

## DISLOCATION-DIFFUSION MECHANISM OF FATIGUE CRACK FORMATION

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## INTRODUCTION

When a metal is loaded, dislocations move from the interior towards the surface. The causes and consequences of this phenomenon are varied and numerous [1 - 3]: (a) in a field of external loads, the dislocations move with certain velocity, depending on material structure, stress, temperature, etc.; (b) near to the surface there are forces which attract dislocations; (c) oxide-coatings may cause the process of dislocation escape to be more difficult or easier; (d) dislocations (and point defects) escaping to the surface develop a surface relief, the roughness of which increases with increasing stress amplitude and with increasing number of cycles applied; (e) the surface relief leads to initiation of microcracks.

## CHANGES IN DISLOCATION DENSITY DESCRIBED BY A DIFFUSION EQUATION

Dislocation motion is governed by many complicated processes. These processes involve the displacement, meeting, multiplication, blocking, escaping and annihilation of dislocations themselves, as well as dislocation and point defect/point defect interactions. The exact mathematical description of such processes is not possible, however, the description of average results of displacement of various objects, including dislocations [8], is possible by use of equations of diffusion. If we introduce into the diffusion equations additional terms expressing the effects of so called positive and negative sources, we can describe the additional density changes, caused by multiplication and/or annihilation processes.

This author obtained a system of such equations for the densities of moving and immobile dislocations [4, 5] and for the concentration of point defects and their colonies [6]. The average total density of dislocations,  $\rho$ , is described by the equation

$$\frac{\partial \rho}{\partial N} = D_D \Delta \rho + B \rho - C \rho^2 \quad (1)$$

where  $\Delta$  is the Laplace operator and  $D_D$ ,  $B$  and  $C$  are factors of dislocation diffusion, multiplication and annihilation, respectively. In a specimen with circular cross-section the initial condition is  $\rho(\bar{r}, 0) = \rho_0(\bar{r})$  and boundary condition  $\rho(R, N) = 0$ , where  $\bar{r} = r/R$ , and  $R$  denotes the radius of specimen cross-section. An analysis of the approximate analytical solution of equation (1) makes it possible to evaluate  $\rho(\bar{r}, N)$  in the fatigue process, the role of a surface layer, etc. [5].

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Taking into account the influence of a potential field,  $U(r, \rho)$ , we have the equation

$$\frac{\partial \rho}{\partial N} = D_D \nabla (\nabla \rho + \frac{\rho \nabla U}{kT}) + B\rho - C\rho^2. \quad (2)$$

Considering a flux of dislocations,  $J$ , not influenced by  $\nabla \rho$ , we have

$$J = D_D \rho \frac{\nabla U}{kT} = D_D \rho \frac{\sigma b \ell}{kT} \quad (3)$$

where  $\ell$  is the length of the dislocation segments between pinning points.

Changes in the dislocation density,  $\rho(N)$ , in the whole volume of thicker specimens are controlled by the processes of dislocation multiplication and annihilation, while appreciable changes in  $\rho(\vec{r})$ , caused by diffusion, occur in the thin surface layer only. Thus, we use equation (1) to describe  $\rho(\vec{r}, N)$  in the specimen core and equation (3) or equation (9) to evaluate the dislocation drift from the surface layer to the surface. This approach seems to be the one possible way to treat the problem to a first approximation, since equation (2) can not be solved analytically.

Motion of a dislocation may be treated as a thermally-activated process of kink diffusion [13, 14]. The kink diffusion coefficient,  $D_k$ , is given by a formula:

$$D_k = b^2 \nu \exp\left(-\frac{Q_k}{kT}\right) \quad (4)$$

where  $\nu$  denotes the frequency of atom vibration ( $\nu = 10^{12}-10^{13}$  Hz) and  $Q_k$  is the activation energy for kink motion.

