Phase Field Simulation of Intragranular Microvoids Evolution Due to Surface Diffusion in Stress Field

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Abstract: Based on the bulk free energy density and the degenerate mobility constructed by the quartic double-well potential function, a phase field model is established to simulate the evolution of intragranular microvoids due to surface diffusion in a stress field. The corresponding phase field governing equations are derived. The evolution of elliptical microvoids with different stresses Λ, aspect ratios β and linewidths $\bar{h}$ is calculated using the mesh adaptation finite element method and the reliability of the procedure is verified. The results show that there exist critical values of the stress Λ_c, the aspect ratio β_c and the linewidth $\bar{h}_c$ of intragranular microvoids under equivalent biaxial tensile stress. When $\Lambda \geqslant \Lambda_c$, $\beta \geqslant \beta_c$ or $\bar{h} \leqslant \bar{h}_c$, the elliptical microvoids are instable with an extending crack tip. When $\Lambda < \Lambda_c$, $\beta < \beta_c$ or $\bar{h} > \bar{h}_c$, the elliptical microvoids gradually cylindricalize and remain a stable shape. The instability time decreases with increasing the stress or the aspect ratio, while increases with increasing the linewidth. In addition, for the interconnects containing two elliptical voids not far apart, the stress will promote the merging of the voids.

Key words: phase field method; stress migration; surface diffusion; finite element method; intragranular microvoid

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0 Introduction

With the continuous progress of microelectronics technology, the size of typical integrated circuits has been drastically reduced. The miniaturization poses many challenges, especially when the linewidth of the interconnect lines reaches the submicron or nanometer level. The thermal mismatch stress induced by the difference of thermal expansion coefficients between the interconnect lines and the passivation layer becomes more pronounced. As the thermal mismatch stress increases, the microvoid nucleates, grows, migrates and changes its shape. When the microvoid grows into a crack, it will cut off the entire interconnect line and cause a break. Therefore, it is of practical importance to understand the evolution of stress induced microvoids.

The early research on the failure of interconnect lines is mainly by experimental observation. Hull and Rimmer[1] observed the growth of intergranular microvoids under different stress states within metallic materials and concluded that the microvoids may be generated due to stress migration. Blech and Herring[2] measured the gradient stresses generated by electromigration in aluminium thin-film interconnect lines on silicon nitride substrates using an X-ray instrument. Wilson et al.[3] measured the stresses in copper interconnect lines with linewidth of 50—500 nm using X-ray diffraction (XRD) and found that the stresses increased with decreasing linewidth and that the grain structure of the interconnect lines had a significant effect on the stresses and stress evolution.

Experimental observations form the basis for theoretical analysis and numerical simulation. The first theoretical investigation of the stress driven

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morphological instability in solids is given by Asaro and Tiller[4]. They discussed the linear stability of a planar surface separating a stressed, two-dimensional semi-infinite solid from a fluid and found that the planar surface was unstable to small disturbances with wavelength greater than a characteristic length. The same result was later rediscovered by Srolovitz[5]. The starting point of these theoretical studies is the chemical potential, which consists of strain energy density and surface energy density. Based on the above theory, Sun and Suo et al.[6-7] developed a theoretical model of microvoids evolution due to surface diffusion and derived the thermodynamic potential with shape function to calculate the rate of microvoids evolution using the variational principle. Wang and Suo[8] analyzed the shape instability threshold and the forming time of crack tip using conformal mapping method. Wang and Li[9-13] theoretically analyzed the stability of two- and three-dimensional intra- and interg-ranular microvoids containing internal pressure and providing a theoretical basis for the numerical simulation. In addition, the elliptical voids and inclusions morphological evolution under a gradient stress field[14-16] and the circular void morphological evolution under high current density was also analyzed theoretically[17-18].

Due to the complexity of the material system and the limitation of the two methods, it is difficult for the experimental observation and theoretical analysis to completely solve the problem of microvoid evolution mechanisms. Therefore, numerical simulation becomes an effective method. The commonly used numerical methods to analyze the evolution of microvoids are the sharp interface method and the phase field method. The sharp interface method is a mature numerical simulation method. So far, the evolution of microvoids in a stress field is mostly based on the sharp interface model. For example, based on the weak statement proposed by Sun and Suo[19], the morphological evolution process of microvoids in a stress field, electric field and gradient stress field[20-23] had been studied in the past few years. Moreover, the mesh adaptation finite element method was also used to study the evolution of intra- and inter-granular microcracks under electromigration and stress migration[24-25].

However, when it comes to complex interface problems (e.g. topological changes) or expansion to three dimensions, the sharp interface method for moving boundaries will become more difficult to handle. In recent years, the rapidly developing phase field method has provided a powerful tool for simulating the evolution of microvoids[26-28]. The phase field method overcomes the limitations of the sharp interface method. The morphological information of microvoids is implicitly included in the phase field equation, which avoids the explicit tracking of its interface location and thus has more advantages when dealing with more complex moving boundary problems. It is also easier to extend the phase field method from two dimensions to three dimensions.

