Numerical Analysis of the Effect of Diffusion and Creep Flow on Cavity Growth at the Nano-scale Level

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ABSTRACT

In this study, a unified numerical method, which combines finite element analysis and finite difference analysis, for inter-granular cavity growth analysis is proposed. The numerical method includes three important mechanisms of cavity growth, which are grain boundary diffusion, surface diffusion along the cavity surface, and material creep flow, in simulating cavity growth at high temperature. An incremental cavity shape evolution scheme is used to simulate cavity shape transition from a spherical-shaped cavity to a crack-like cavity. The proposed numerical method was verified against two extreme cases; grain boundary diffusion controlled cavity growth and surface diffusion controlled cavity growth. When extremely fast surface diffusivity is dominant, the current numerical method predicts that the cavity maintains an initial spherical cavity shape. At the opposite extreme condition, that is surface diffusion controlled cavity growth, the current method successfully describes cavity shape change from initial spherical-shape to crack-like shape. Between these extremes, the cavity growth shape may evolve into different shapes including a diamond.

Keywords: creep, cavity growth, surface diffusion.

1 INTRODUCTION

Because of the complex physical phenomena, in most cases of numerical analysis for cavitation by diffusion, one of the two extreme cases, fast grain boundary diffusion or fast surface diffusion, is assumed. When grain boundary diffusivity is much faster than surface diffusivity (surface diffusion controlled process), the cavity shape will be similar to a crack because the atomic flow rate along the cavity surface is not fast enough to reduce surface curvature at the cavity tip. On the other hand, when surface diffusivity is much faster than grain boundary diffusivity (grain boundary diffusion controlled process), the cavity shape will be a spherical cap shape. Spherical cap refers to a sphere cut by a plane centered above or on the sphere center.

Despite its apparent importance, little analysis has been performed on continuous cavity growth analysis including grain boundary and surface diffusion mechanisms and viscoplastic deformation of the grain material. The numerical studies of these combined effects on the cavity growth will provide basic understanding of these synergies, and they will be useful in identifying the critical conditions where the combined effects become important. In this study, the effect of the ratio of the surface and grain boundary diffusivity and material viscoplastic deformation on the cavity growth rate is examined numerically. More details can be found in reference [1].

2 NUMERICAL MODEL

The atomic flow rates are proportional to driving forces, which are chemical potential gradients of the atom. When tensile stress is applied on the grain boundary, atoms diffuse from the cavity surface to the grain boundary due to the chemical potential gradient. As atoms diffuse from the cavity wall to the grain boundary, the grain boundary should accommodate the diffused atoms.

The chemical potential of the atom on the cavity surface 'μ_s' and that on the grain boundary 'μ_{gb}' respectively, are given by

$$\mu_s = -\gamma_s(\kappa_1 + \kappa_2)\Omega$$

$$\mu_{gb} = -\sigma_n\Omega\,.$$

The atomic volume, surface energy at cavity surface, principal curvatures of the cavity surface, and normal stress along the grain boundary are respectively represented by 'Ω', 'γ', 'κ_1', 'κ_2', and 'σ_n'. The driving force of the surface diffusion denoted by 'F_s' and that of the grain boundary diffusion denoted by 'F_{gb}', respectively, are

$$F_s = -\frac{\partial \mu_s}{\partial S}$$

$$F_{gb} = -\frac{\partial \mu_{gb}}{\partial r}$$

where 'S' is the curvilinear coordinate along the cavity surface and 'r' is the radial coordinate from the center of the cavity. Assuming the linear kinetic law, the surface and grain boundary atomic flow rates, denoted by 'j_s' and 'j_{gb}', respectively, are

