Molecular Dynamics. A same configured model with some small voids is simulated by using FEM. In this simulation, the mechanical properties, which are given by the potential function of the Molecular Dynamics, are used. If there is only one seed, one void grows simply from the seed. In this study, we observed the void growing and the void vanishing by the influence from the other voids. The behaviors of the voids initiation by the two methods, which are microscopic and macroscopic method, are compared to each other.

SIMULATIONS BY FEM

The void formations in an infinite long compressible elastic cylinder under axis-symmetric stretch are examined by Biwa [4]. In this theory, the strain energy function W for homogeneous isotropic nonlinear elastic solid is given as constitutive relation.

$$W(\lambda_1,\lambda_2,\lambda_3) = \frac{\mu}{k}\left| \lambda_1^{-k}+\lambda_2^{-k}+\lambda_3^{-k}-3+k(\lambda_1\lambda_2\lambda_3-1) \right| \tag{1}$$

where, λ_i (i=1, 2, 3) is the principle stretches. Young's modulus, the bulk modulus and Poisson's ratio of Ni can be given as 110[GPa], 180[GPa] and 0.398 for EAM potential, respectively. Then, the material constants μ and k are set to 154[GPa] and 0.513, respectively. We consider the square plate, which side length is denoted as A, and make five holes with radius B_i (i = 1, 2, 3, 4, 5) , as shown in Fig.1.

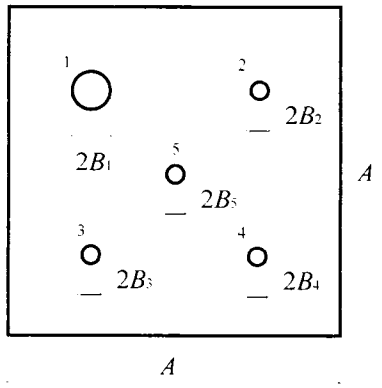
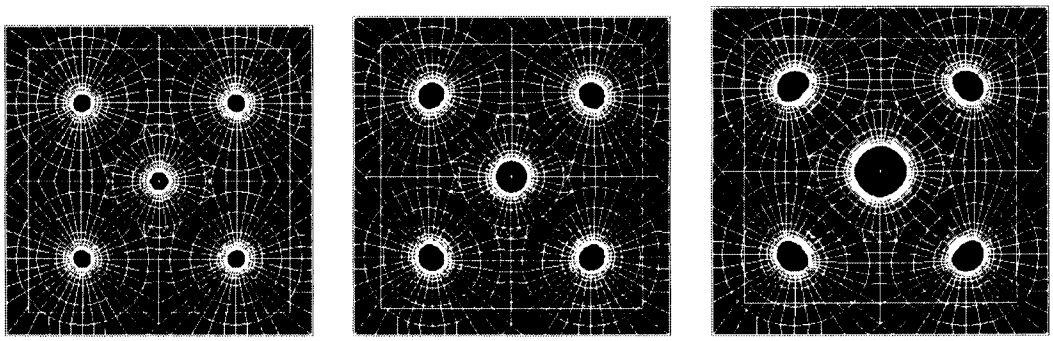


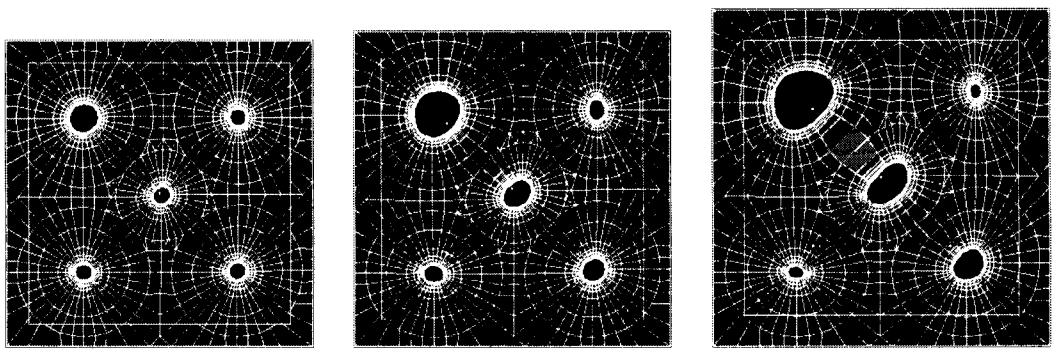
Figure 1: Simulation model.

By using the energy function W as shown in Eq.(1), FEM simulations are proceeded with plain strain condition. The stepwise uniform stretch is applied by moving boundary of this square in plane strain condition. Two types of radius Bi/A = 0.002145 or 0.00357 are used as the initial void. The number of combination to set two radii to five holes is twelve in consideration with symmetry. We tried every combinations and the typical results are shown in Fig. 2.



