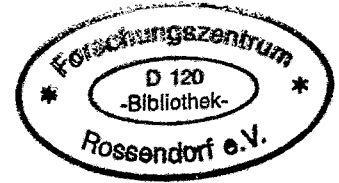


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Nucleation of dislocation loop at the crack tip**

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**Analytical Description of Brittle-to-Ductile  
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Nucleation of dislocation loop at the crack tip**

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### **Abstract**

Nucleation of dislocation loop at the crack tip in a material subjected to uniaxial loading is investigated. Analytical expression for the total energy of rectangular dislocation loop at the crack tip is found. Dependence of the nucleation energy barrier on dislocation loop shape and stress intensity factor at the crack tip is determined. It is established that the energetic barrier for nucleation of dislocation loop strongly depends on the stress intensity factor. Nucleation of dislocation loop is very sensitive to stress field modifiers (forest dislocations, precipitates, clusters of point defects, *etc*) in the crack tip vicinity.

# 1 Introduction and overview

The ductile-to-brittle transition (DBT) is a classic phenomenon exhibited by almost all materials with *possible* exception of *fcc* metals. The change in fracture behaviour from (quasi)brittle cleavage to ductile failure is always accompanied by significant increase of dislocation density at the near crack surface region [1]. A number of experimental observations unambiguously demonstrate noticeable cold-working of crack surfaces due to nucleation of dislocations at the crack tip [1, 2].

There are two possible ways of energy release from the crack tip region during fracture process. The first one is the formation of a new surface that results in crack growth. The second possible process is the local plastic flow at the near crack tip region. There are two time scales involved. Depending on the relation between typical time of crack growth ( $\tau_{cr}$ ) and typical time of plastic deformation ( $\tau_d$ ) one of the following cases can be realized. Provided typical time of crack surface formation is significantly less than that of deformation ( $\tau_{cr} \ll \tau_d$ ) brittle cleavage of material occurs. Comparable time scales ( $\tau_{cr} \simeq \tau_d$ ) result in ductile failure. High deformation rate at the crack tip region ( $\tau_{cr} \gg \tau_d$ ) prohibits crack growth because all the work of external forces absorbed by solid is dissipated through local plastic deformation at the crack tip.

In order to establish particular process taking place it is convenient to estimate typical times. Assuming that typical time of crack growth is independent on the structural environment evolution and is taken into consideration as an external parameter the typical time of deformation is evaluated. It consists of the time of dislocation nucleation ( $\tau_f$ ) and the time of dislocation motion ( $\tau_m$ ):

$$\tau_d = \tau_f + \tau_m. \quad (1)$$

In the existing models DBT is considered either as a competition between crack propagation and thermally activated generation of a dislocation (assumption  $\tau_f \gg \tau_m$ ) [3]-[6] or as a thermally activated motion of dislocation (assumption  $\tau_f \ll \tau_m$ ) [7, 8]. The latter limiting case is realized in covalent crystals (*e.g.* in silicon) where temperature dependent dislocation motion occurs at temperature range up to the melting point. The former case is more appropriate for metals at relevant temperatures because of athermal pattern of dislocation motion at DBT temperature

range.

According to general approaches of statistical mechanics typical time of the process ( $\tau_d$ ) is connected with appropriate activation energy ( $W_\Sigma$ ) through Arrhenius dependence:

$$\tau_d \sim \exp\left(-\frac{W_\Sigma}{kT}\right). \quad (2)$$

Within suggested point of view the problem of change of fracture behaviour is reduced to evaluation of the nucleation energetic barrier for dislocation at the crack tip. Presented contribution consists of several parts. In the first part a brief description of recent models of dislocation formation and equilibrium at the crack tip region is given. In the second part a new model of rectangular dislocation loop nucleation at the crack tip is proposed. The next section deals with evaluation of nucleation energy barrier and eduction of typical dimensions of 'critical' dislocation loop. Subsequent text includes analysis and discussion of the obtained results, conclusions and suggestions for further considerations.

## 2 Recent models

In order to estimate the nucleation energy of dislocation at the crack tip region various shapes of dislocation line, location of dislocation and crack, and loading geometry have been suggested.

