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Degradation of mechanical properties of structural reactor materials induced by formation of stress concentrators

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Abstract

The paper deals with the crack nucleation and stability in strain fields of stress concentrators (e.g. voids, gas bubbles, secondary phase precipitates). A general equation describes critical and subcritical crack length as a function of external (applied loading) and internal (stress concentrator type, normal traction, elastic properties of matrix, etc.) parameters. For the critical crack an analog of the Griffith criterion is found. The reduction of fracture stress due to different types of internal stress concentrators was evaluated.

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1. Introduction

Severe degradation of mechanical properties of nuclear reactor materials, the so-called high temperature irradiation embrittlement (HTIE), is regarded as one of the most important problems in radiation physics. It reduces operating temperature, working stress, and/or life time of a reactor. Although HTIE has been studied for more than 30 years, its driving mechanisms are still far from being understood. A number of approaches relate HTIE to structural evolution of the materials under environmental conditions [1–4].

Modern structural reactor materials have complicated chemical composition and operate in hard environmental conditions (thermal cycling, fast particle irradiation, alternate loading, etc.) Such a complex influence results in the microstructural change of a material, redistribution of its components, formation and growth of secondary phase precipitates, gas bubbles and voids. These macroscopic structural imperfections are regarded as stress concentrators. According to transmission and scanning electron microscopy observations [4], the preferable nucleation regions for stress concentrators are structural inhomogenities, namely, grain boundaries (GB) and triple grain junctions (TGJ) oriented normally to the applied stress. Taking into account noticeable local stress field modifications by stress concentrators, their presence can not only facilitate crack nucleation and propagation but also change the fracture mode from intergranular to transgranular and from viscous to brittle. The change of the fracture mode is the tentative proof of HTIE.

In this paper we consider the nucleation and stability of a crack formed at a stress concentrator. The results obtained is applied to the description of the behavior of cracks formed at different types of stress concentrators often met in application-relevant materials.

2. Formulation of the problem

Here we discuss nucleation of a crack on a stress concentrator in terms of two-dimensional geometry (plain strain). Even though in application-relevant situations both the loading geometry and the shape of stress concentrators are usually three-dimensional, the simplification used here makes it possible to elucidate qualitative behavior of cracks at stress concentrators, avoiding inevitable complications of three-dimensional geometry. Moreover, in certain cases the two-dimensional approach adopted here is directly applicable to

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real situations, such as the nucleation of cracks at armoring fibers in composite materials. Another example is crack formation at the chains of secondary phase precipitates or gas bubbles along TGJ in metals.

Let us assume that an infinite matrix is subjected to a mode I loading with a constant external tension, σ, applied along the Oy axis of a Cartesian coordinate system (see Fig. 1). A wedge crack is formed at the circular stress concentrator with radius R. The crack is simulated with a cut of length, L, along the Ox axis. The center, O, of the coordinate system is chosen in the center of the crack. The edges of the circle and the crack are subjected to normal tractions, p_1, and p_2, respectively.

The condition of mechanical stability of a crack of length L requires the force balance at the crack surface to be fulfilled:

$$\begin{aligned} &\sigma_{ij} n_j\big|_S + P_i(x) = 0, \quad i,j = \mathrm{X},\mathrm{Y}; \\ &S = \{-L/2 \leqslant x \leqslant L/2,\ y = 0\}, \end{aligned} \tag{1}$$

where $\mathbf{n}$ is a unit vector of the outward normal to the crack surface, S; $\mathbf{P}(x)$ is the total traction at the crack surface caused by both external and internal loading. The absence of a shear stress resulting from the symmetry of the problem makes it possible to reduce Eq. (1) to the following form:

$$\sigma_{yy}(x) = -P(x), \tag{2}$$

where $P(x)$ is the component of the traction normal to the crack. In our case $P(x)$ can be written as (see Fig. 1)

$$P(x) = -p_2 - \sigma^0_{yy}(x) + S(h(x)), \tag{3}$$

where $S(h(x))$ is the adhesive force acting in the crack tip (in the region d, $a \ll d \ll L$, where a is the interatomic distance) [5] and $\sigma^0_{yy}(x)$ is the stress acting in the plane $y = 0$ in the sample without the crack. According to the general approach of linear theory of elasticity [6], $\sigma^0_{yy}(x)$ is straightforwardly obtained in the form

$$\begin{aligned} \sigma^0_{yy}(x) = \frac{\sigma}{2}\Bigg[2 + \left(1 + \frac{2p_1}{\sigma}\right)\left(\frac{R}{x + R + (L/2)}\right)^2 \\ + 3\left(\frac{R}{x + R + (L/2)}\right)^4 \Bigg]. \end{aligned} \tag{4}$$

