

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, 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.

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.

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

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

$$\sigma_{yy} - \sigma_{xx} + 2i\sigma_{xy} = 2[\overline{z}\Phi'(z) - \Psi(z)] \quad (5)$$

$$2\mu(u'_x + u'_y) = iz \left[\kappa\Phi(z) - \overline{\Phi(z)} + \overline{z}\Phi'(z) + \frac{\overline{z}}{z}\Psi(z) \right] \quad (6)$$

where $u'_x = \partial u_x / \partial \theta$, $u'_y = \partial u_y / \partial \theta$, $\Phi'(z) = d[\Phi(z)]/dz$, the overbar represents the complex conjugate, μ is the shear modulus of the bulk solid, ν is Poisson's ratio of the bulk solid, $\kappa = 3 - 4\nu$ 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

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

where $\sigma_{\theta\theta}^0$ and $\varepsilon_{\theta\theta}^0$ denote surface stress and strain, μ^0 and λ^0 are surface Lamé 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.

$$u_r^0 + iu_\theta^0 = R_2\varepsilon \quad |\zeta| = R_2 \quad (8)$$

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 mismatches 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

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

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

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

$$\Phi_2(z) = \frac{\gamma'_0 + \gamma'_1}{z} + \Gamma_1 + \Phi_{20}(z) \quad (11)$$

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

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

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

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

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

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

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

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

$$f_x - if_y = (b_y + ib_x) [\Phi_0(z_0) + \overline{\Phi_0(z_0)}] + (b_y - ib_x) [\overline{z_0} \Phi'_0(z_0) + \Psi_0(z_0)] \quad (17)$$

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 Quissaunee and Santare [12], the perturbation complex potentials are calculated as follows:

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

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

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

$$f_g = f_x \cos(\theta + \varphi) + f_y \sin(\theta + \varphi) \quad (20)$$

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 σ_{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:

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

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

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

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

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

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

It is found that the remote critical stress is independent of location from which the dislocation will be emitted, which is accord with the result of Zeng et al. [15].

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 been 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 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\AA [16]. In addition, let $\nu_1 = \nu_2 = 0.25$. 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 with different ratios of the shear modulus of the matrix and the effective medium and surface elasticity. One should notice that, when nanovoid size is fixed, the smaller the chosen ratio of the shear modulus is, the larger nanovoid volume fractions 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 fractions in the nanoporous materials make the dislocation emission take place more easily, relative most probable critical emission angle more pronouncedly depart from the direction 45° . They mean that the distinct softening behavior can be happened and then significantly enhances capability of dislocation emission from nanovoid surface in the nanoporous materials. 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. So it is well shown that the ductility of the material increases with increasing nanosize void volume fraction and the porosity would evidently affect the ductility of structural materials.

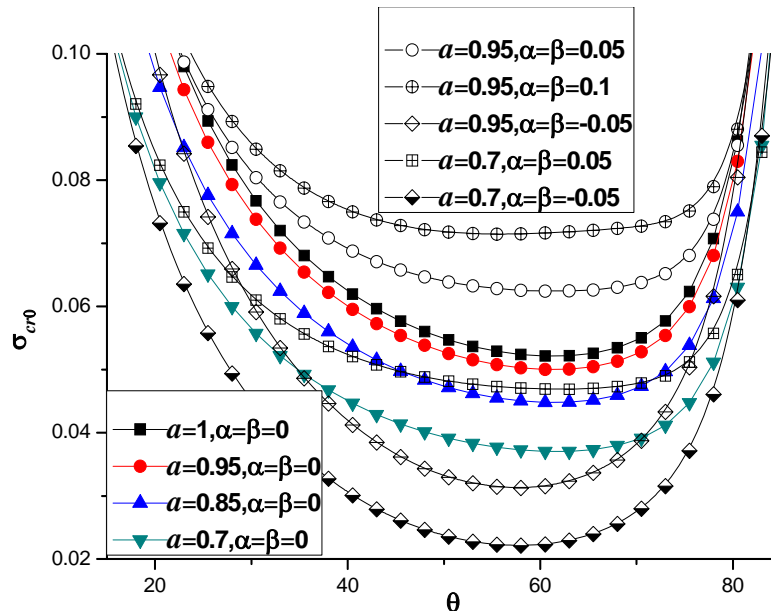


Fig. 2 Dependences of normalized critical stress σ_{cr0} on emission angle θ with different ratios of the shear modulus of the matrix and the effective medium $a = \mu_2/\mu_1$ and surface elasticity for $\rho_0 = b_z$, $\varepsilon = 0$, $j_1 = 1$, $j_2 = j_3 = 0$, $b = 8$, $c = 1.5$, $\delta = 0$.

Fig.3 shows normalized critical stress for dislocation emission to take place as a function of emission angle 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, 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. Under the condition of constant void volume fraction, the larger the neighboring number of nanovoids is, the higher the critical stress becomes. It indicates that 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 improves the ductility of the nanoporous materials. The larger the positive surface residual stress is, the more easily the dislocation emitted from nanovoid surface is. The larger neighboring number of nanovoids under the same void volume fraction has a greater role in the critical stress required for dislocation emission.