### 2.1 2D model of equilibrium of edge dislocation at the crack tip

Equilibrium of edge dislocation at the crack tip region was considered within two dimensional geometry (plain strain) in the framework of force balance approach [4]. Material with crack is subjected to mode I loading in the direction normal to the crack plane. Edge dislocation is located at the distance  $r$  from the crack tip. Slip plane of dislocation makes angle  $\theta$  with the crack plane, see Fig.1.

The equilibrium position for the edge dislocation comes from the force balance between the stress field from the crack tip that pushes dislocation away and the mirror forces from the free surface of the crack that attracts dislocation back. The main drawback of this approach is related to the geometry applied. Two dimensional

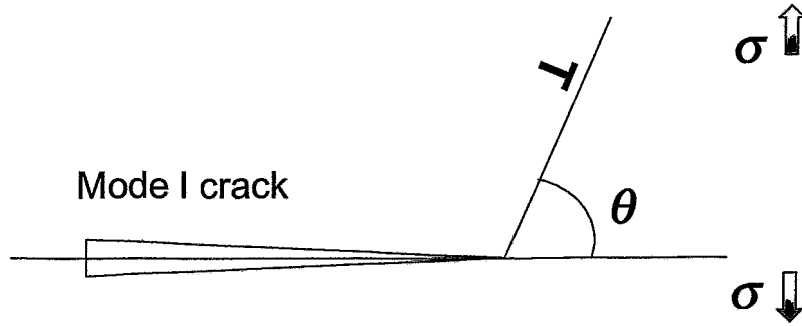


Figure 1: Geometry of 2D approach to evaluation of equilibrium position of edge dislocation emitted by mode I crack.

consideration supposes infinite solid, crack and edge dislocation in the direction normal to the plane of Figure 1. Therefore, the total energy of the edge dislocation is also infinite. It means that infinite dislocation cannot be emitted from the crack tip by thermal fluctuations.

## 2.2 3D model of dislocation loop generation from a crack tip

Advanced model of dislocation loop nucleation at the crack tip has been proposed recently [5]. Material with crack is subjected to mode II loading in the direction parallel to the plane of the crack. Circular dislocation loop is nucleated at the crack tip. Slip plane of the dislocation coincides with crack plane, see Figure 2.

Nucleation energy barrier for circular dislocation loop formation at the crack tip region has finite value. However, the circular shape of the loop can be less preferable from the energetic point of view in comparison with *e.g.* rectangular one.

## 3 Nucleation of dislocation loop at the crack tip

Within the general problem of ductile-to-brittle transition we propose to consider nucleation of rectangular dislocation loop at the crack tip. Geometry of the problem is shown in Figure 3. Material with wedge crack is loaded with external

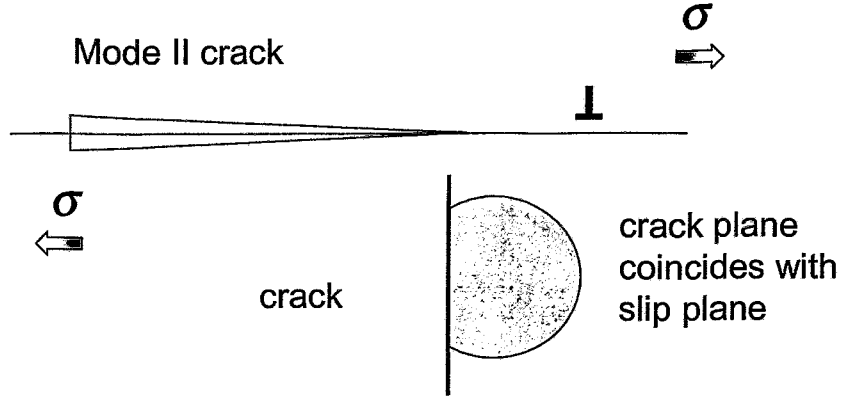


Figure 2: Geometry of 3D approach [5] to evaluation of the energy of circular dislocation loop emitted by mode II crack.

stress  $\sigma$  normal to the crack surface. Rectangular dislocation loop with 'height'  $a$  (pure screw segments) and 'width'  $L$  (pure edge segment) is nucleated at the crack tip. Here we neglect dislocation line tension effects changing the shape of the loop. Slip plane of the loop makes angle  $\theta$  with the plane of the crack. The most preferable direction of the loop nucleation is determined by the maximum of actual stress and should be established within the problem treatment.