In order to find the dependence of crack length L on the parameters of the problem the well-known technique to simulate a crack by a pile-up of virtual dislocations [7] is applied. Equilibrium crack length L is defined by the equation

$$\frac{\mu}{2\pi(1-\nu)} \int_{-L/2}^{L/2} \frac{\omega(\xi)}{\xi - x}\, \mathrm{d}\xi = \sigma_{yy}(x), \tag{5}$$

where μ and ν are the shear modulus and Poisson's ratio, respectively, $\omega(\xi)$ is the density of virtual dislocations related to the displacement of the crack edges, $h(x)$, as

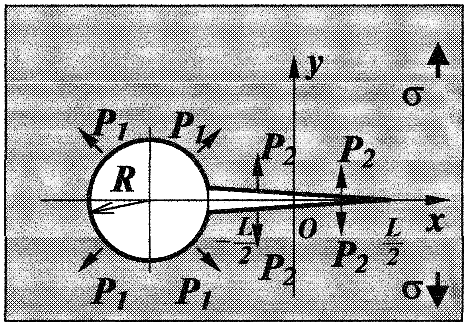

Fig. 1. Geometry of the problem.

$$\omega(x) = \frac{\mathrm{d}h(x)}{\mathrm{d}x}. \tag{6}$$

3. Solution

In order to find $\omega(x)$ from Eqs. (3)–(5), let us define non-dimensional variables

$$\eta = \frac{2x}{L}, \quad \rho = \frac{2R}{L} \tag{7}$$

and use the expansion of the function $\sigma_{yy}(\eta)$ over the Chebyshev polynomials T_n [8]:

$$\sigma_{yy}(\eta) = \sum_{n=0}^{\infty} Q_n T_n, \tag{8}$$

where

$$\begin{aligned} Q_0 &= \frac{1}{\pi}\int_{-1}^{1} \frac{\sigma_{yy}(\eta)\, \mathrm{d}\eta}{\sqrt{1-\eta^2}}, \\ Q_n &= \frac{2}{\pi}\int_{-1}^{1} \frac{\sigma_{yy}(\eta) T_n(\eta)\, \mathrm{d}\eta}{\sqrt{1-\eta^2}}. \end{aligned} \tag{9}$$

Eq. (5) represents a Hilbert transformation of $\omega(x)$. Since Chebyshev polynomials are the characteristic functions for the transformation, the density $\omega(x)$ is obtained by reconversion in the form [8]

$$\omega(\eta) = \frac{2(1-\nu)}{\mu}\left[-\frac{Q_0 \eta}{\sqrt{1-\eta^2}} + \sqrt{1-\eta^2}\sum_{n=1}^{\infty} Q_n U_{n-1}(\eta) \right]. \tag{10}$$

The first term in the summation in Eq. (10) diverges at the crack tips, whereas the other terms are limited there. So, the stress evaluated from Eq. (5), after substitution of Eq. (10), diverges as well, if the condition $Q_0 = 0$ is not satisfied. If the coefficient $Q_0 \neq 0$, then according to Eq. (8) σ_{yy} becomes infinite at the crack tips, i.e. infinitesimal loading will suffice to provide crack propagation and fracture of the material. To avoid this, one should require that

$$\int_{-1}^{1} \frac{\sigma_{yy}(\eta)\, \mathrm{d}\eta}{\sqrt{1-\eta^2}} = 0. \tag{11}$$

This condition coincides with that introduced in Refs. [9,7]. The requirement, Eq. (11), is the condition of mechanical stability of the crack (analogous to the Griffith criterion).

4. The criterion of a crack stability

The criterion of mechanical stability of a crack formed at a stress concentrator, as defined by Eq. (11), can be written in the form

$$(p_2+\sigma) + \left(p_1 + \sigma\left(\frac{1}{2}+\frac{3}{8}\frac{\rho}{\rho+2}\right)\right)\frac{\rho+1}{\rho+2}\sqrt{\frac{\rho}{\rho+2}} + \sigma\frac{3}{8}\frac{\rho}{\rho+2}\frac{1+3(\rho+1)^2}{(\rho+2)^2} - \frac{\sqrt{2}K}{\pi\sqrt{L}} = 0, \tag{12}$$

where K is the stress intensity factor [10], defined by

$$K = \int_0^\infty \frac{S(h(x))}{\sqrt{x}}\, \mathrm{d}x. \tag{13}$$

Criterion (12) describes the behavior of brittle and quasibrittle cracks irrespective of the crack formation mechanism (fatigue, hardening, strain, intergranular crack, etc.). Moreover, it describes critical and subcritical (smaller than the Griffith one) cracks.

