Edge dislocation emission from nanovoid with the effect of neighboring nanovoids and surface stress

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Abstract Experimental evidence, molecular dynamics simulations and theoretical analyses of nanovoid growth and coalescence in ductile materials indicate that nanovoid growth, coalescence, and stain localization depend strongly on distribution and volume fraction of the nanovoids in ductile porous materials. In the light of this mechanism, a generalized self-consistent theoretical model to describe the dislocation emitted from nanovoid accounting for the effect of neighboring nanovoids is suggested. The explicit solution to the critical stress is derived by means of the complex variable method. The influence of the nanovoid size, volume fraction and uniform distribution density of neighboring nanovoids in the effective medium as well as the surface effect on the critical condition required for dislocation emission from nanovoid surface is discussed.

Keywords dislocation emission; neighboring nanovoid interactions; nanovoid volume fractions; surface stress

1. Introduction

The effect of preexisting volume defects, such as voids and cracks, is generally to lead to an increase in ductility and a reduction in the load carrying capacity of the porous material. A critical mechanism of ductile damage usually involves the nucleation, growth and coalescence of nanovoids, as a result of the applied loading conditions, in a plastically deforming porous materials. According to what we know, there is lacking study about nanovoid growth by dislocation mechanisms, which depends on the size and distribution of the nanovoids in nanoporous materials. In order to quantitatively estimate the interaction of multiple nanovoids in the particular case of porous solids, a generalized self-consistent analytical approach is utilized to study the effects of neighboring defect interactions, and void distribution and volume fractions on the dislocation emission from nanovoid surface, in which a large number nanovoids are statistically homogeneously distributed. It is also a feasible choice for two-dimensional situations in which the voids are roughly cylindrical and near uniformly distributed. The size-effect modeled here pertains to the surface elasticity theory of Gurtin-Murdoch on the nanometer scale. The explicit solution to the critical stress is derived by means of the complex variable method. The influence of the nanovoid size, the surface effect, nanovoid content and uniform distribution density of neighboring nanovoids in the effective medium on the critical condition required for dislocation emission from nanovoid surface is discussed.

2. Modeling and solution

In this section, we present a framework for a generalized self-consistent theory accounting for the effect of neighboring nanovoids in ductile nanoporous materials, based on the dynamics of void nucleation and growth. For a two-dimensional case, the constitutive model for the material is divided into three regions: the inner circular region representing the nanovoid phase, the intermediate annular region representing the matrix phase, and the infinitely extended outer region representing composite phase or effective medium. Elastic deformation under plane strain conditions is assumed and the nanovoids are assumed to be and remain cylindrical, and are statistically homogeneously distributed so that their shape is characterized by a single parameter.

Lubarda [1, 2] have modified previous analysis by using the expression for the image force on a dislocation emitted from the surface of the void. In this case, the stress fields of an edge dislocation emitted from the surface of the void correspond to the imposed displacement discontinuity along the cut from the surface of the void to the center of the dislocation. The geometrical structure is shown in Fig. 1. One edge dislocation with Burgers vector B_0 was emitted from the surface of the circular nanovoid to the point z_0 in the matrix phase, and $z_0=\left(R_1+\rho e^{i\theta}\right)e^{i\varphi}$. The rest edge dislocation with Burgers vector B_1 is located at the surface of the circular nanovoid, and $z_1=R_1e^{i\varphi}$. They are both assumed to be straight and infinite along the direction perpendicular to the xy -plane, and $B_0=-B_1=b_x+ib_y=b_z e^{i(\varphi+\theta)}$, $b_z=\sqrt{b_x^2+b_y^2}$.