The total energy of dislocation loop at the crack tip includes several terms:

$$W_{\Sigma} = W_{\sigma} + W_l + 2W_f + W_i, \quad (3)$$

where  $W_{\sigma}$  is the energy of the edge segment of rectangular dislocation loop in the actual stress field;  $W_l$  is the energy of ledge formation;  $W_f$  is the formation energy of a screw segment of rectangular dislocation loop and  $W_i$  is the energy of interaction of the screw segments of the loop.

In order to calculate the first term of Eq.3 the actual stress field and the most preferable direction of loop nucleation have to be found.

Asymptotic behavior of shear stress  $\sigma_{r\theta}^c(r, \theta)$  at the crack tip region is given by the following relation [9]:

$$\sigma_{r\theta}^c(r, \theta) = \frac{K_I}{\sqrt{\pi r}} \sin \theta \cos \frac{\theta}{2}, \quad (4)$$



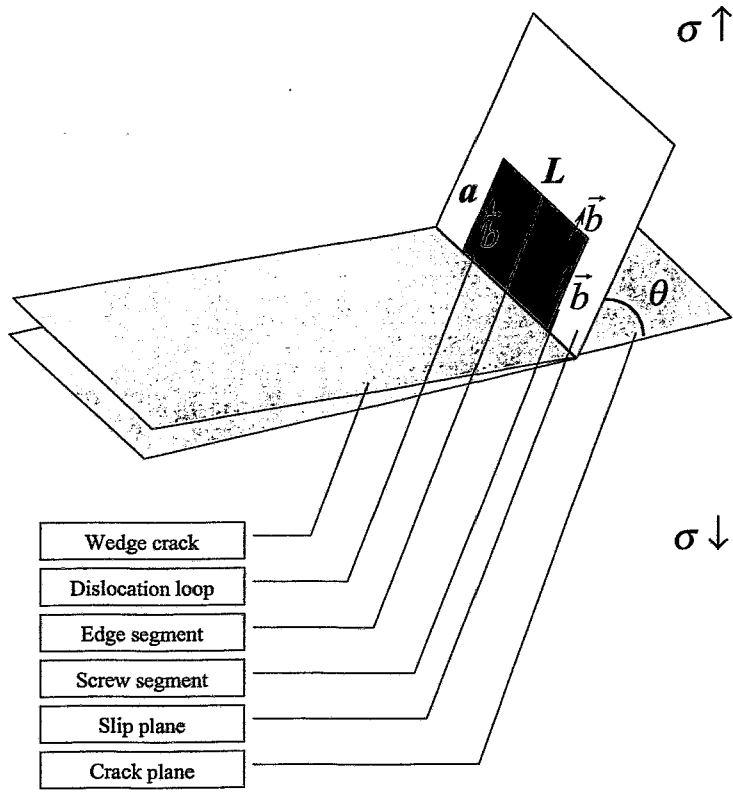


Figure 3: Geometry of the suggested approach to evaluation of nucleation energy of dislocation loop at the crack tip.

where  $K_I$  is the stress intensity factor at the crack tip,  $r$  and  $\theta$  are appropriate coordinates in polar coordinate system with the origin at the crack tip.

Dependence of  $\sigma_{r\theta}^c(r, \theta)$  is shown in Fig.4 and respective contour plot is given in Fig.5. The distance from the crack tip is normalized by the value of Buerger's vector  $b$ . The magnitude of shear stress is given in units of  $K_I/\sqrt{\pi b}$ . Direction of the maximum of  $\sigma_{r\theta}^c(r, \theta)$  makes angle  $\theta \approx 70.5^\circ$  with the plane of the crack and can be evaluated via obvious technique [9].