In the case when the crack is the Griffith one, K is equal to the fracture toughness of the material, K_g, evaluated from Ref. [10]:

$$K_g = \sqrt{\frac{\gamma E}{\pi(1-\nu^2)}}, \tag{14}$$

where γ is the specific energy of the crack surface.

Let us analyze the asymptotic behavior of a Griffith crack formed on a stress concentrator. First of all, let us rewrite Eq. (12) in a dimensionless form

$$\left(\frac{p_2}{\sigma_g}+s\right) + \left(\frac{p_1}{\sigma_g} + s\left(\frac{1}{2}+\frac{3}{8}\frac{\rho}{\rho+2}\right)\right)\frac{\rho+1}{\rho+2}\sqrt{\frac{\rho}{\rho+2}} + s\frac{3}{8}\frac{\rho}{\rho+2}\frac{1+3(\rho+1)^2}{(\rho+2)^2} - \sqrt{\frac{1}{l}} = 0, \tag{15}$$

where $l = L/L_g$ is the dimensionless crack length, $L_g = 2K_g^2/\pi\sigma_g^2$ the length of the Griffith crack, σ_g the applied stress corresponding to the Griffith crack, and $s = \sigma/\sigma_g$ is the dimensionless external loading.

Let us analyze a 'Griffith' crack (the length $l = 1$). In the case when $\rho \gg 1$ the stress required to initiate the unstable crack growth is reduced as compared to the Griffith one as

$$s = \frac{1}{3}\left[1 - \left(\frac{p_1}{\sigma_g}+\frac{p_2}{\sigma_g}\right) + \frac{1}{\rho}\left(2\frac{p_1}{\sigma_g} + \frac{19}{6}\left(1-\frac{p_2}{\sigma_g}\right)\right)\right]. \tag{16}$$

In the opposite case when $\rho \ll 1$, for the same crack length $l = 1$, the critical stress is given by

$$s = \left(1-\frac{p_2}{\sigma_g}\right) + \frac{\sqrt{\rho}}{2\sqrt{2}}\left(\frac{p_2}{\sigma_g} - \frac{p_1}{\sigma_g} - \frac{1}{2}\right) + \frac{p_1}{\sigma_g}\frac{1}{16}\rho. \tag{17}$$

An important particular case corresponds to $\rho = 1$, when the crack size is equal to the diameter of the stress concentrator:

$$s = \frac{1}{1+5/12\sqrt{3}+13/72}\left(1 - \left(\frac{2}{3\sqrt{3}}\frac{p_1}{\sigma_g}+\frac{p_2}{\sigma_g}\right)\right) \approx 0.704\left(1 - \left(\frac{2}{3\sqrt{3}}\frac{p_1}{\sigma_g}+\frac{p_2}{\sigma_g}\right)\right). \tag{18}$$

5. Applications

Although the proposed approach deals with brittle crack nucleation and propagation, the results obtained can be applied for description of quasibrittle crack evolution, when the crack tip emits dislocations. In order to take into account material plasticity effect on the crack behavior and fracture, the stress intensity factor (14) renormalization is sufficient. The case of extended plasticity is not discussed here. It is proposed to apply the results obtained for investigation of embrittlement of relevant materials.The embrittlement is one of the main problems of radiation materials science. Appearing of stress concentrators can result in change of fracture mode from viscous to brittle and lead to strong embrittlement.

Let us apply the developed model for a description of the crack formation on particular types of stress concentrators, namely secondary phase precipitates, gas bubbles, voids.