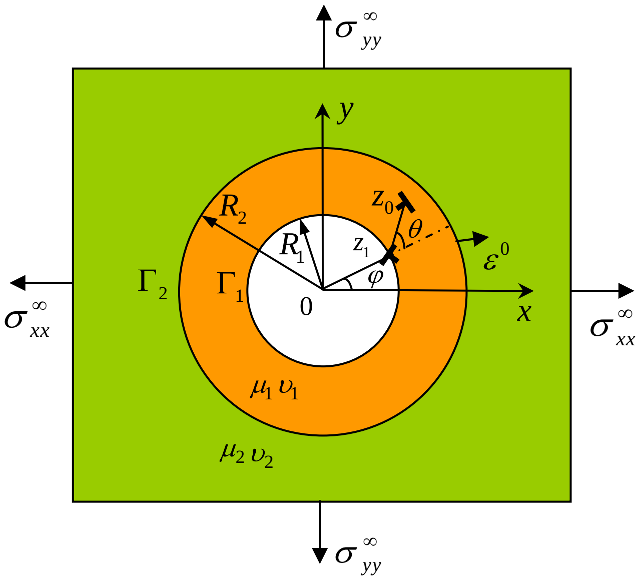

Fig.1 Dislocation emitted from the nanovoid surface in generalized self-consistent model

For the current problem, the elastic strain and stress in the two materials produced by lattice mismatch and dislocations can easily be calculated using the theory of elasticity. For nanovoid surface, surface stress resulting from a surface free energy and a constant residual stress was suggested in the Gurtin-Murdoch model [3-5]. So according to Sharma et al. [6], the equilibrium equation and the constitutive relations on the surface Γ_1 and the interface Γ_2 can be expressed as

$$\left[\sigma_{rr1}(t)+i\sigma_{r\theta 1}(t)\right]^-=\frac{1}{R_1}\left[\sigma^0_{\theta\theta 1}(t)-i\frac{\partial\sigma^0_{\theta\theta 1}(t)}{\partial\theta}\right] \tag{1}$$

$$\left[\sigma_{rr2}(\zeta)+i\sigma_{r\theta 2}(\zeta)\right]^- - \left[\sigma_{rr1}(\zeta)+i\sigma_{r\theta 1}(\zeta)\right]^+=0 \tag{2}$$

$$\left[u_{r1}(\zeta)+iu_{\theta 1}(\zeta)\right]^+ - \left[u_{r2}(\zeta)+iu_{\theta 2}(\zeta)\right]^-=u_r^0+iu_\theta^0 \tag{3}$$

where u_r and u_q are the displacement components, s_{rr} and s_{rq} are the stress components in the polar coordinates, u_r^0 and u_θ^0 are the displacements induced by growth or shrink of neighboring voids. In addition, $|t|=R_1$, $|\zeta|=R_2$. The symbols R_1 and R_2 are the inner and outer radii of the intermediate annular region (the matrix phase).

For plane strain problem, stress fields and displacement fields may be expressed in terms of Muskhelishvili's complex potentials [7] $\Phi(z)$ and $\Psi(z)$

$$\sigma_{yy}+\sigma_{xx}=2\left[\Phi(z)+\overline{\Phi(z)}\right] \tag{4}$$

$$\sigma_{yy}-\sigma_{xx}+2i\sigma_{xy}=2\left[\bar{z}\Phi'(z)-\Psi(z)\right] \tag{5}$$

$$2\mu\left(u_x'+u_y'\right)=iz\left[\kappa\Phi(z)-\overline{\Phi(z)}+\bar{z}\overline{\Phi'(z)}+\frac{\bar{z}}{z}\overline{\Psi(z)}\right] \tag{6}$$

where $u_x'=\partial u_x/\partial\theta$, $u_y'=\partial u_y/\partial\theta$, $\Phi'(z)=d\left[\Phi(z)\right]/dz$, the overbar represents the complex conjugate, μ is the shear modulus of the bulk solid, υ is Poisson's ratio of the bulk solid , $\kappa=3-4\upsilon$ for plane strain state.

Under the assumption that the interface adheres to the bulk without slipping, and in the absence of body forces, according to Sharma et al. [6] based on Gurtin and Murdoch surface/interface model, the constitutive equation in the surface region is given as

$$\sigma_{\theta\theta}^0=\tau^0+\left(2\mu^0+\lambda^0-\tau^0\right)\varepsilon_{\theta\theta}^0 \tag{7}$$

where $\sigma_{\theta\theta}^0$ and $\varepsilon_{\theta\theta}^0$ denote surface stress and strain, μ^0 and λ^0 are surface Lame constants, τ^0 is the residual surface tension.