$$j_s = M_s F_s$$

$$j_{gb} = M_{gb} F_{gb}$$

where 'M_s' and 'M_{gb}' are given by

$$M_s = \frac{D_s}{kT},$$

$$\text{where } D_s = D_{so}\delta_s \exp(-\frac{Q_s}{RT}),$$

$$M_{gb} = \frac{D_{gb}}{kT},$$

$$\text{where } D_{gb} = D_{gbo}\delta_{gb} \exp(-\frac{Q_{gb}}{RT}),$$

and "D_s", "D_{gb}", "k", "T", "$D_{so}\delta_s$", "$D_{gbo}\delta_{gb}$", "Q_s", "Q_{gb}", and "R" respectively, are the surface diffusivity, grain boundary diffusivity, Boltzman constant, absolute temperature, surface diffusion coefficient, grain boundary diffusion coefficient, activation energy for surface diffusion, activation energy for grain boundary diffusion, and gas constant.

In this analysis, cavity growth rates and cavity shape evolution are calculated by combining finite element and finite difference methods for a given time step. First, an extension of the finite element method by Needleman and Rice [3] is used to calculate the atomic flux (j_{gb} at cavity tip = j_o) by grain material deformation assisted grain boundary diffusion. In addition, the cavity shape change by grain material deformation, "jacking" effect for a given cavity geometry, and cavity tip stress, are included. When the "jacking" is not included material flux at the cavity tip is expressed as $2j_s = j_{gb}$, satisfying matter conservation law. However, material flow into the grain boundary contributes to the additional cavity volumetric growth. Therefore, this additional diffusion flux is included in the proposed numerical method (it has been neglected in many prior studies). A form of the open ended finite difference method is used to update cavity shape for a given time step.

After the cavity shape evolves for the current time step, the chemical potential of the atom at the cavity tip is calculated approximately from the value of principal curvatures of the node next to the cavity tip. At the next time step, the cavity tip stress, which is used for the FEM portion of the analysis, is calculated from the cavity tip curvatures obtained from previous FDM analysis and the same procedure is repeated until cavity coalescence occurs. Elastic-power law type material constitutive equations are assumed for creep flow. Figure 1 shows the structure of numerical calculation procedure (see [1]).

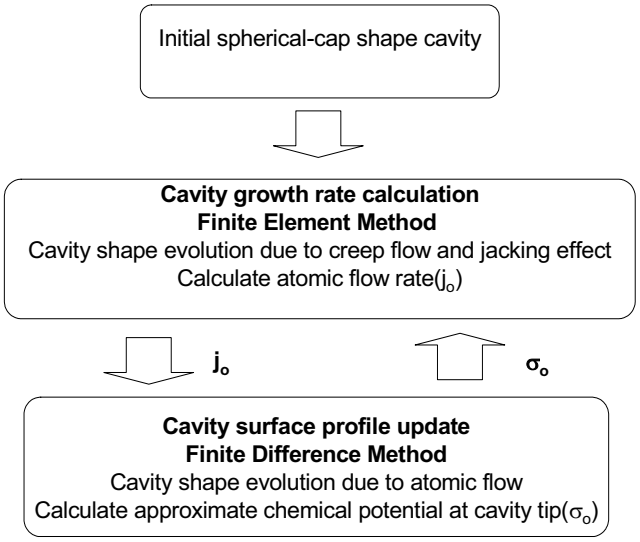

Figure 1. Illustration of numerical calculation structure for single cavity growth model. The unified numerical method, which combines finite element method and finite difference method, starts with the known spherical-cap shape cavity geometry. For the given time step, which is chosen to be sufficiently short, finite element method and finite difference method are employed to simulate cavity shape evolution (see [1] for details).

3 DIFFUSION GROWTH RESULTS

First results for grain boundary diffusion controlled growth are provided followed by combined growth.