Mirror forces  $\sigma_{r\theta}^m(r, \theta)$  from the crack surface act on the edge dislocation and attract it back to the crack. The value of mirror forces (per unit length) versus edge

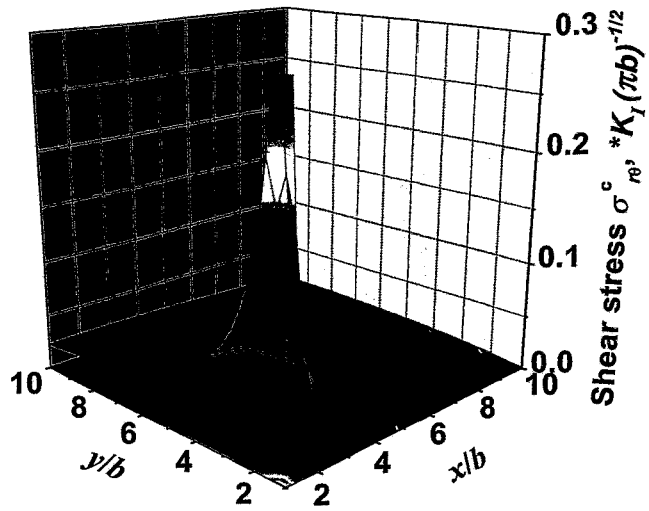


Figure 4: Shear stress. The value of  $\sigma_{r\theta}^c(r, \theta)$  is normalized by factor  $K_I/\sqrt{\pi b}$ .

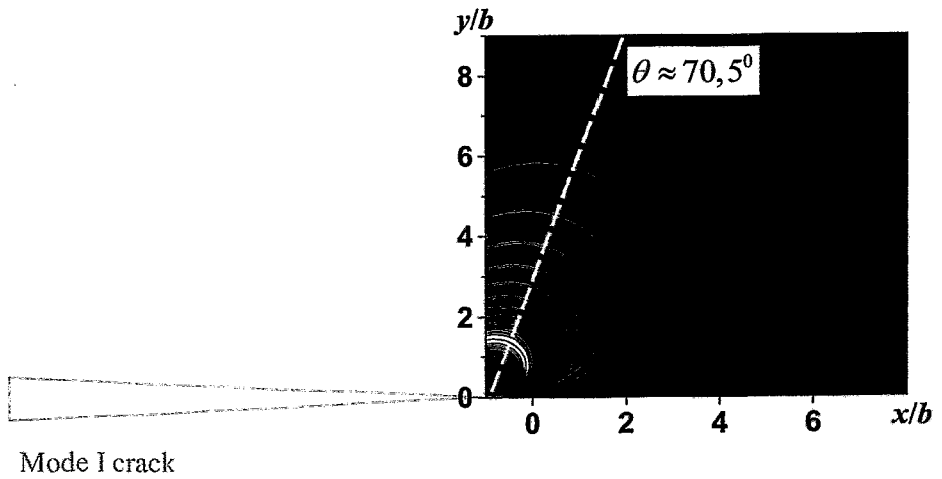


Figure 5: Shear stress  $\sigma_{r\theta}^c(r, \theta)$  contour plot. Direction of the maximum stress makes angle  $\theta \approx 70.5^\circ$  with  $x$  axis and is indicated by dash line.

dislocation position is given by the following relation [9]:

$$\sigma_{r\theta}^m(r, \theta) = \frac{L_I}{\sqrt{\pi r}} \sin \theta \cos \frac{\theta}{2}, \quad (5)$$

where

$$L_I = -\frac{b\mu}{2(1-\nu)\sqrt{\pi r}} \sin \theta \cos \frac{\theta}{2}, \quad (6)$$

where  $\mu$  is shear modulus, and  $\nu$  is the Poisson ratio.

Dependence of  $\sigma_{r\theta}^m(r, \theta)$  is shown in Fig.6 and appropriate contour plot is given in Fig.7. The dependence is more sharp than  $\sigma_{r\theta}^c(r, \theta)$ , and  $\sigma_{r\theta}^m(r, \theta)$  quickly decreases with increase of the distance  $r$  from the crack tip.

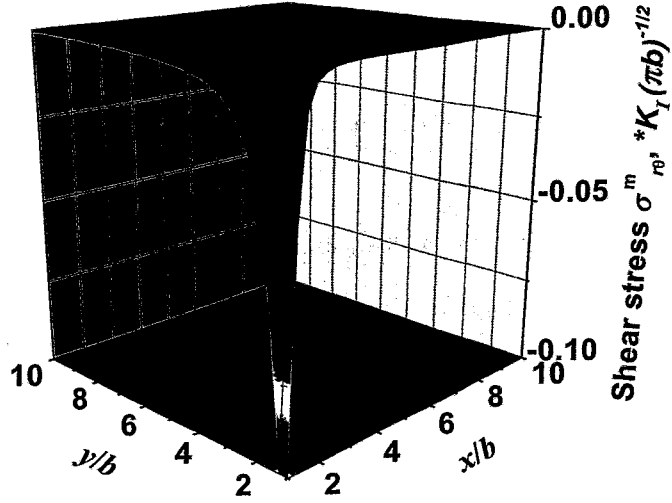


Figure 6: Mirror stress  $\sigma_{r\theta}^m(r, \theta)$ . The value of  $\sigma_{r\theta}^m(r, \theta)$  is normalized by factor  $K_I/\sqrt{\pi b}$ .