The bulk free energy plays an important role in the phase field model and directly determines the construction and composition of the total free energy of the system[26]. At present, for the analysis of the evolution of microvoids morphology in the interconnect lines, there are two principal forms of the bulk free energy density, which are the quartic double-well potential function and the nonsmooth double-obstacle potential function. Using the quartic double-well potential function, Yeon et al.[29] presented a phase field model for the surface corrugation of elastically stressed films where surface diffusion is a dominant mass transport mechanism. The method was also used to analyze such problems as void migration driven by temperature gradients[30], electromigration-induced thermal grooving evolution on grain boundaries[31-32] and non-isothermal coalescence in polycrystalline sintering[33]. Meanwhile, using the nonsmooth double-obstacle potential function, Barrett et al.[34] derived the phase field equations for stress migration induced surface diffusion based on degenerate mobility and solved the governing equations using the finite element method. Bhate et al.[35-36] proposed a phase field model and used the mesh adaptation method to capture the interfacial layer information to analyze the morphological evolution of microvoids under electro- and stress migration induced surface diffusion and bulk diffusion, respectively. Li et al.[37] analyzed the effects of electrical conductivity and anisotropic surface energy on the migration and evolution of inclusions under the electric field. Subsequently, this method was extended to research the morphological evolution of inclusions in piezoelectric films under mechanical and electric loads[38].

For the phase field method using the nonsmooth double-obstacle potential function, the order parameter only needs to be calculated within the interface layer, which improves computational efficiency. But it brings some disadvantages. The first is the need to introduce algorithms for capturing the interface layer, such as dynamic mesh method or narrowband interface method, which needs to capture the node information of the interface layer and update the mesh after a certain time of calculation. Secondly, when coupling the stress field, different mesh densities need to be consistence with different stress conditions. However, the quartic double-well potential function is capable of continuously and synchronously coupling the external fields. And its computational effort and efficiency are rapidly improving with the development of adaptive grid technology[39]. The evolution of microvoids in a stress field based on a phase field model with a quartic double-well potential function and degenerate mobility has not been reported in the literature. Therefore, in this paper, the evolution of elliptical microvoids in a stress field is investigated based on the modified phase field method using the quartic double-well potential function and the degenerate mobility.

The plan for the rest of the article is as follows: in the first part, the phase field model and the governing equations are introduced; in the second and third parts, the results and discussions are presented, and the effects of different stresses, aspect ratios and linewidths on the evolution of elliptical microvoids are investigated.

1 Phase Field Model and Governing Equations

1.1 Phase field model

The phase field model is illustrated in Fig.1 and the interconnect line is idealized as an isotropic linear elastic model of a two-dimensional single crystal, which is subjected to biaxial tensile stresses σ_x and σ_y on its external boundary. a and h_0 are the long semi-axis and short semi-axis of the elliptical microvoid, respectively. L and H are the length and the width of the interconnect line. As shown in Fig.1, the order parameters $\phi=+1$ and $\phi=-1$ represent the two equilibrium phases with the minimum bulk free energy. In this paper, they correspond to the metallic conductor and the microvoid respectively. For physically reasonable values of the material parameters, we may divide the region R into three portions. Let R_+ denote the region occupied by solid material ($\phi=+1$), R_- denote the region occupied by void ($\phi=-1$), and R_I denote the interface region. We denote the two extreme contours, associated with $\phi=-1$ and $\phi=+1$ by Γ_- and Γ_+, respectively. The bisecting contour $\phi=0$ is denoted by Γ. s represents the local coordinate direction along the hole tangent direction, and r the local coordinate direction perpendicular to the hole tangent direction.

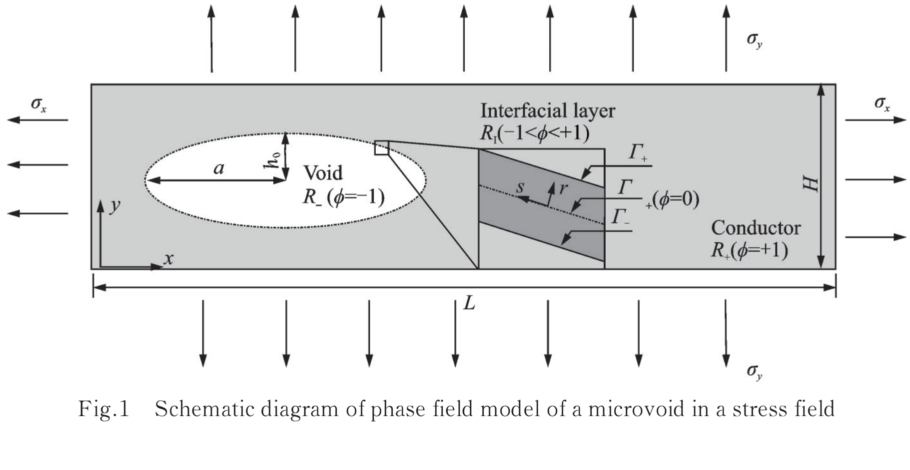


Fig.1 Schematic diagram of phase field model of a microvoid in a stress field

This paper adopts some basic assumptions as follows:

(1) The isotropic surface diffusion is the only material transport mechanism in the microvoids evolution.