According to Gao [8], the uniform eigenstrains could be represented to express the displacements produced by the mismatch strains ε of the matrix and the effective medium.

$$u_r^0+iu_\theta^0=R_2\varepsilon \qquad |\zeta|=R_2 \tag{8}$$

where ε is dilatational or shrunk eigenstrain of neighboring voids in the matrix phase. The effective medium plasticity mismatches ε may be produced due to the yield stress and the strain hardening exponent on the nanovoid growth and coalescence. It is possible, of course, that to be attributed to mismatchs of the thermal expansion coefficient between the constituents.

According to Muskhelishvili [7], two complex potentials $\Phi_1(z)$ and $\Psi_1(z)$ in the matrix can be taken the following forms

$$\Phi_1(z)=\frac{\gamma_0}{z-z_0}+\frac{\gamma_1}{z-z_1}+\Phi_{10}(z) \tag{9}$$

$$\Psi_1(z)=\frac{\overline{\gamma_0}}{z-z_0}+\frac{\gamma_0\overline{z_0}}{\left(z-z_0\right)^2}+\frac{\overline{\gamma_1}}{z-z_1}+\frac{\gamma_1\overline{z_1}}{\left(z-z_1\right)^2}+\Psi_{10}(z) \tag{10}$$

Two complex potentials $\Phi_2(z)$ and $\Psi_2(z)$ in the effective medium can be taken the following forms

$$\Phi_2(z)=\frac{\gamma_0'+\gamma_1'}{z}+\Gamma_1+\Phi_{20}(z) \tag{11}$$

$$\Psi_2(z)=\frac{\overline{\gamma_0'}+\overline{\gamma_1'}}{z}+\Gamma_2+\Psi_{20}(z) \tag{12}$$

where $\gamma_k=-i\mu_1 B_k/\left[\pi(1+\kappa_1)\right]$, $\gamma_k'=-i\mu_2 B_k/\left[\pi(1+\kappa_2)\right]$ $(k=0,1)$, $\Gamma_1=\left(\sigma_{xx}^\infty+\sigma_{yy}^\infty\right)/4$, $\Gamma_2=\left(\sigma_{yy}^\infty-\sigma_{xx}^\infty+2i\sigma_{xy}^\infty\right)/2$

(σ_{xx}^∞, σ_{yy}^∞ and σ_{xy}^∞ are the remote stresses). $\Phi_{10}(z)$, $\Psi_{10}(z)$, $\Phi_{20}(z)$ and $\Psi_{20}(z)$ are holomorphic and the first two can be expanded in Laurent series

$$\Phi_{10}(z)=\sum_{k=0}^{\infty}a_k z^k+\sum_{k=1}^{\infty}b_k z^{-k} \tag{13}$$

$$\Psi_{10}(z)=\sum_{k=0}^{\infty}c_k z^{k-2}+\sum_{k=1}^{\infty}d_k z^{-k-2} \tag{14}$$

where the unknown coefficients a_k, b_k, c_k and d_k could be determined from the boundary conditions (1)-(3).

According to the work of Fang and Liu [9] and Zhao et al. [10], by a sufficient number of calculations, the explicit expressions of two complex potentials $\Phi_1(z)$ and $\Psi_1(z)$ in the matrix can be given

$$\Phi_1(z)=\frac{\gamma_0}{z-z_0}+\frac{\gamma_1}{z-z_1}+\sum_{k=0}^{\infty}a_k z^k+\sum_{k=1}^{\infty}b_k z^{-k} \tag{15}$$

$$\Psi_1(z)=\frac{\overline{\gamma_0}}{z-z_0}+\frac{\gamma_0\overline{z_0}}{(z-z_0)^2}+\frac{\overline{\gamma_1}}{z-z_1}+\frac{\gamma_1\overline{z_1}}{(z-z_1)^2}+\sum_{k=0}^{\infty}c_k z^{k-2}+\sum_{k=1}^{\infty}d_k z^{-k-2} \tag{16}$$

3. Critical stress for dislocation emission

According to Hirth and Lothe [11] and Peach-Koehler formula, the image force acting on the dislocation can be written as

$$f_x-if_y=\left(b_y+ib_x\right)\left[\Phi_0(z_0)+\overline{\Phi_0(z_0)}\right]+\left(b_y-ib_x\right)\left[\overline{z_0}\Phi_0'(z_0)+\Psi_0(z_0)\right] \tag{17}$$

where f_x and f_y are the force acting on the edge dislocation with Burgers vector B_0 in the x and y directions, respectively. $\Phi_0(z_0)$ and $\Psi_0(z_0)$ are the perturbation complex potentials in the matrix.