The energy of the edge segment of dislocation loop in the actual stress field in the crack vicinity is equal to:

$$W_\sigma = bL \int_{\xi_{pm}b}^a (\sigma_{r\theta}^c + \sigma_{r\theta}^m) dr = \frac{\mu b^3 L}{2\pi b} \left[ \frac{4\pi K_I}{\mu\sqrt{\pi b}} \left( \sqrt{\frac{a}{b}} - \sqrt{\xi_{pm}} \right) - \frac{\sin \theta \cos \frac{\theta}{2}}{1-\nu} \ln \frac{a}{e(\xi_{pm}b)} \right], \quad (7)$$

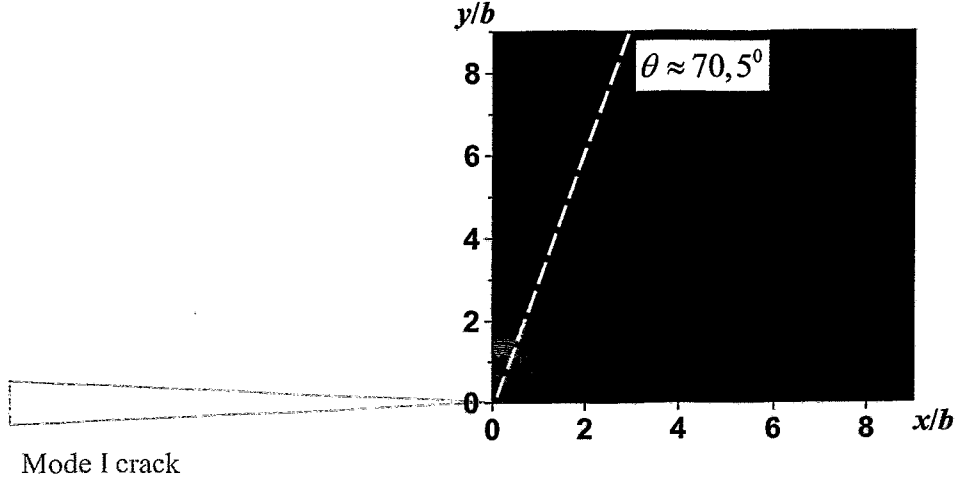


Figure 7: Mirror stress contour plot. The most preferable direction of the loop nucleation is indicated by dash line.

where  $\xi_{pn}b$  is the dimension of dislocation core,  $e$  is the base of natural logarithm.

The energy of ledge formation is given by the following relation:

$$W_l = bL\gamma, \quad (8)$$

where  $\gamma$  is the specific energy of free surface formation.

The energy of formation of screw segments of dislocation loop is equal to [10]

$$W_f = \frac{\mu b^3 a}{4\pi b} \ln \frac{a}{e(\xi_{pn}b)}. \quad (9)$$

And the energy of interaction of screw segments of the dislocation loop is given by [10, 11]

$$W_i = \frac{\mu b^3 a}{4\pi b} \left\{ \ln \frac{a + \sqrt{L^2 + a^2}}{L} - \frac{2 - \nu}{1 - \nu} \left[ \sqrt{1 + \frac{L^2}{a^2}} - \frac{L}{a} \right] \right\}. \quad (10)$$

## 4 Nucleation energy barrier

The energy of formation of rectangular dislocation loop (3) vs its height ( $a$ ) and width ( $L$ ) for stress intensity factor  $K_I = 0.4K_{Ic}$  is shown in Figure 8. Linear

dimensions of dislocation loop are normalized by length of Buerger's vector  $b$ . The energy of dislocation loop is represented in units of  $\mu b^3 / 2\pi$ .