(2) The model studied in this paper is a plane strain problem.

(3) The stress is uniformly distributed on the stress boundary and the deformation of the line satisfies the line elastic deformation.

1.2 Governing equations

For the surface diffusion mechanism, the order parameter of the conserved field needs to satisfy the law of mass conservation and energy dissipation. According to the Gurtin principle of microcode equilibrium[40], the expression for the total free energy function of the system F in a stress field is

$$F(\phi,\epsilon)=\int_V\left\{\frac{\gamma_s}{A\epsilon}\left(f_b(\phi)+\frac{1}{2}\epsilon^2\left|\nabla\phi\right|^2\right)+W(\boldsymbol{\varepsilon},\phi)\right\}\mathrm{d}V \tag{1}$$

where γ_s is the surface energy per unit area, ϵ the parameter controlling the thickness of the interface, $A=2\sqrt{2}/3$ the dimensionless parameter[41] and $W(\boldsymbol{\varepsilon},\phi)$ the strain energy density of the system, which can be expressed as

$$W(\boldsymbol{\varepsilon},\phi)=\frac{1}{2}\boldsymbol{\sigma}:\boldsymbol{\varepsilon}=\frac{1}{2}\boldsymbol{\varepsilon}:\boldsymbol{C}(\phi)\boldsymbol{\varepsilon} \tag{2}$$

where $\boldsymbol{C}(\phi)$ is the second-order elasticity tensor with order parameter, $\boldsymbol{\sigma}$ the stress tensor, $\boldsymbol{\varepsilon}$ the strain tensor, and the bulk free energy density function $f_b(\phi)$ is

$$f_b(\phi)=\frac{1}{4}\left(1-\phi^2\right)^2 \tag{3}$$

The chemical potential μ is defined by the variational derivative of F with respect to ϕ

$$\mu=2\Omega\frac{\delta F}{\delta\phi}=2\Omega\left[\frac{\partial F}{\partial\phi}-\nabla\cdot\frac{\partial F}{\partial\nabla\phi}\right]=\frac{2\Omega\gamma_s}{A\epsilon}\left(f_b'(\phi)-\epsilon^2\nabla^2\phi\right)+2\Omega\frac{\partial W}{\partial\phi} \tag{4}$$

where the factor 2 is the change of the order parameter from $+1$ to -1, i.e., the transition from solid material to voids across the interfacial layer, F the free energy functional density of the system and Ω the volume of the atom.

The driving force of atomic migration $\boldsymbol{f}$ is related to the gradient of μ

$$\boldsymbol{f}=-\nabla\mu \tag{5}$$

where the negative sign indicates that the direction of driving force is opposite to the chemical potential gradient, so that atoms migrate from the high chemical potential region to the low chemical potential region.

The gradients of strain energy and surface curvature cause material to be deposited or removed locally, and the surface motion will occur where unbalanced flux exists. The number of atoms per time crossing a unit length on the surface is determined by

$$\boldsymbol{J}=\frac{M(\phi)D_s}{B\epsilon}\boldsymbol{f} \tag{6}$$

where $B=2\sqrt{2}/3$ is the dimensionless parameter[41] and D_s the atomic mobility for surface diffusion. In addition, $M=M(\phi)$ denotes the degenerate coefficient[42] associated with ϕ, shown as

$$M(\phi)=\left(1-\phi^2\right)^2 \tag{7}$$

Based on the law of conservation of mass, the derivative of ϕ with respect to time t is related to the divergence of the diffusion flux $\boldsymbol{J}$, shown as

$$\frac{\partial\phi}{\partial t}=-\nabla\cdot\boldsymbol{J} \tag{8}$$

Coupling Eq.(4) to Eq.(8) yields the phase field equations combining the thermodynamic and kinetic laws, which are the modified fourth-order nonlinear Cahn-Hilliard equations

$$\frac{\partial\phi}{\partial t}=\nabla\cdot\left(M(\phi)D_s\nabla\left(\frac{9\Omega\gamma_s}{4\epsilon^2}\left(f_b'(\phi)-\epsilon^2\nabla^2\phi\right)+\frac{3\sqrt{2}\,\Omega}{2\epsilon}\frac{\partial W}{\partial\phi}\right)\right) \tag{9}$$

Based on the phase-field governing equation, the morphological evolution and migration of void depend on the gradient of strain energy along the surface. At each time, we solve the distribution of strain energy for a given void morphology.