According to Qaissaunee and Santare [12], the perturbation complex potentials are calculated as follows:

$$\Phi_0(z_0)=\frac{\gamma_1}{z-z_1}+a_{01}+a_{02}\Gamma_1+a_1 z+\left(a_{21}+a_{22}\Gamma_2\right)z^2+\sum_{k=3}^{\infty}a_k z^k+b_1 z^{-1}+\left(b_{21}-b_{22}\overline{\Gamma_2}\right)z^{-2}+\sum_{k=3}^{\infty}b_k z^{-k} \tag{18}$$

$$\Psi_0(z_0)=\frac{\overline{\gamma_1}}{z-z_1}+\frac{\gamma_1\overline{z_1}}{(z-z_1)^2}+\left(c_{01}-c_{02}\Gamma_1\right)z^{-2}+c_1 z^{-1}+c_{21}+c_{22}\Gamma_2+\sum_{k=3}^{\infty}c_k z^{k-2}+d_1 z^{-3}+\left(d_{21}-d_{22}\overline{\Gamma_2}\right)z^{-4}+\sum_{k=3}^{\infty}d_k z^{-k-2} \tag{19}$$

Based on Stagni [13], the primary physical interest lies on the component of the force along the Burgers vector direction (glide force) which are given by

$$f_g=f_x\cos(\theta+\varphi)+f_y\sin(\theta+\varphi) \tag{20}$$

Adopting the criterion from Lubada et al. [14], it is assumed that the dislocation with Burgers vector B_0 will be emitted from the surface of the void if its equilibrium distance ρ from the surface of the void is equal to the dislocation core cut-off radius ρ_0 (one half of the dislocation width, which represents the extent of the dislocation core spreading). In the equilibrium dislocation position, the glide force vanishes, namely $f_g = 0$. In the present study, we consider the remote applied critical stress is the stress required to keep dislocation with Burgers vector B_0 in equilibrium position. A lower stress would suffice to keep the dislocation in the equilibrium at the distance greater than ρ_0, i.e., the equilibrium position of the dislocation is unstable, and the dislocation would be driven away from the void indefinitely, or until it is blocked by an obstacle. The angle $\theta = \theta_{cr}$ at which the dislocation is emitted from nanovoid corresponds to the minimum value of the applied stress $\sigma_{cr}^{\min}$. So by letting $\rho = \rho_0$ specifies the stress required to emit the dislocation from the surface of the nanovoid.

When considering the effect of the remote axial loading, we suppose that $\sigma_{xx}^{\infty} = \sigma$, $\sigma_{yy}^{\infty} = j_1\sigma$, $\sigma_{xy}^{\infty} = j_2\sigma$, it yields $\Gamma_1 = (1+j_1)\sigma/4$, $\Gamma_2 = (j_1 - 1 + 2ij_2)\sigma/2$. The following expression for the critical stress σ_{cr} can be expressed as follows:

$$\sigma_{cr} = \frac{\mathrm{Re}\left[f_{img}\right]\cos(\theta+\varphi) - \mathrm{Im}\left[f_{img}\right]\sin(\theta+\varphi)}{\mathrm{Im}\left[M\right]\sin(\theta+\varphi) - \mathrm{Re}\left[M\right]\cos(\theta+\varphi)} \tag{21}$$

where $f_{img} = \left(b_y + ib_x\right)\left[\Phi_{0d}(z_0) + \overline{\Phi_{0d}(z_0)}\right] + \left(b_y - ib_x\right)\left[\overline{z_0}\Phi'_{0d}(z_0) + \Psi_{0d}(z_0)\right]$

$$\Phi_{0d}(z_0) = \frac{\gamma_1}{z - z_1} + a_{01} + a_1 z + a_{21} z^2 + \sum_{k=3}^{\infty} a_k z^k + b_1 z^{-1} + b_{21} z^{-2} + \sum_{k=3}^{\infty} b_k z^{-k}$$