5.1. Voids

In order to check the approach, it is applied to the description of Griffith crack formation at a void with no internal loading: $p_1 = p_2 = 0$. However, the presence of the stress concentrator results in the reduction of the fracture stress (see Fig. 2) according to

$$1 + \left(\frac{1}{2}+\frac{3}{8}\frac{\rho}{\rho+2}\right)\frac{\rho+1}{\rho+2}\sqrt{\frac{\rho}{\rho+2}} + \frac{3}{8}\frac{\rho}{\rho+2}\frac{1+3(\rho+1)^2}{(\rho+2)^2} - \frac{1}{s} = 0. \tag{19}$$

The same data have been obtained numerically in Refs. [11–14]. Some calculations have been carried out in Ref. [15]. The asymptotic behavior of Eq. (19) for $\rho \gg 1$ is given by (see Fig. 2)

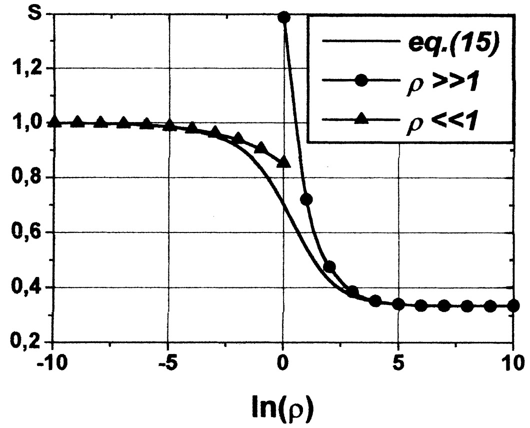

Fig. 2. Dependence of dimensionless fracture stress on the ρ and asymptotic functions.

$$s = \frac{1}{3}\left(1 + \frac{19}{6}\frac{1}{\rho}\right), \tag{20}$$

whereas at $\rho \ll 1$ Eq. (19) takes the form (see Fig. 2):

$$s = 1 - \frac{\sqrt{\rho}}{4\sqrt{2}}. \tag{21}$$

The stress s inducing crack nucleation ($\rho \to \infty$) is given by

$$s = \frac{1}{3}, \tag{22}$$

i.e. three times less than that in the bulk of material (the well-known result, see e.g. Refs. [11–15]).

5.2. Gas bubbles

Gas bubbles are typical in materials irradiated in nuclear reactors, where helium is generated by nuclear (n, α) reactions. Because of the low solubility in metals, it segregates into helium bubbles. Helium bubble formation often results in severe degradation of the mechanical properties of structural reactor materials as a result of high temperature helium embrittlement (HTHE).

In the case of crack formation at a gas bubble the internal loads are defined by the gas pressure and $p_2 = p_1 = P$. The dependence of fracture stress s on the internal gas pressure and ρ is shown in Fig. 3. The strong reduction of s due to the internal gas pressure is clearly seen. The most significant effect occurs for large ρ. According to Eq. (16) the asymptotic behavior of Eq. (12) is given by

$$s = \frac{1}{3}\left[1 - \frac{2P}{\sigma_g} + \frac{1}{\rho}\left(2\frac{P}{\sigma_g} + \frac{19}{6}\left(1 - \frac{P}{\sigma_g}\right)\right)\right]. \tag{23}$$

The critical stress for crack nucleation at a bubble ($\rho \gg 1$) is reduced (in comparison with the Griffith crack) to

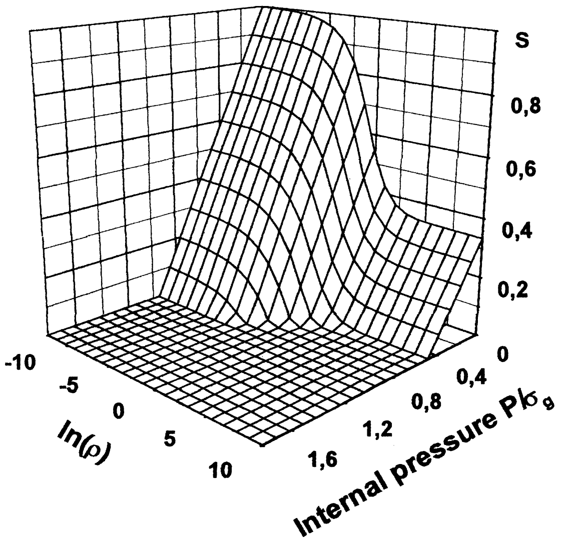

Fig. 3. Dependence of dimensionless fracture stress on the ρ and internal gas pressure.

$$s = \frac{1}{3}\left(1 - 2\frac{P}{\sigma_g}\right). \tag{24}$$

It is seen that at the internal gas pressure $P = \sigma_g/2$ the stress, s, for fracture initiation vanishes, i.e. an infinitesimal external applied stress will suffice to provide crack propagation. Let us investigate the change of actual gas pressure P acting during crack evolution.