The equations to solve the stress field are

$$\nabla\cdot\boldsymbol{\sigma}=0 \tag{10}$$

$$\boldsymbol{\sigma}=\boldsymbol{C}(\phi)\boldsymbol{\varepsilon}=2G(\phi)\boldsymbol{\varepsilon}+\lambda(\phi)(\mathrm{tr}\boldsymbol{\varepsilon})\boldsymbol{I} \tag{11}$$

$$G(\phi)=G_0(1+\phi)/2,\lambda(\phi)=\lambda_0(1+\phi)/2 \tag{12}$$

where $G(\phi)$ and $\lambda(\phi)$ are the shear modulus function and the Lame function of the order parameter, respectively. trϵ is the trace of the second-order strain tensor and $\boldsymbol{I}$ the unit tensor. In the microvoid region, the shear modulus and the Lame constant are zero. In the solid region, the shear modulus is G_0, and the Lame constant is λ_0.

Based on the governing equations of the phase field model, the corresponding program is developed through the open-source finite element framework Moose[43]. For the convenience of description, the dimensionless process is $\bar{x}=x/h_0$, $\bar{y}=y/h_0$, $\bar{h}=H/h_0$, $\beta=a/h_0$, $\tau=tD_s\Omega\gamma_s/h_0^4$, $\overline{\nabla}=h_0\nabla$, $\overline{W}=W\epsilon/\gamma_s$, $\Lambda=\sigma^2h_0^2/\gamma_sE$. Then, the dimensionless phase field method governing equation can be written as

$$\frac{\partial\phi}{\partial\tau}=\overline{\nabla}\cdot\left(M(\phi)\overline{\nabla}\left(\left(\frac{3h_0}{2\epsilon}\right)^2\left(f_b'(\phi)-\frac{\epsilon^2}{h_0^2}\overline{\nabla}^2\phi+\frac{2\sqrt{2}}{3}\frac{\partial\overline{W}}{\partial\phi}\right)\right)\right) \tag{13}$$

For each time step $\Delta\tau$, the calculations proceed as follows:

(1) Solve the elasticity problem on the current configuration, obtaining the strain energy density at all of the element nodes.

(2) Compute the new configuration by iterative calculation in space to obtain the values of the order parameters that satisfy the residual requirements.

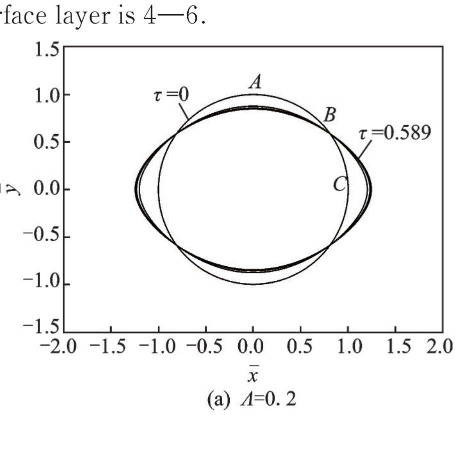
(3) Update the adaptive time step.

2 Numerical Simulation and Discussion

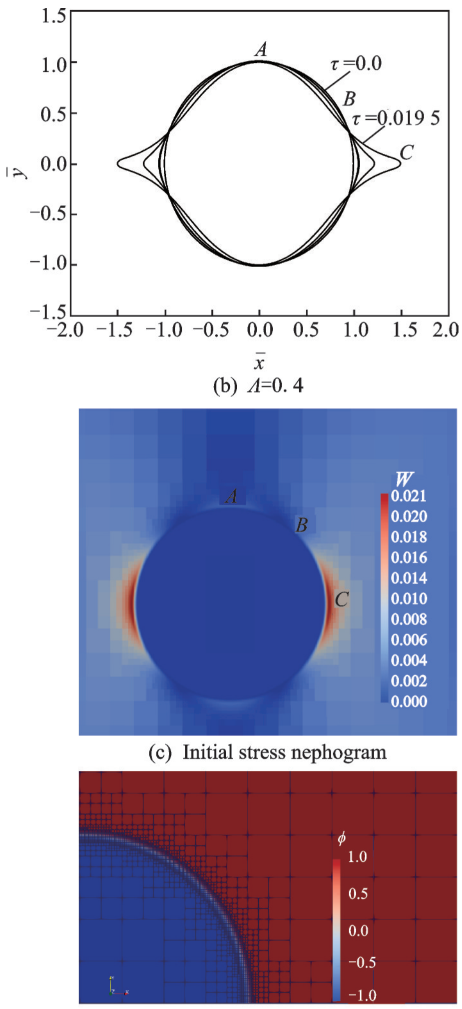
It is known from diffusion theory that atoms migrate from a region of high chemical potential to a region of low chemical potential due to the presence of chemical potential differences. The chemical potential of each point on the surface of the intragranular microvoid is related to the external stress, aspect ratio and linewidth. Therefore, in this section, the phase field method proposed in this paper is used to analyze the evolution of intragranular microvoid under equivalent biaxial tensile stress with different stresses, different aspect ratios and different linewidths.