2.1 Grain Boundary Diffusion

In this study, numerical analysis of an initial spherical-shaped cavity was carried out for $D_s/D_{gb} = 171$ (fast surface diffusion), $a_l/b = 0.1$ and $a_l/L=0.316$. The equilibrium dihedral angle was chosen to be 70° and the creep exponent was taken to be 4.5. 'a' is cavity radius and 'b' is cavity spacing. Figure 2 shows the cavity radius increase with non-dimensional time, '$t\dot{\varepsilon}_e^{cr}$', where '$\dot{\varepsilon}_e^{cr}$' is the equivalent creep strain rate. From Fig. 2, it is clear that the proposed numerical method can reproduce Needleman and Rice [3] result exactly without the assumption of fast surface diffusivity. When the 'jacking' effect is not included, the present model overestimates cavity coalescence time. Therefore, it is also clear that the 'jacking' effect and creep flow of the surrounding grain material can cause significant difference in calculating cavity growth rates and cavity shape evolution especially when 'a+L' is smaller than 'b'. Chen and Argon [4] assumed that the grain boundary displacement ('jacking' effect) due to matter flow is constant over diffusion distance 'L'. However, Needleman and Rice [3] pointed out that material accommodation occurs mainly at cavity tip when creep deformation occurs. Also, when the diffusivity ratio is between the two extreme values (i.e. combined grain boundary diffusion/surface diffusion dominant) the cavity shape can evolve into more a complicated one, not spherical or crack-like one, due to the 'jacking effect'. This effect will be more important as 'a/L' increases since more severe matter accommodation occurs at the cavity tip. This is further explained in the next section. Analytical predictions are similar to the current numerical result up to a/b = 0.5. This gives us confidence in the model. Many other cases and results are presented in reference [1].

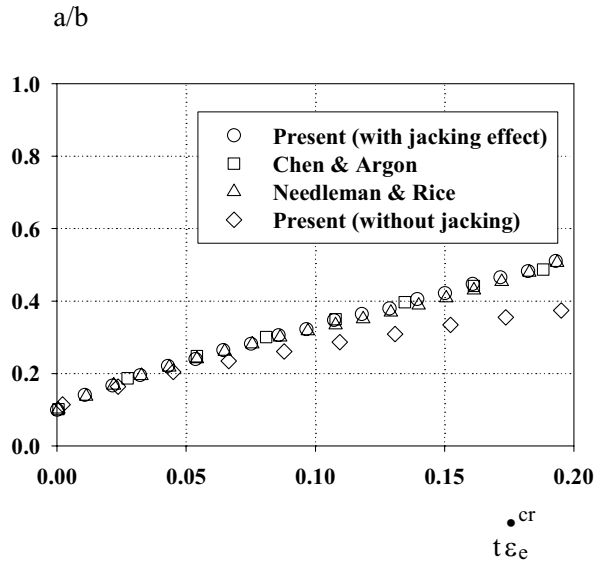

Figure 2. Normalized cavity major radius with time for a_I/L=0.316, a_I/b_I=0.1, and D_s/D_{gb}=171 (fast surface diffusion). When a/b is 0~0.5, the present numerical results (with jacking effect), which simulate cavity shape evolution, reproduce the Needleman and Rice results. In this range, the Chen and Argon analytical results also matches with the Needleman and Rice results. When jacking effect is not considered, the present result deviates with the other three results. That implies jacking effect is significant in this a/L range. Also, when a/b is 0.5~1.0, the present results still matches well with the Needleman and Rice results. However, Chen and Argon result starts to deviate with the Needleman Rice results.

2.2 Surface Diffusion

When surface diffusion controls cavity growth, the cavity elongates in the direction of the normal to the applied stress and the cavity growth kinetics change. In presenting the results, time is expressed in units of

$$t_s = \frac{a_I^4}{M_s \Omega \gamma_s}$$

and stress is expressed in non-dimensional form as

$$\Sigma = \frac{\sigma a_I}{\gamma_s}.$$

The diffusivity ratio is expressed as

$$f = \frac{D_{gb}}{D_s}.$$

The ratio of the applied normal stress to Young's modulus, σ_∞ / E, is 10^{-4} and initial "a_I/b_I" is 0.1. The capillarity angle at cavity tip is assumed to be 70°.