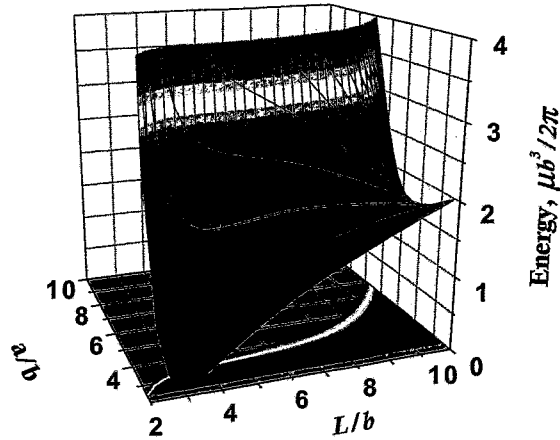


Figure 8: Formation energy of rectangular dislocation loop at the crack tip *vs* dislocation loop height  $a$  and width  $L$ . Stress intensity factor  $K_I = 0.4K_{gc}$ . The value of nucleation energy barrier is too high for nucleation through thermal fluctuations.

Substitution of typical values of iron into Eq.3 results in the nucleation energy barrier (the energy corresponding to the saddle point of the surface) of the order of several  $eV$ . So, there is no nucleation of dislocation through thermal fluctuations at this level of stress concentration at the crack tip.

Small increase of stress intensity factor up to  $K_I = 0.42K_{gc}$  leads to significant decrease of the nucleation barrier down to the value of approximately  $0.8 eV$ . Appropriate dependence of the total energy is shown in Figure 9.

Further increase of actual stress intensity factor results in disappearance of the nucleation barrier, see Fig. 10, and therefore spontaneous nucleation of dislocation loops at the crack tip occurs.

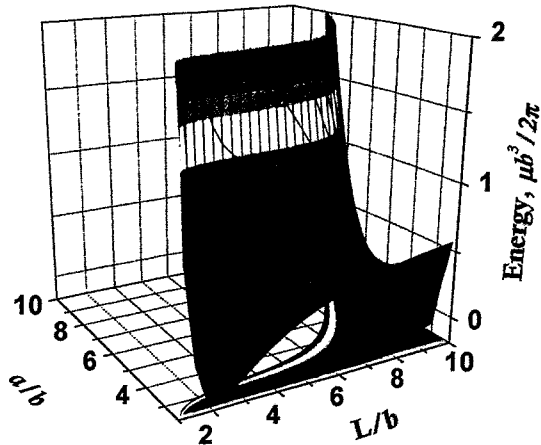


Figure 9: Formation energy of rectangular dislocation loop at the crack tip (nucleation through thermal fluctuations). Stress intensity factor  $K_I = 0.42K_{gc}$ .

## 5 Discussion

Investigation of dislocation loop nucleation at the mode II crack tip within Peierls concept proposed by J.P.Rice [5] gives stress intensity factor of  $K_{II} = 0.9K_{gc}$  leading to spontaneous dislocation loop nucleation. Our consideration results in approximately two times less value:  $K_I \approx 0.43K_{gc}$ . With the exception of loading geometry the main distinction of the suggested approach in comparison with that of J.P.Rice is in the different shape of emitted loop. 3D model [5] proposed by J.P.Rice suggests circular shape of the loop with one describing parameter (dislocation loop radius  $R$ ) whereas in the current model rectangular dislocation loop with 'width'  $a$  and 'length'  $L$  is considered. It is obvious, that this particular geometry of the problem allows to generate more preferable loop configuration from the energetic point of view.

According to the obtained analytical results spontaneous nucleation of dislocation at the crack tip occurs provided stress intensity factor achieves value  $K_I \gtrsim 0.43K_{gc}$ . It is significantly less than the critical stress intensity factor  $K_{gc}$ . So, one

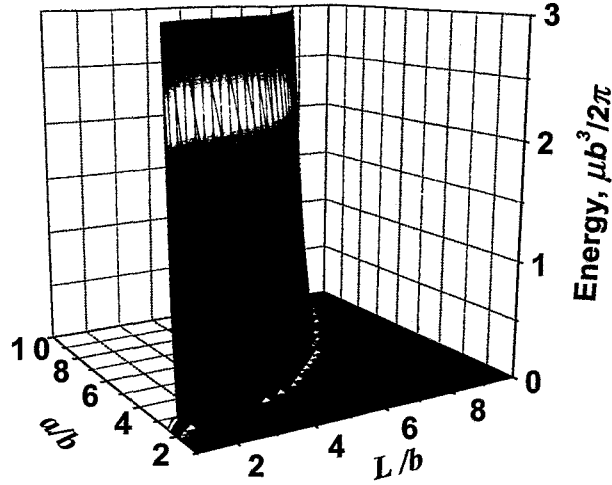


Figure 10: Formation energy of rectangular dislocation loop at the crack tip (spontaneous nucleation). Stress intensity factor  $K_I = 0.46K_{gc}$ .