2.1 Effect of stress field

Fig.2 gives a graphical representation of the evolution of a circular void subjected to y-directional tensile stress, the stress nephogram of the model at the initial moment and the schematic diagram of the adaptive grid at the initial time for a quarter model. It can be seen from Fig.2 that the curvature of each point on the microvoid surface κ is equal at the initial time and $\kappa_C=\kappa_B=\kappa_A$. However, the strain energy density of each point is different because of the stress concentration. We can find that $W_C>W_A>W_B$, which indicate that the atoms will migrate from point C to point A and point B. When the stress is relatively small (Fig.2(a)), the circular microvoid will become elliptical microvoid. At the same time, the curvature of the microvoid becomes different $\kappa_C>\kappa_B>\kappa_A$, which impedes further ellipticalization of the shape. And the circular microvoid will remain a stable elliptical void. When the stress is relatively high (Fig.2(b)), the strain energy dominates, and the instability is formed by the gradual formation of crack tips at the end of the void due to the atom migration. As can be seen from Fig.2, there exists a critical stress Λ_c. When the stress is larger than the critical stress, the microvoid will collapse into a crack. In addition, Fig.2(d) gives the schematic diagram of the adaptive grid at the initial time for a quarter model. The adaptive grid is updated synchronously with the evolution of the microvoid. The mesh refinement level of the transition between the surface layer is 4—6.



(a) Λ=0.2



(b) Λ=0. 4

(c) Initial stress nephogram

(d) Schematic diagram of the adaptive grid

Fig.2 Evolution of intragranular circular microvoid, the initial stress nephogram for $\Lambda=0.4$, $\sigma_x=0$ and the schematic diagram of the adaptive grid for a quarter model

Fig. 3 shows the variation of the critical stress as a function of the stress ratio σ_x/σ_y. Below the curve, the voids remain stable; above the curve, the voids are unstable and the crack tips will appear. It can be seen that the solution of the phase field method due to surface diffusion in the stress field is basically consistent with the curve of the theoretical solution. Therefore, the algorithm in this paper is reliable.

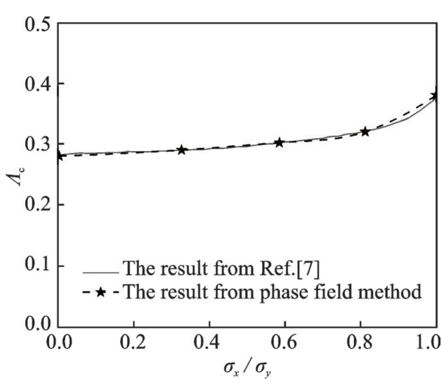
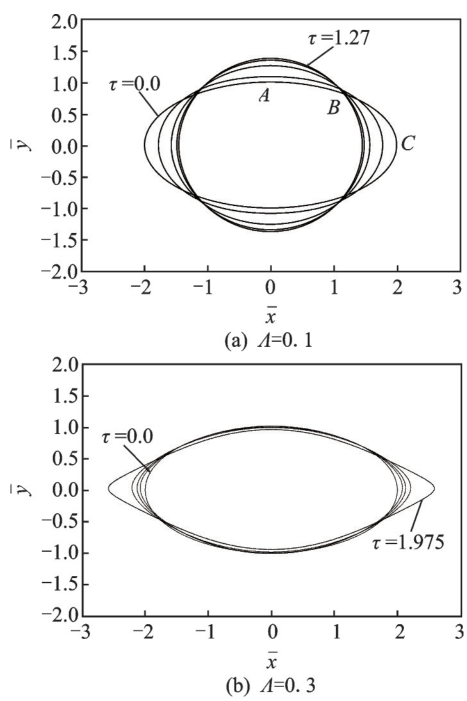


Fig.3 Λ_c as a function of the stress ratio σ_x/σ_y

Fig. 4 shows the evolution of intragranular microvoid for $\beta=2$, $\bar{h}=20$ as the stress increases ($\Lambda=0.1, 0.3$). As shown in Fig.4, the evolution of elliptical microvoid under different stresses is basically the same as that of the circular microvoid. The only difference between the circular microvoid and the elliptical microvoid is that the curvature of the microvoid surface is different at the initial time. For the elliptical microvoid, atoms migrate from the relatively flat surface to the tip (Fig.4(a)). That is, the atoms migrate from point A to point B and then from point B to point C. When the stress is relatively small, the elliptical microvoid will gradually cylindricalize and maintain a stable form. But, the elliptical microvoid will form crack tips at both ends and gradually destabilize when the stress is large. Therefore, there exists a critical stress Λ_c as shown in Fig.5. In addition, it can be seen from Fig.5 that the critical stress decreases with increasing the aspect ratio. The elliptical microvoid will destabilize and form a cusp when $\Lambda \geqslant \Lambda_c$. The elliptical microvoid will cylindricalize and remain stable when $\Lambda < \Lambda_c$.