We can get a similar equation for  $D_D$ :

$$D_D = b^2 \nu_D \exp\left(-\frac{Q_D}{kT}\right) \quad (5)$$

where  $\nu_D$  denotes the vibration frequency of dislocation segments ( $\nu_D = 10^6-10^{11}$  Hz [12]) and  $Q_D$  is the activation energy for dislocation motion. If the dislocation moves in a potential field, dislocation jump frequency is equal to:

$$\nu_D \exp\left(-\frac{Q_D + W_D}{kT}\right) \quad (6)$$

Here  $W_D = \sigma H$  denotes the work done by the sum of external and internal stresses,  $\sigma = \sigma_{ex} + \sigma_{in}$ , and  $H = b\ell b'$  is an "activation volume" where  $b'$  is the distance that the dislocation moves in vibrations. As the dislocation jump frequency in the direction favoured by the external stress is greater than in the reverse direction there is a drift velocity,  $v$ , for the affected dislocations given by:

$$v = b \nu_D \exp\left(-\frac{Q_D}{kT}\right) \sinh\left(-\frac{\sigma b \ell b'}{kT}\right) = D_D \sinh\left(-\frac{\sigma b \ell b'}{kT}\right) \frac{1}{b} \quad (7)$$

which for small stresses,  $\sigma \ll kT/H$ , reduces to

$$v = D_D \frac{\sigma b \ell b'}{kT}. \quad (8)$$

Dislocation flux,  $J$ , is then:

$$J = \rho v = \rho D_D \sinh\left(-\frac{\partial H}{kT}\right) \frac{1}{b} = \rho D_D \frac{\sigma b \ell b'}{kT}. \quad (9)$$

In cyclic stress the sign of  $J$  varies periodically. If a given micro-region of a material is loaded symmetrically, the difference between the dislocation flux in the positive and negative directions is nil. If stress conditions are not symmetric, a net flux occurs. Such a situation always exists in the surface layer, where - even if external loads are symmetric - local forces acting upon dislocations are not symmetric because of the influence of the surface.

Numerical solution of equation (1) made possible an estimation of:

(a) approximate values of  $B$ ,  $C$  and  $D_D$  for various materials; (b) mutual relations between the values of these factors; (c) rates of dislocation density increase till saturation; (d) the influence of various factors (e.g., initial dislocation density, diameter of specimen) on the rate of increase of dislocation density, etc. [8].

The value of the dislocation multiplication factor,  $B$ , strongly influences the rate of increase in dislocation density,  $\rho(N)$ . A comparison of computed results with available experimental data shows that the factor  $B$  has the following values: in copper single crystals  $B = 1 - 0.5$ ; in copper and aluminum polycrystals  $B = 10^{-1}-10^{-2}$ ; in aluminum alloys  $B = 10^{-2}-10^{-4}$ ; in steels and steel-like materials  $B = 10^{-4}-10^{-6}$ .

The value of the dislocation diffusion coefficient,  $D_D$ , is estimated from equation (1) and equation (5). An analysis of equation (1) made by assuming  $D_D$  to be constant shows that dislocation density can increase if  $D_D$  is not too large in comparison with  $B$ , namely if:

$$B > D_D \lambda_1; \quad \lambda_1 = \frac{5.78}{R^2}. \quad (10)$$

No increase in dislocation density over the whole cross-section occurs if  $B/D_D \lambda_1 \approx 1$ . From this condition, necessary to stop the process of dislocation density growth in whisker-like simple crystals ( $R = 2.5 \mu\text{m}$ ), we obtain  $D_D = 10^{-12} B$  and, as in such a material  $B = 1$ ,  $D_D = 10^{-12}$ . Using this value of  $D_D$  we have  $B/D_D \lambda_1 = 10^6-10^{10}$  for thicker specimens ( $R = 0.001 - 0.1 \text{ m}$ ). The surface layer of such specimens is very thin, of the order of a micrometer. It is only in this layer that dislocation diffusion influences the average dislocation density  $\rho(\vec{r}, N)$  and in the remaining part of the cross-section the distribution of  $\rho(\vec{r})$  is constant. As in various materials, under similar loading conditions, the  $B/D_D \lambda_1$  relation is almost the same [8], the thickness of the surface layer does not depend on material.