Fig.3 shows the cavity shape when a = 0.1, 0.3, 0.5, and 0.7 for f = 1 and f =10, respectively. For the results in Fig. 3, the initial cavity size divided by cavity spacing (a_I/b) was equal to 0.1. The values of a/b = 0.3, 0.5, and 0.7 occur after cavity growth is dominated by surface diffusion. Since a cavity becomes crack-like as it grows, as shown in Fig. 3, the first primary curvature increases at cavity tip. The nodes on the cavity surface were marked along the cavity surface in Fig. 3. Initially, 15 nodes existed along cavity surface with the same separation distance. As the cavity shape becomes more crack-like, more nodes exist along the high curvature area according to the node 'removal-creation' rule explained earlier. Nodes on the flat surface are removed when $\Delta\beta$ is less than 2° and moved to higher curvature area. This node 'removal-creation' procedure is accurate enough to simulate crack-like cavity evolution. Results not shown here show that the cavity becomes more crack-like when f = 10 than when f = 1. Therefore, the normal stress at the cavity tip (sintering stress) for f = 10 becomes higher than that for f = 1.

Based on the results from section 2.1 and 2.2, current numerical model is validated against two extreme cases; grain boundary and surface diffusion controlled cavity growth cases. With confidence in the accuracy of the model, we perform analyses in regimes where surface and grain boundary diffusion are both important.

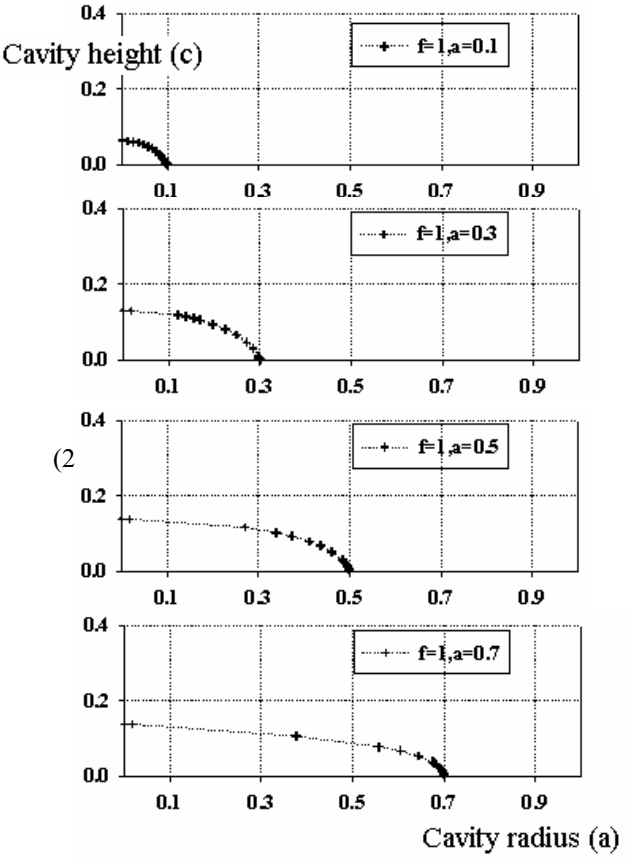

Figure 3. Cavity growth behavior for surface diffusion dominated cavity growth. Note the crack like nature.