(a) Λ=0. 1

(b) Λ=0. 3

Fig.4 Evolution of the intragranular microvoid for $\beta=2$, $\bar{h}=20$

Fig. 6 shows the variation of instability time with stress. From Fig.6, it can be seen that the instability time decreases with the increase of the aspect ratio and the stress. When $\Lambda > 0.4$ and $\beta > 3$, the microvoid will destabilize rapidly. Fig.7 shows the evolution process of the microvoid aspect ratio with time under the two kinds of external loads in Fig.4. When the microvoid is unstable, the evolution of the aspect ratio with time can be seen as the evolution of cracked tip growth with time. From Fig.7, it can be seen that when $\Lambda = 0.3$ and $\tau > 1.5$, the cracked tip expands rapidly and eventually leads to the void destabilization.

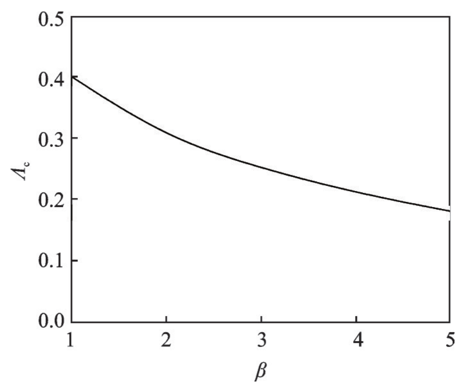


Fig.5 Λ_c as a function of $\beta(\bar{h} = 20)$

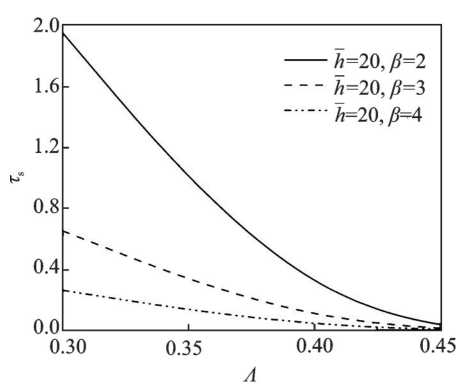


Fig.6 τ_s as a function of Λ

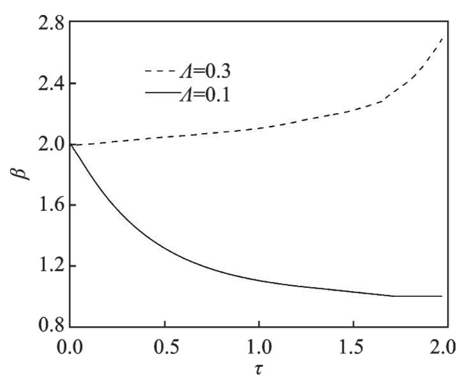


Fig.7 β as a function of τ

2.2 Effect of the initial aspect ratio

Fig.8 shows the evolution of the intragranular microvoid for $\Lambda = 0.2$, $\bar{h} = 20$ as the initial aspect ratio increases ($\beta = 2, 3$). As shown in Fig.8, there exists a critical aspect ratio β_c. When $\beta \geqslant \beta_c$, the elliptical microvoid will form a cracked tip and cause instability. When $\beta < \beta_c$, the elliptical microvoid will gradually cylindricalize and maintain a relatively stable shape. The critical aspect ratio decreases rapidly with increasing the stress (Fig.9). Fig.10 shows the variation of the instability time with increasing the aspect ratio. It can be seen that the instability time decreases with increasing the aspect ratio or the stress. In addition, the instability time is approximately 0 when $\beta \geqslant 3.5$, which means that the microvoid will be unstable instantly.