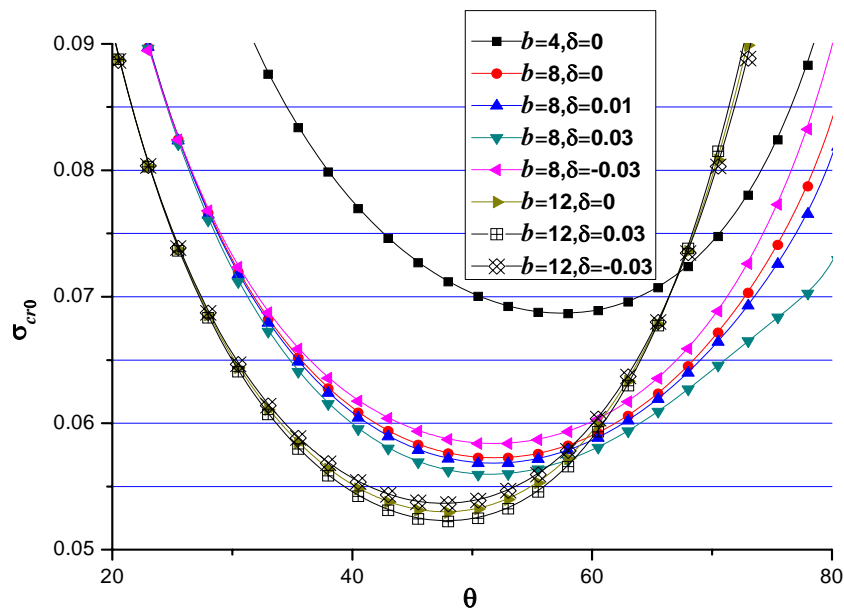


Fig. 3 Dependences of normalized critical stress σ_{cr0} on emission angle θ with different nanovoid sizes and surface residual stresses for $\rho_0 = b_z$, $\varepsilon = 0$, $j_1 = 1$, $j_2 = j_3 = 0$, $a = 0.9$, $c = 1.5$, $\alpha = \beta = 0$.

In this case in Fig. 4, namely $a = 0.9$, it means that the void volume fraction keeps the same, and c characterizes the distance of neighboring nanovoids or the uniform distribution density of the neighboring nanovoids. The larger physical quantity c , it demonstrates the larger neighboring

distance or the rougher distribution of the neighboring nanovoids under the same void volume fraction. From Fig. 4, it is found that the critical stress decreases clearly, while the relative most probable critical angle for dislocation emission increases as the physical quantity c increases. That is, with the initial void volume fraction and nanovoid size keep the same, the distinct hardening behavior can be happened and then significantly suppresses capability of dislocation emission from nanovoid surface in the nanoporous materials with improving the uniform distribution density of the neighboring nanovoids. 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 at nanoscale void distribution plays a role in determining the deformation behavior of ductile metals.

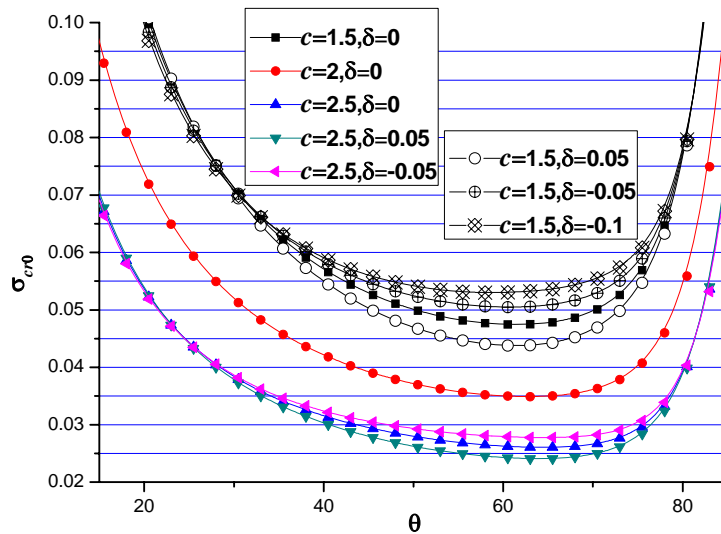


Fig. 4 Dependences of normalized critical stress σ_{cr0} on emission angle θ with different uniform distribution densities of the neighboring nanovoids and surface residual stresses for $\rho_0 = b_z, \varepsilon = 0, j_1 = 1, j_2 = j_3 = 0, a = 0.9, b = 8, \alpha = \beta = 0$.

5. Conclusions

In conclusion, when nanovoid size is fixed, the larger nanovoid volume fractions in the nanoporous materials make the dislocation emission take place more easily. Under the condition of constant void volume fraction, the larger the neighboring number of voids is, the higher the critical stress becomes. With the initial void volume fraction and nanovoid size keep the same, the distinct hardening behavior can be happened and then significantly suppresses capability of dislocation emission from nanovoid surface in the nanoporous materials with improving the uniform distribution density of the neighboring nanovoids. Softening or hardening of nanovoid surface due to surface effect has a pronounced effect on the critical condition for dislocation emission.

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