The value of  $D_D = 10^{-12}$  is obtained in the presence of an ultimate stress  $\sigma = \sigma_{ex} + \sigma_{in}$ . In such conditions the value of  $Q_D - W_D$  in equation (6) seems to be reduced to zero and then from equations (5) and (6) with  $b = 2.5 \times 10^{-10} \text{ m}$  we obtain  $\nu_D = 1.6 \times 10^7 \text{ Hz}$ . This result is in good agreement with published

data [12]. As in metals  $Q_D = 1.6 \times 10^{-19}$  J, we have finally at room temperature  $D_D = 10^{-28}$ .

If  $B/D_D \lambda_1 \gg 1$ , then the maximal dislocation density (density of the saturation state),  $\rho_{lim}$ , does not depend on the value of  $D_D$ . Our calculations show that in such a case  $\rho_{lim}$  can be expressed by the simple formula

$$\rho_{lim} = \frac{B}{C} \quad (11)$$

It is known from many experiments that  $\rho_{lim} = 10^{13} - 10^{17} m^{-2}$ . It means that  $C = (10^{-17} - 10^{-13})B$ , and finally  $C = 10^{-24} - 10^{-13}$ .

As in a given material  $\rho_{lim}$  depends on stress amplitude, the B/C ratio increases with increasing applied stress. On the other hand, this ratio is almost the same in various materials, as the dislocation density under similar loading conditions is not very dependent on material.

The processes of diffusion or thermal conduction are such that after a sufficiently long time they do not depend on the initial conditions. In other words, they depend only on the values of factors controlling the given process. In our case these factors are the coefficients B, C,  $D_D$  and  $\lambda_1$ .

The experiments of Feltner and Laird [7] show that the average dislocation density attained after cycling, as well as dislocation distribution (dislocation cell dimensions) in materials of wavy (three dimensional) slip mode do not depend on the initial dislocation density and distribution or on load history. It means that the process of changes in dislocation density has, indeed, a diffusional character and in saturation conditions there ought to be a dynamic equilibrium between the processes of dislocation multiplication, diffusion and annihilation. Thus, in these materials the average dislocation density depends on the actual stress amplitude only and values of the constants B, C and  $D_D$ , independent of external conditions [8].

On the other hand, the dislocation density and distribution in materials of strictly planar (two dimensional) slip mode depends strongly on prior history [7], and this shows that in these materials the factors B, C and  $D_D$  change markedly when influenced by external conditions [8]. Lukáš and Klesnil have shown [10], however, that the extremely high dislocation density in wavy slip mode material produced by grinding, cannot be changed by later cycling. It means also that these materials may be sensitive to load history and in specific conditions the B, C and  $D_D$  factors need not remain constant.

Our numerical calculations of the changes in dislocation saturation density with sudden increase and decrease of stress (strain) amplitude (for example: low, high, low) for materials with stable or unstable B, C and  $D_D$  factors give results which are in full agreement with experimental data on the effects of changes in amplitude and/or temperature on the saturation density in copper and Cu + 7.5% Al-alloy, obtained by Feltner et al [7] and by Polák [9].

## RATE OF FATIGUE CRACK FORMATION

Making use of the mechanism of dislocation diffusion described above it is possible to estimate the flux of dislocations escaping toward a free surface. It may be expressed by equation (3) or (9); it is especially high in the surface layer, as load asymmetry is greater there than elsewhere and the value of  $\ell$  is high too (as the saturation density is never reached). Let us consider a microcrack lying in the plane perpendicular to the specimen axis. The formation of an intrusion and such a microcrack of an area,  $A_C$ , ( $A_C \max = A - A_F$ ), is possible if in a specific microregion of the surface layer a number of dislocations, S, of known length, L, and Burgers vector, b, escapes to the surface. Thus:

$$A_C = S L b \quad (12)$$

As the number of dislocations (of known L and b) escaping to the surface in unit time is J, we can express the number of cycles, N, during which the crack area develops to the size of  $A_C$ , dividing equation (12) by equation (3):