2.3 Transition From Equilibrium Mode to Crack-like Mode

The grain material deformation not only assists the grain boundary diffusion but also changes the cavity shape. Therefore the cavity shape evolution can not be simply predicted based on simple analytical results. Fig. 4 shows cavity shapes in the case of (a_l/L) =1.0 and α= 1.0 when a/b = 0.3, 0.5, 0.7, and 0.9. The cavity shape is completed by reflecting nodes on the symmetric part of axis-symmetric geometry. When a/b = 0.3, the initial spherical-shaped cavity maintains its original shape with slightly increased aspect ratio. When a/b = 0.5 and 0.7, some nodes have negative curvature value because of cavity elongation at the cavity tip in the r-direction due to material diffusion and cavity elongation at the cavity top in z-direction due to the 'jacking' effect. When a/b = 0.9, the node with negative curvature fades away due to small '$\Delta\beta$' and cavity shape become V-shaped. These results are based on the assumption that the sintering stress is zero. When the sintering stress is considered, it is expected that the current numerical method predicts the cavity shape evolution and the final cavity coalescence time for general case in a physically more realistic manner. These 'diamond' shaped cavities have been observed in experiments.

3 CONCLUSIONS

In this study, a unified numerical method, which combines finite element analysis and finite difference analysis, for inter-granular cavity growth analysis was proposed. The numerical method includes three important mechanisms of cavity growth, which are grain boundary diffusion, surface diffusion along the cavity surface, and material creep flow, in simulating cavity growth at high temperature. The proposed numerical method was verified against two extreme cases; grain boundary diffusion controlled cavity growth and surface diffusion controlled cavity growth. When extremely fast surface diffusivity is dominant, the current numerical method predicts that the cavity maintains an initial spherical cavity shape, which was assumed by Needleman and Rice[19].

The present cavity growth rate prediction differs from the prediction by Chen and Argon[5] especially when 'a/b' is larger than 0.5. It is thought that this discrepancy is due to neglect of the proper 'jacking' effect in Chen and Argon model. At the opposite extreme condition, that is surface diffusion controlled cavity growth, the current method successfully describes cavity shape change from initial spherical-shape to crack-like shape. Although, in this method, the node next to cavity tip was used to calculate cavity tip normal stress, it was good approximation under physically reasonable diffusivity ratios.

It was shown that the cavity shape change is a complicated function of material diffusivity ratio, 'a/L', and cavity tip geometry when creep flow effects on cavity growth are important. It was shown that the cavity shape transition occurs gradually and the cavity growth rate during the transition phase is much higher than the prediction by Chen and Argon. As a/L increases, local accommodation at the cavity tip affects not only cavity shape but the overall cavity growth rate. This grain boundary displacement, which causes 'jacking' at the cavity tip, has been assumed to have a constant value in most research studies to date. Other results, including those compared with experiment, are presented in reference [1].

4 REFERENCES

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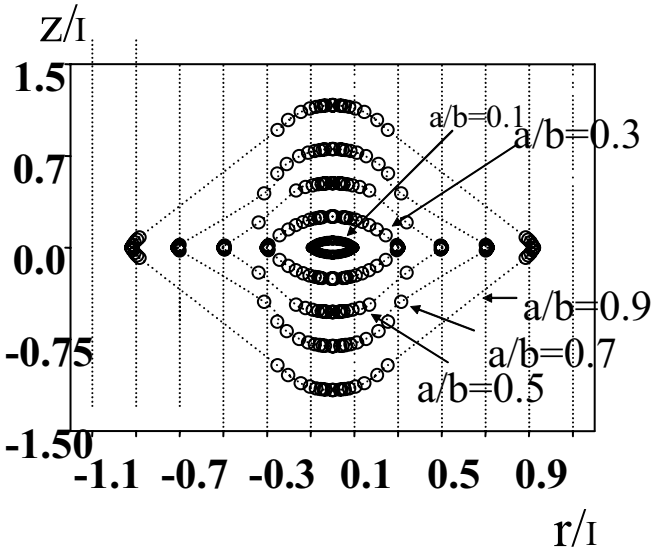

Figure 4. Cavity evolution from spherical-cap shape to V-shape for a_l/L=1, α=1. Initial spherical-cap shape cavity maintains its original shape until a/L=0.3. When a/L reaches to 0.5, cavity shape changes to V-shape, since surface diffusivity is slow and material creep flow effect is significant.