$$\Psi_{0d}(z_0) = \frac{\overline{\gamma_1}}{z - z_1} + \frac{\gamma_1 \overline{z_1}}{(z - z_1)^2} + c_{01} z^{-2} + c_1 z^{-1} + c_{21} + \sum_{k=3}^{\infty} c_k z^{k-2} + d_1 z^{-3} + d_{21} z^{-4} + \sum_{k=3}^{\infty} d_k z^{-k-2}$$

$$\begin{aligned} M = {} & \left(b_y + ib_x\right)\left[\begin{array}{l}\left(a_{02} + \overline{a_{02}}\right)(1+j_1)/4 + a_{22}(j_1 - 1 + 2ij_2) z_0^2/2 - b_{22}(j_1 - 1 - 2ij_2) z_0^{-2}/2 \\ + \overline{a_{22}}(j_1 - 1 - 2ij_2)\overline{z_0^2}/2 - \overline{b_{22}}(j_1 - 1 + 2ij_2)\overline{z_0^{-2}}/2\end{array}\right] \\ & + \left(b_y - ib_x\right)\left[\begin{array}{l}a_{22} z_0 \overline{z_0}(j_1 - 1 + 2ij_2) + b_{22} z_0^{-3}\overline{z_0}(j_1 - 1 - 2ij_2) + c_{02} z_0^{-2}(1+j_1)/4 \\ + c_{22}(j_1 - 1 + 2ij_2)/2 - d_{22} z_0^{-4}(j_1 - 1 - 2ij_2)/2\end{array}\right]\end{aligned}$$

4. Condition for dislocation emission

The critical stress required to emit the dislocation from the surface of the nanovoid can be determined accurately and explicitly given by Eq. (21). In this section considerable attention has be paid to elaborating the influence of the nanovoid size, the surface effect, nanovoid content and uniform distribution density of neighboring nanovoids in the effective medium on the critical condition required for dislocation emission from nanovoid surface. In this paper, we suppose that the normalized critical stress for the edge dislocation emitted from nanovoid surface by the shear modulus of the matrix $\sigma_{cr0} = \sigma_{cr}/\mu_1$, the intrinsic lengths of the nanovoid surface $\alpha = \mu_1^0/\mu_1$, $\beta = \lambda_1^0/\mu_1$ and $\delta = \tau_1^0/\mu_1$, the ratio of the shear modulus of the matrix and the effective medium $a = \mu_2/\mu_1$, the radius of the nanovoid $b = R_1/b_z$, the relative spacing between neighboring nanovoids or uniform distribution density of neighboring nanovoids $c = R_2/R_1$. Former studies have indicated that the surface properties can be either positive or negative, depending upon the material type and the surface crystallographic orientation. According to their results, the absolute values of intrinsic lengths α, β and δ are nearly $1\mathring{\mathbf{A}}$ [15]. In addition, let $\upsilon_1 = \upsilon_2 = 0.25$. The present study focuses exclusively on the effect of nanovoid content and uniform distribution density of neighboring nanovoids in the effective medium on the critical condition for splitting of dislocation from nanovoid surface, providing a remote equal biaxial loading.

Fig. 2 shows the critical stress to induce dislocation emission from the nanovoid surface as a function of emission angle θ with different ratios of the shear modulus of the matrix and the effective medium $a = \mu_2/\mu_1$ and surface elasticity. One should notice that, when nanovoid size b is fixed, the smaller the chosen ratio of the shear modulus a is, the larger nanovoid volume fraction the nanoporous materials contain. The figure presents the critical stress required to emit dislocation decreases, while relative most probable critical angle for dislocation emission increases as the ratio of the shear modulus decreases. That is to say, when nanovoid size is fixed, the larger nanovoid volume fraction in the nanoporous materials makes the dislocation emission take place more easily, and relative most probable critical emission angle more pronouncedly depart from the direction 45°. They mean that the distinct softening behavior can be happened and the interaction among neighboring nanovoids becomes important as nanovoid volume fraction increases. Therefore, it can significantly enhance capability of dislocation emission from nanovoid surface, favor the nanovoid growth, and then result in decreased ductility of the nanoporous materials. So it is well shown that the ductility of the material depresses with increasing nanosize void volume fraction and the porosity would evidently affect the ductility of structural materials, in agreement with the analysis by Tvergaard and Hutchinson [16]. We have observed a strong influence of surface effect on critical condition for dislocation emission. The positive surface elasticity increases the critical stress and the relative most probable critical angle for dislocation emission, while the negative surface elasticity reduces them. And the larger positive value of surface elasticity makes the dislocation emission from nanovoid take place more difficultly.