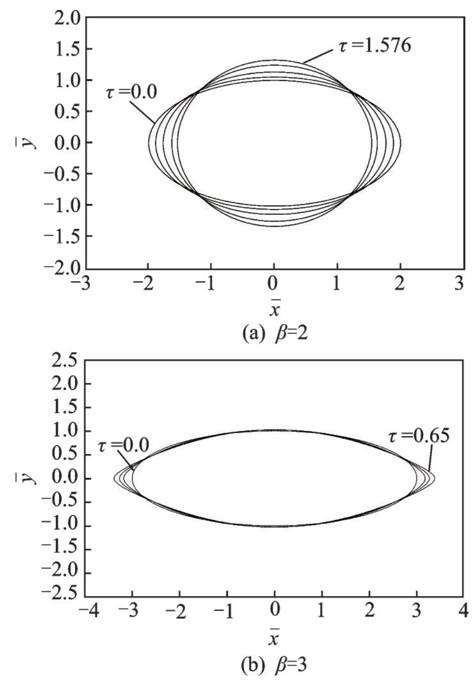


Fig.8 Evolution of intragranular microvoid for $\Lambda = 0.2$, $\bar{h} = 20$

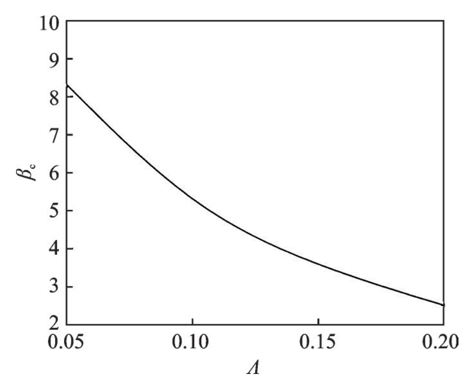


Fig.9 β_c as a function of $\Lambda(\bar{h} = 20)$

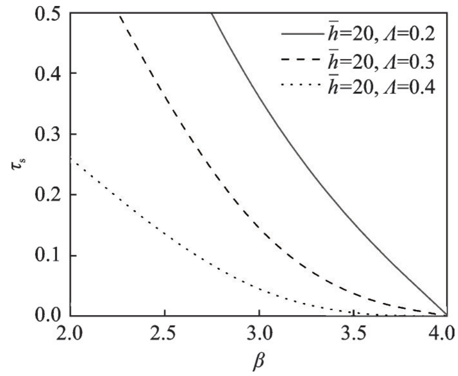


Fig.10 τ_s as a function of β

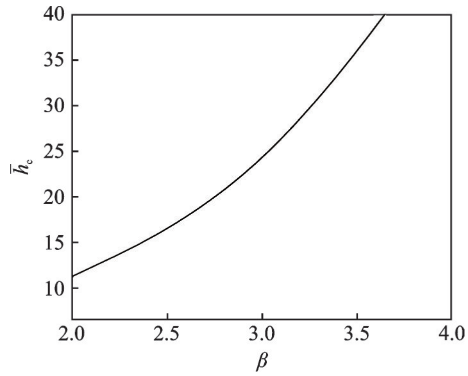


Fig.12 $\bar{h}_c$ as a function of $\beta(\Lambda = 0.2)$

2.3 Effect of linewidth

Fig.11 shows the evolution of the intragranular microvoid for $\Lambda = 0.2$, $\beta = 2$ as the linewidth decreases ($\bar{h} = 20, 8$). As displayed in Fig.11, there exists a critical linewidth $\bar{h}_c$. When $\bar{h} \leqslant \bar{h}_c$, the elliptical microvoid will form a cracked tip and be instability. When $\bar{h} > \bar{h}_c$, the elliptical microvoid will gradually cylindricalize and maintain a relatively stable shape. As shown in Fig. 12, the critical linewidth increases as the aspect ratio increases. And the effect of linewidth can be eliminated when the aspect ratio is greater than 3.6, which means that regardless of the linewidth, the microvoid will be unstabe. Fig. 13 shows the variation of the instability

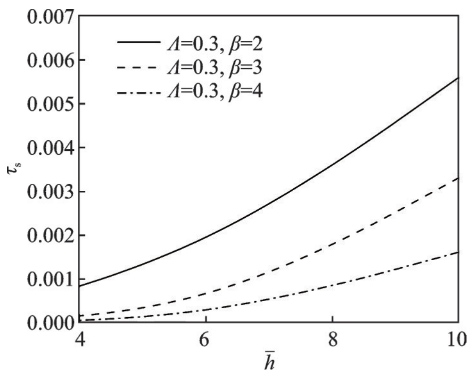


Fig.13 τ_s as a function of $\bar{h}$

time with increasing the linewidth. It is obvious that the instability time decreases as the aspect ratio increases and increases as the linewidth increases. When the linewidth is relatively small, the microvoid will quickly become unstable.

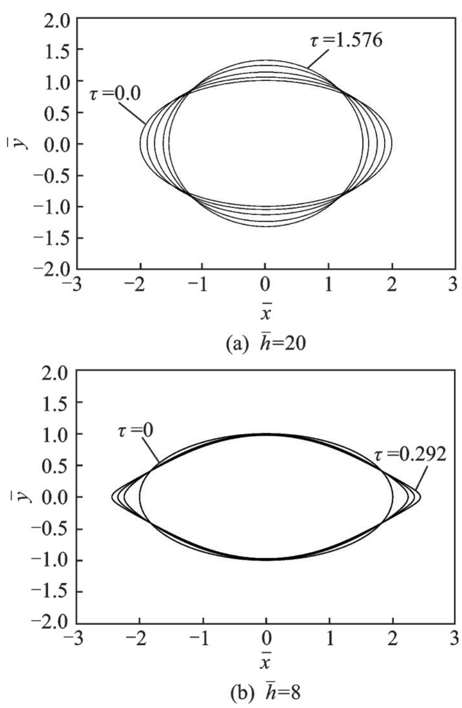
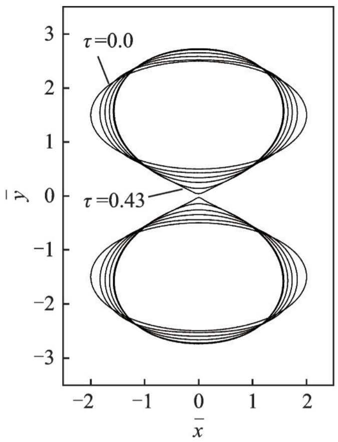
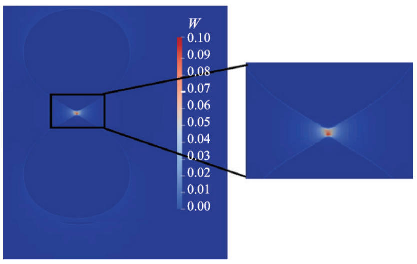