Stretch = 1.171 1.206 1.240

(a) $B_1/A = B_2/A = B_3/A = B_4/A = B_5/A = 0.002145$



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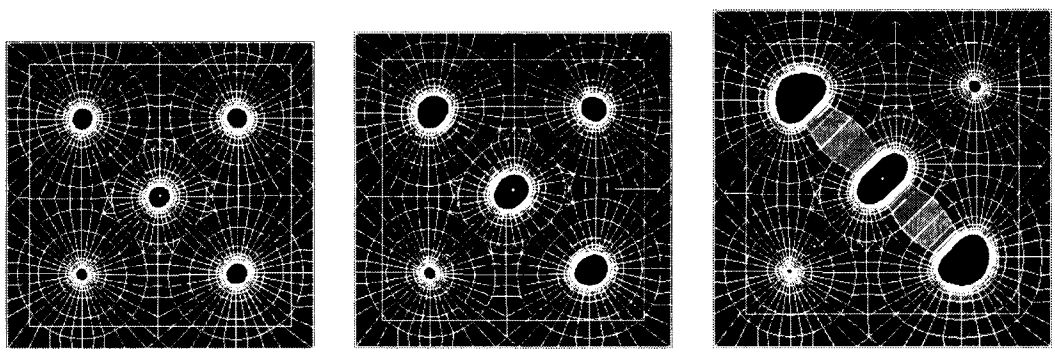
(b) $B_1/A = 0.00357$, $B_2/A = B_3/A = B_4/A = B_5/A = 0.002145$



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(c) B1/A = B2/A = B4/A = B5/A = 0.00357, B3/A= 0.002145

Figure 2: Void growth from the five seeds.

We found that, the void in the neighborhood of the slightly big void, that is void along the diagonal line, grows into bigger. The other voids are growing within small stretch, but they are shrinking by the growth of the bigger voids. Figure 3 shows relationships between the stretch and the radius of the voids for case (a), (b) and (c) in Fig.2. The growth of the void is reduced by growing of the void in diagonal line. For example, the radius of void B_2 in (b) and (c) is reducing after stretch 1.2 by growing of void B_1.

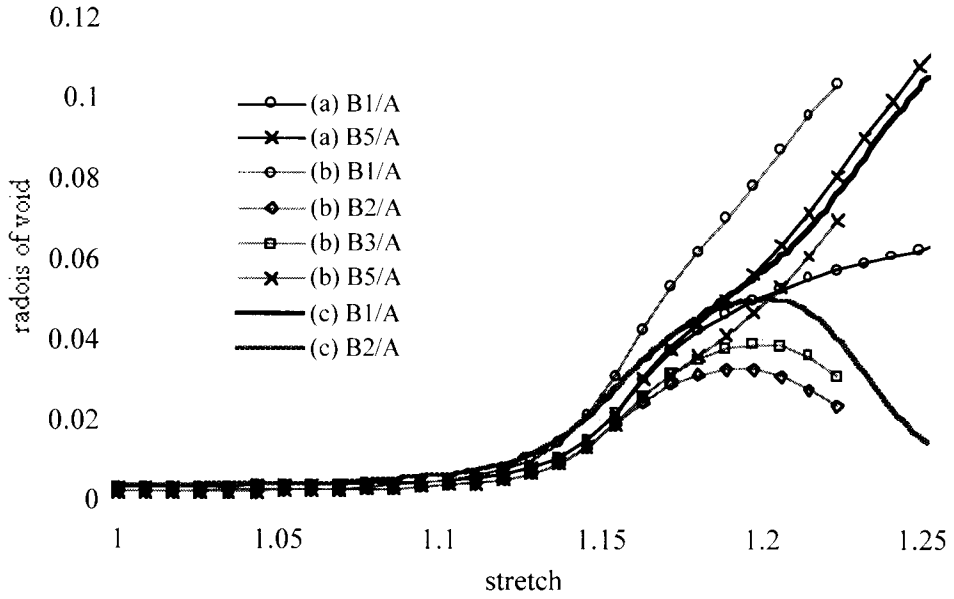
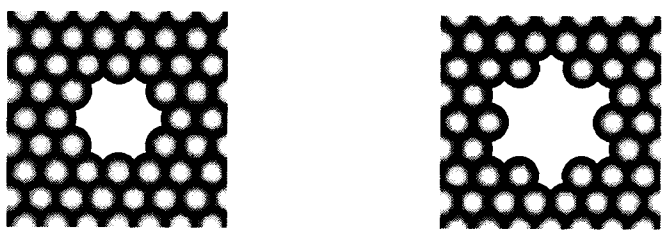


Figure 3: Relationship between stretch and radius of the voids with the initial hole radius as (a) $B_1/A = B_2/A = B_3/A = B_4/A = B_5/A = 0.002145$, (b) $B_1/A = 0.00357$, $B_2/A = B_3/A = B_4/A = B_5/A = 0.002145$ and (c) $B_1/A = B_2/A = B_4/A = B_5/A = 0.00357$, $B_3/A = 0.002145$.