Let us assume that the gaseous impurity behavior satisfies the following equation of state:

$$PV = \text{const}, \tag{25}$$

where the cross-section, V, of the cavity (crack and bubble) is determined by

$$V = V_b + V_{cr} = \pi R^2 + \int_{-L/2}^{L/2} h(x)\,dx. \tag{26}$$

In order to estimate the crack contribution to the total volume of the system (and consequently reduction of the internal gas pressure P due to crack formation) the dependence of the V_{cr}/V_b ratio on the ρ for different external loadings and internal pressure of the gaseous impurity is outlined (see Fig. 4). It is clear that the crack contribution, V_{cr}, to the total cavity volume, V, can be neglected for all physically possible cases we are interested in. Therefore, according to Eq. (25) the actual gas pressure P is invariable throughout the crack propagation process.

5.3. Secondary phase precipitates

Secondary phase precipitates are a common feature of structural materials. They can be formed by thermal

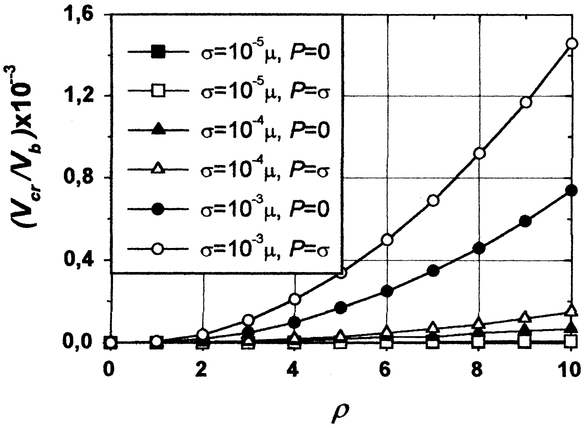

Fig. 4. Dependence of the V_b/V_{cr} ratio on the ρ at different internal and external loadings.

treatment in order to improve service properties of the structural material or arise due to environmental effects. For example, improper heat treatment and/or hard thermal conditions induce diffusional redistribution of chromium from the bulk of the grain to the grain boundaries in stainless steels and result in $Cr_{23}C_6$ precipitate formation. The presence of these precipitates at the grain boundaries leads to embrittlement of steels. Similar processes occurring in titanium alloys lead to σ-phase formation and result in strong embrittlement. Irradiation is an additional factor activating diffusional redistribution of material components.

The dependence of dimensionless tensile stress s on the normal traction p on the secondary phase-matrix interface and ρ is given by

$$s+\left(\frac{p}{\sigma_g}+s\left(\frac{1}{2}+\frac{3}{8}\frac{\rho}{\rho+2}\right)\right)\frac{\rho+1}{\rho+2}\sqrt{\frac{\rho}{\rho+2}} + s\frac{3}{8}\frac{\rho}{\rho+2}\frac{1+3(\rho+1)^2}{(\rho+2)^2}-1=0 \tag{27}$$

and illustrated in Fig. 5. The crack evolution is noticeably influenced by the precipitate only for sufficiently large ρ values:

$$s=\frac{1}{3}\left[1-\frac{p}{\sigma_g}+\frac{1}{\rho}\left(2\frac{p}{\sigma_g}+\frac{19}{6}\right)\right]. \tag{28}$$

The critical stress for crack nucleation at a secondary phase precipitate is given by

$$s=\frac{1}{3}\left(1-\frac{p}{\sigma_g}\right). \tag{29}$$

In contrast to HTHE discussed above, the internal loading necessary for spontaneous fracture is two times higher. Nonetheless, in relevant applications, precipitates are more probable candidates for the reason of spontaneous fracture than gas bubbles. Indeed, the precipitates can be larger (10 or even 100 μm) than the

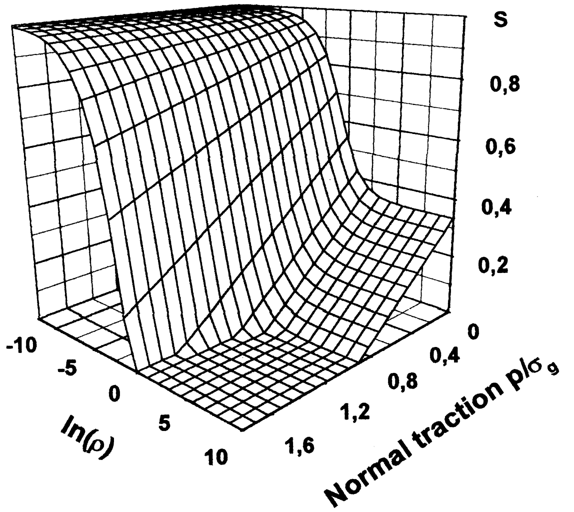

Fig. 5. Dependence of dimensionless fracture stress on the ρ and normal traction on secondary phase-matrix interface.

bubbles, and stress acting at the matrix–precipitate interface is independent of the size of the precipitate, whereas the internal helium pressure reduces with increase of the bubble size.