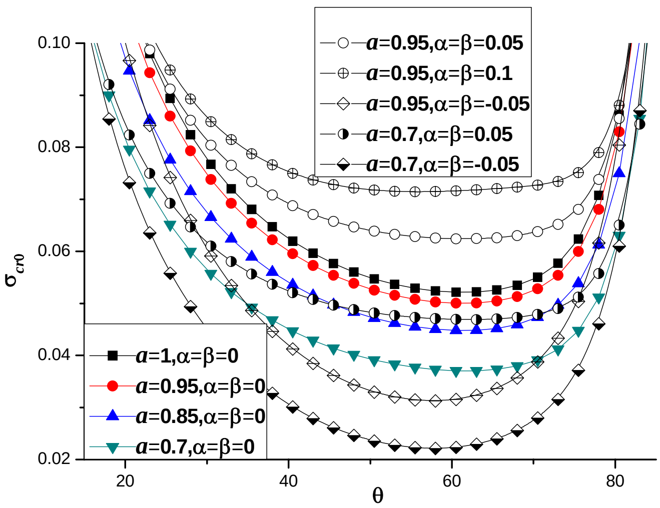

Fig. 2 Dependences of normalized critical stress σ_{cr0} on emission angle θ with different ratios of the shear modulus of the matrix and the effective medium $a = \mu_2/\mu_1$ and surface elasticity for $\rho_0 = b_z$, $\varepsilon = 0$, $j_1 = 1$, $j_2 = j_3 = 0$, $b = 8$, $c = 1.5$, $\delta = 0$.

Fig.3 shows normalized critical stress for dislocation emission to take place as a function of emission angle θ with different nanovoid sizes and surface residual stresses. When the nanovoid volume fraction is given, if the nanovoid size decreases, there must be larger number of same-size neighboring nanovoids. The figure shows the critical stress and relative most probable critical angle for dislocation emission decrease as the nanovoid size increases. That is to say, when the nanovoid volume fraction is fixed, the larger nanovoid size in the nanoporous materials makes the dislocation emission take place more easily, relative most probable critical emission angle less pronouncedly depart from the direction 45°. In other words, the dependence of critical stress on the neighboring number of nanovoids under the same void volume fraction can evidently be observed. Given the same void volume fraction, improved critical stress is accompanied with an increase in the neighboring number of nanovoids. The larger neighboring number of nanovoids under the same void volume fraction has a greater role in the critical stress required for dislocation emission. This is because the load-carrying capacity and the stress resistivity of materials can be enhanced by redistributing a large void into multiple small ones at nanoscale. These results are reasonable agreement with that of molecular dynamics simulations by Mi et al. [17]. As well-evident from the Fig. 3, we know that the negative surface residual stress would increase the critical stress, while the positive one reduces it. It means that the nanovoid surface characterized by the positive surface residual stress clearly promotes dislocation emission and lessens the ductility of the nanoporous materials. The larger the positive surface residual stress is, the more easily the dislocation emitted from nanovoid surface is.