SIMULATIONS BY MD

The simulation model is constructed with fcc crystal of Ni atoms. The axial direction is set along [111] direction. By applying the periodical boundary condition with periodic length 6.097 Å to the axial direction, the model forms the infinite long bar with square cross section 100.6 × 100.6 Å. The number of atoms without void is 5692. The equilibrium lattice constant at the absolute temperature 0K is 3.52Å. The movement of atoms, which constructs the outer surface of the bar within 4 Å from the edge, is fixed in order to apply the stretch. Two types of the initial void, as shown in Fig. 4, are introduced by taking the atoms. The time step $\Delta t = 0.001$ [ps] and the stretch 1.001 is applied by every 100 time steps, that is, the relaxation time 0.1 [ps] is applied by every stretch step. Embedded Atom Method [5] is used as the inter-atomic potential. At first, the simulation model is relaxed at the initial temperature 0K. Next, the model is subjected to the uniform stretch by moving the fixed atoms along the cross section of the bar. While the external load is applied, the temperature control is not carried out.

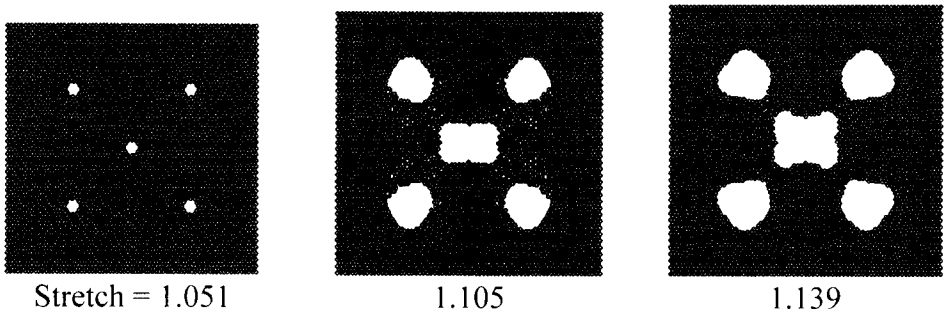


(I) small void (II) big void

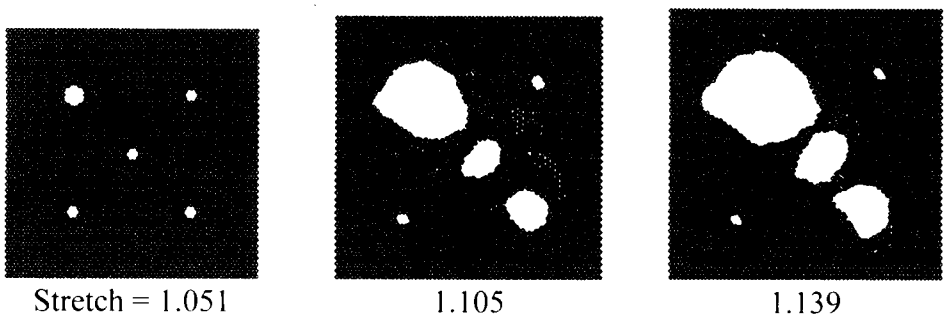
Figure 4 : Two types of initial void.

Figure 5 shows the snapshots of the simulations with the stretch 1.051, 1.105 and 1.139. We can observe the similar manner of the voids growing to the results by FEM in Fig. 2. In this MD simulation, smaller initial void can not grow. In case (c), such the void is vanished by growing of the other voids. The radius of the initial voids is relative to the width of this plate with about 0.04. Thus, this relative radius of the initial voids is ten times larger than the one in the FEM simulations. Then, the growth of the small void is disturbed by

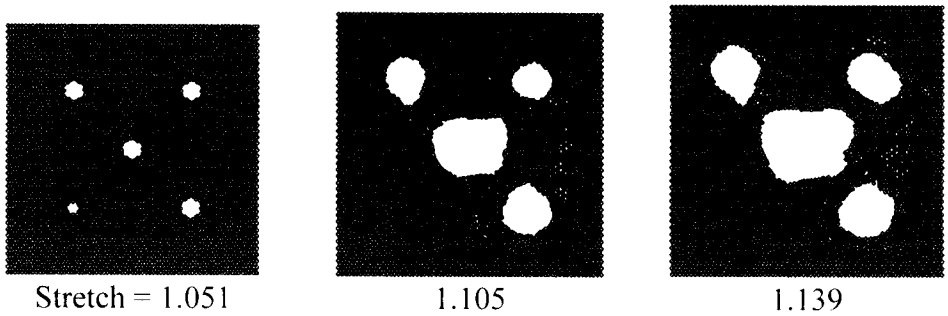
the big voids at smaller stretch.



(a) All holes are type I (small).



(b) The hole 1 is type II (big), and the other holes are type I (small).



(c) The hole 2 is type I (small), and the other holes are type II (big).

Figure 5: Void growth from the five origins.

CONCLUSIONS

The growth of five initial seeds, whose radius is slightly different, in the square plate is simulated by FEM and MD. Very different void growth by the difference of the initial void radius could be observed. Moreover, the manner of growth by FEM is similar to the one by MD, although the scale and the method of the simulation are very different. It might be some formulas in the growing of the void from multiple seeds. If we can find such the formulas, it could be possible to discover the process from micro to mezzo.

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