Fig.11 Evolution of the intragranular microvoid for $\Lambda = 0.2$, $\beta = 2$

In addition, the interconnect line does not always contain just one void, and sometimes contains two or more voids. Fig.14 shows the morphological evolution of two intragranular microvoids for $\Lambda = 0.1$, $\beta = 2$. The vertical distance between the centers of the two elliptical voids is 3. The atoms migrate from the region with high strain energy to the region with low strain energy (Fig.14(b)), and eventually the two elliptical voids evolve into symmetrical "heart-shaped" voids on top and bottom. That is, the tensile stress can promote the merging of two voids that are not far apart. Therefore, it is understandable that if the microvoids in the interconnect line evolve and combine to form larger voids, it is more likely to lead to the formation of microcracks and the open circuit failure of the interconnect line.



(a) Λ=0.1, β=2



(b) Final stress nephogram

Fig.14 Evolution of two intragranular microvoids and the final stress nephogram

Because of the interaction between multiple voids, the interconnect line with multiple microvoids is a complex system, which will be analyzed in detail in the next work. The phase field simulation of the double-void problem here is only to demonstrate the applicability of the method to the multi-void problem. Due to the microscale of the interconnect line, especially the harsh multi-physical field coupling of its service conditions, the variability of its service behavior is caused, which greatly increases the complexity of the characterization and evaluation of its service behavior. In this paper, we focus on the phase field simulation of the void evolution under stress induced surface diffusion in the interconnect line. The research on the failure behavior of multiple voids under multi-physical field will be carried out in the following work.

3 Conclusions

The governing equations of the phase filed method are derived to simulate the evolution of microvoids due to surface diffusion in a stress field. The reliability of the procedure is verified. And the evolution of the elliptical microvoids under different stresses, different aspect ratios and different linewidths is studied in detail. The main conclusions are as follows:

(1) Due to surface diffusion induced by stress migration, the elliptical microvoids have two trends: Firstly, the elliptical microvoids gradually cylindricalize and maintain a stable form; secondly, the elliptical microvoids form a crack tip and will collapse into a crack.

(2) There exist critical values of the stress field Λ_c, the initial aspect ratio β_c and the linewidth $\bar{h}_c$. When $\Lambda \geqslant \Lambda_c$, $\beta \geqslant \beta_c$ or $\bar{h} \leqslant \bar{h}_c$, the intragranular microvoid can form crack tips and have a tendency to cause a failure of interconnects; conversely, the intragranular microvoid will gradually cylindricalize.

(3) The higher of the stress Λ, the larger of the aspect ratio β or the smaller of the linewidth $\bar{h}$, the more easily to cause instability of the intragranular microvoid in interconnects, and the smaller time is required for destabilization.

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应力场诱发表面扩散下晶内微孔洞演化的相场模拟

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摘要：基于四次双阱势函数的体自由能密度和退化的迁移率，建立了一个相场模型来模拟应力场中表面扩散诱发的晶内微孔洞的演化，推导了相应的控制方程。使用自适应网格的有限单元法计算了不同应力Λ，不同形态比β和不同线宽$\bar{h}$下椭圆形微孔洞的演化，并验证了程序的可靠性。结果表明，在等轴双向拉应力作用下，晶内微孔洞存在临界应力值Λ_c，临界形态比β_c和临界线宽$\bar{h}_c$。当$\Lambda \geqslant \Lambda_c$、$\beta \geqslant \beta_c$或$\bar{h} \leqslant \bar{h}_c$时，椭圆形微孔洞逐渐形成裂纹尖端而失稳。当$\Lambda < \Lambda_c$、$\beta < \beta_c$或$\bar{h} > \bar{h}_c$时，椭圆形微孔洞逐渐呈现圆柱化并保持稳定。失稳时间随着应力或形态比的增大而减小，随着线宽的增大而增大。此外，对于包含两个相距不远的椭圆形微孔洞的内连导线，其应力促进孔洞的合并。

关键词：相场法；应力迁移；表面扩散；有限元法；晶内微孔洞