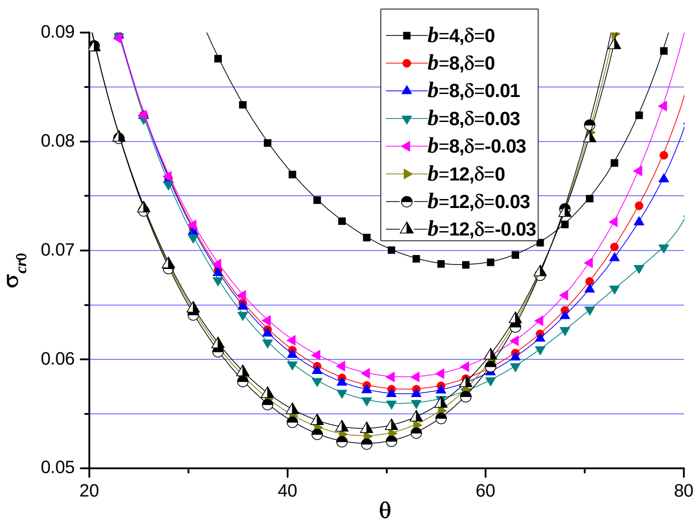

Fig. 3 Dependences of normalized critical stress σ_{cr0} on emission angle θ with different nanovoid sizes and surface residual stresses for $\rho_0 = b_z$, $\varepsilon = 0$, $j_1 = 1$, $j_2 = j_3 = 0$, $a = 0.9$, $c = 1.5$, $\alpha = \beta = 0$.

In this case in Fig. 4, namely $a = 0.9$ and $b = 8$, it means that for given void volume fraction and nanovoid size, c characterizes the spacing of neighboring nanovoids or the uniform distribution density of the nanovoids. The smaller physical quantity c defines the smaller neighboring spacing or the denser distribution of the nanovoids under the same void volume fraction and nanovoid size. As is seen from Fig. 4, the critical stress decreases clearly, while the relative most probable critical angle for dislocation emission increases as the physical quantity c decreases. That is, the initial void volume fraction and nanovoid size remain constant, the distinct softening behavior can be happened and then significantly promotes capability of dislocation emission from nanovoid surface in the nanoporous materials with improving the uniform distribution density of the neighboring nanovoids. In other words, increasing nanovoid spacing can impede the nanovoid growth and increase ductility. These conclusions are further confirmed by the earlier experiment from Dubensky and Koss [18], and the finite element analysis from Gao et al. [19]. It is also visibly indicates that the larger the negative surface residual stress is, the harder the dislocation emitted from nanovoid surface becomes. These observations demonstrate that the density of nanovoid concentration and the surface residual stress have a significant effect on determining the deformation behavior of ductile materials.

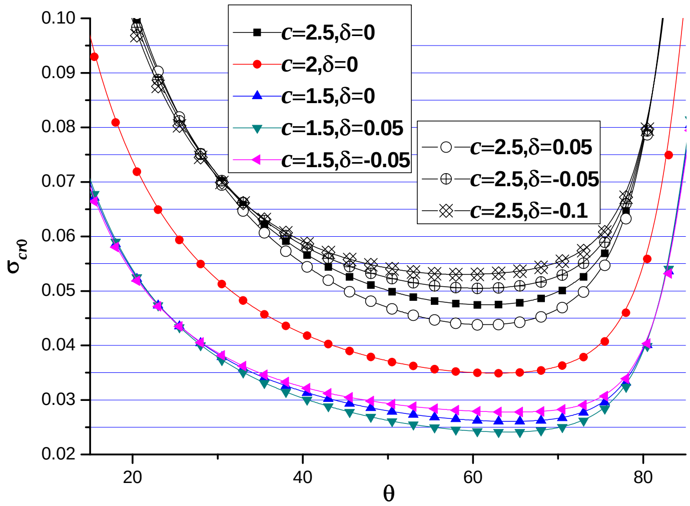

Fig. 4 Dependences of normalized critical stress σ_{cr0} on emission angle θ with different uniform distribution densities of the neighboring nanovoids and surface residual stresses for $\rho_0 = b_z$, $\varepsilon = 0$, $j_1 = 1$, $j_2 = j_3 = 0$, $a = 0.9$, $b = 8$, $\alpha = \beta = 0$.

5. Conclusions

In conclusion, when nanovoid size is fixed, the larger nanovoid volume fraction in the nanoporous materials makes the dislocation emission take place more easily, relative most probable critical emission angle more pronouncedly depart from the direction 45°. Under the condition of constant void volume fraction, the larger the neighboring number of voids is, the higher the critical stress becomes. For given void volume fraction and nanovoid size, the distinct softening behavior can be happened and then significantly promotes capability of dislocation emission from nanovoid surface in the nanoporous materials with improving the uniform distribution density of the neighboring nanovoids.

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