can conclude that crack propagation is always accompanied by ejection of dislocation (at least in iron), *i.e.* quasi-brittle fracture occurs. This preliminary conclusion is consistent with experiments that demonstrate cold-working of crack surfaces at any temperatures. Experimentally measured values of the specific surface energy are approximately two orders of magnitude higher in comparison with that of the ideal surface:  $\gamma \simeq 10^2 \gamma_{ideal}$ .

Nucleation energy barrier demonstrates extremely sharp dependence on the stress intensity factor, see Fig. 11. 10 per cent decrease of the actual stress intensity factor  $K_I \approx 0.43K_{gc}$  in the vicinity of crack tip increases nucleation energy barrier from near zero values up to several eV and lock dislocation loop nucleation. Such behaviour entails very high sensitivity of the dislocation nucleation (and therefore fracture toughness of material) on the structural surrounding at the crack tip. Any structural inhomogeneities like precipitates, voids, gas bubbles, grain boundaries, forest dislocations and their pile-ups affect stress distribution at the crack tip and influence on the nucleation of dislocation loops.

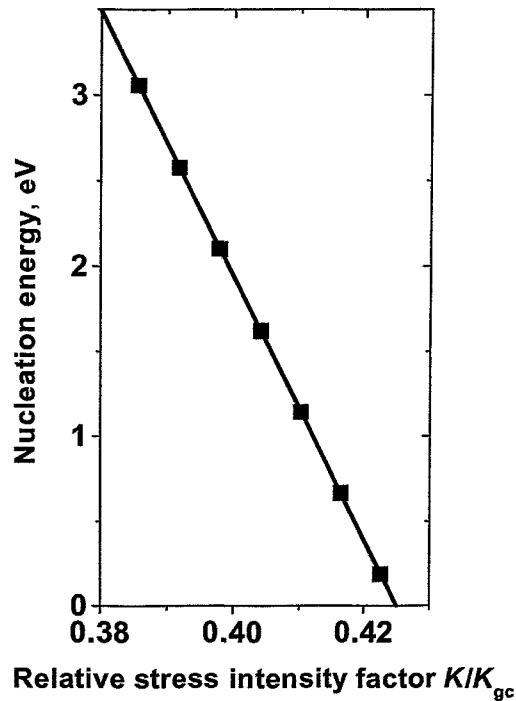


Figure 11: Nucleation energy barrier vs stress intensity factor.

## 6 Further considerations

Structural inhomogeneities can affect dislocation loop nucleation at the crack tip in two ways. The first one is the direct influence on the stress distribution at the crack tip region. However, another indirect effect also occurs. All structural imperfections decelerate or lock moving dislocations. Forming pile-ups modify stress field in the crack vicinity and prohibit further ejection of dislocation loops. Effect of stress intensity factors on the nucleation of dislocation loops and dynamic screening of crack tip by moving dislocations is the problems for further consideration in the framework of the general problem of ductile to brittle transition of solids:

- Nucleation of dislocation loop at the crack tip in the presence of forest dislo-



cations in surrounding.

- Effect of finite dislocation velocity.
- Effect of weak obstacles.
- Effect of strong obstacles.
- Reasons for linear dependence of nucleation energy barrier on stress intensity factor.

## 7 Conclusions

- Spontaneous nucleation of dislocation loops in metals is possible at stress intensity factors of the order of  $0.4K_{gc}$ . Ejection of at least one dislocation is possible in accordance with experimental observations.
- The shape of the loop is of fundamental importance for nucleation.
- Nucleation energy barrier exhibits strong dependence on the stress concentration at the crack tip region.
- Nucleation of dislocation loop at the crack tip is very sensitive to structural environment (dislocation density, precipitates, *etc.*)

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