$$N = \frac{A_C F kT}{\sigma \rho D_D b \ell} \quad (13)$$

where F denotes frequency of cycling. As  $A_C \max = A - A_F$ , we have

$$N_f = \frac{(A - A_F) F kT}{\sigma \rho D_D b \ell} \quad (14)$$

The rate of crack area development is given by the formula<sup>1</sup>

$$\frac{dA_C}{dN} = \frac{\sigma \rho}{F kT} D_D b \ell \quad (15)$$

Influence of Various Parameters Upon the  $dA_C/dN$  Rate

As we see, the mechanism of fatigue crack formation, i.e., of its initiation and growth, appears to be invariable over the whole range of N,  $0 \leq N \leq N_f$ , however it can be more or less intensive, depending on actual values of factors in the above equations. The value of the flux is very low in the initial stage of cycling, but it increases rapidly with increasing N and is extremely high at the crack tip, because the dislocation density in the vicinity of the crack tip is especially high [1, 2, 11], and  $\sigma$  is extremely high there, also. Thus, generally  $dA_C/dN$  as a function of N is not constant, but it may be almost constant in separate  $\Delta N$  ranges. Such a state is especially possible when the saturation density is already achieved

1. It seems almost certain that point defects contribute to the formation of a fatigue crack, too, and the number of point defects escaping to the surface ought to be some function of the number of escaping dislocations. In order to study this problem it is necessary to solve a system of equations describing point defect concentrations which is connected with the system of equations of dislocation densities. We do not deal with that problem in the present paper.

( $\sigma$ ,  $\rho$ ,  $\ell$  are constant), but there is not crack formed yet and then there are no reasons for the increase of these parameters. In this stage, well known as Stage II,  $dA_c/dN = \text{const.}$  As we said, in all other stages there cannot be a constant  $dA_c/dN$  value.

These conclusions show good agreement with the data in the literature. Thus, it follows from [11] that fatigue crack propagation rate increases with increasing maximum excess dislocation density,  $\delta\rho$ , at the crack tip, and  $\delta\rho$  increases with increasing crack size.

On the other hand, it follows from the above considerations that  $dA_c/dN$  ought to depend on the material (differing dislocation mobility), although  $\rho$  is almost independent of the material.

The values of  $D_D$  and  $J$  depend on many parameters, both natural (e.g., material type) and specifically created (e.g., various treatments). Thus, equations (3) and (5) show that  $J$  strongly depends on  $\sigma$  and  $T$ . The increase both of  $\sigma$  and of  $T$  leads to rapid increase of  $J$ ; in such a case the rate of crack growth increases and  $N_f$  decreases.

The environment and the surface oxide both have a large effect on the values of flux  $J$  and on the rate of fatigue crack development. As the moving dislocations approach the surface, they interact with the oxide coating. Depending on oxide coating thickness and on water vapor presence in the environment, the dislocations may or may not escape to the surface [1]; the value of  $J$  is then higher or less, respectively.

The chemical-thermal treatment causes the introduction of great numbers of new obstacles into the surface layer. Thus, the value of  $\ell$  in equation (3), the value of  $J$  and crack growth rate (equation (15)) decreases and  $N_f$  - according to equation (14) - increases.

Cold-working of the surface layer increases the number of new dislocations. Thus, the value of  $\ell$  in equation (3) or (15) decreases and, as a consequence,  $dA_c/dN$  decreases and  $N_f$  increases.

However, if stress amplitude is sufficiently high, both chemical-thermal and cold-working treatments cannot prolong the fatigue life to infinity, because the value of  $J$  cannot be diminished to zero [8]. Even if the dislocation density produced by cold-working in the surface layer is extremely high (and  $\ell$  is extremely small), the dislocations nearest to the surface are able to leave the crystal. They open up a way toward the surface for distant dislocations which can now escape from the interior, too, and the process of dislocation diffusion develops, although more slowly than in virgin material. Invention of such a treatment which would provide more stable diminution of the dislocation flux toward the surface would be very desirable.

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