It should be pointed out that there are a lot of precipitate–matrix systems where the normal traction p is negative, and the influence of a precipitate on crack nucleation and evolution is more complicated. Dependence of the fracture stress s on the ρ value and the negative normal traction p is shown in Fig. 6. An absolute increase of the normal traction p results in a respective enlargement of the critical stress. However, the actual value of the fracture stress can be either smaller or larger than the Griffith one depending on the ρ value (see Fig. 7). Curve 1 in Fig. 7 corresponds to zero normal traction. Curves 2, 3 and 4 can be divided into two

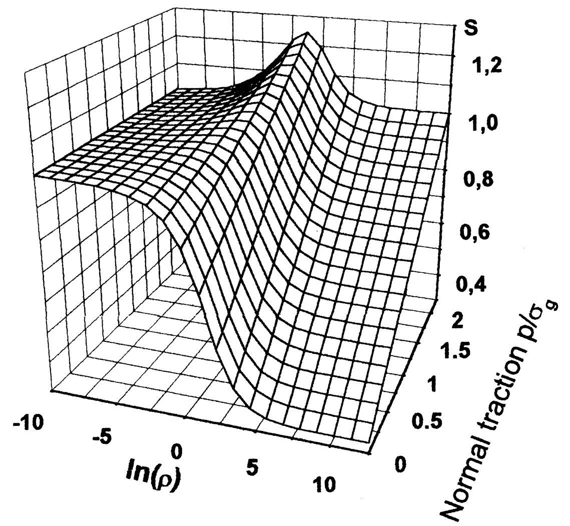

Fig. 6. Dependence of dimensionless fracture stress on the ρ and negative normal traction on secondary phase-matrix interface.

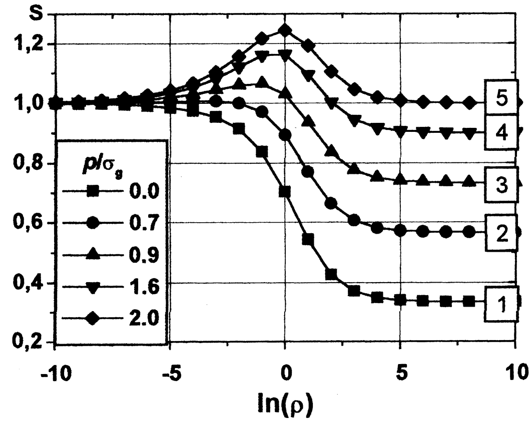

Fig. 7. Characteristic cross-sections of Fig. 6.

regions. In the first region, $\rho \leqslant \rho_c$ (where $\rho_c = \rho_c(p/\sigma_g)$), dimensionless fracture stress, s, is larger than the Griffith one. In the second region, $\rho \geqslant \rho_c$, fracture stress is less than the Griffith one. In the cases described by curves 2, 3 and 4 the preferable crack nucleation location is at the precipitate, but crack propagation for all values $\rho < \rho_c$ is obstructed by the local stress field induced by the inclusion. Curve 5 illustrates the case when the actual fracture stress is larger than the Griffith one for any values of the ρ parameter. In this case crack nucleation can occur everywhere except the secondary phase precipitate.

6. Conclusions

The paper deals with the problem of crack formation at stress concentrators. A general equation for the critical and subcritical crack length as a function of external and internal parameters is suggested. In the case of a critical crack this equation reduces to an analog of the Griffith criterion. In the limiting case of crack nucleation when $\rho \gg 1$ the critical stress is found for different types (voids, gas bubbles, secondary phase precipitates) of stress concentrators. It has been found that the internal stress concentrators can noticeably decrease the fracture stress of the material. The complicated influence of secondary phase precipitates having negative normal traction on crack evolution is established. A detailed investigation of this problem is to be carried out elsewhere.

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