

Statistical Model of Submicrocrack Evolution under Cyclic Loading

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Abstract To describe the damage evolution under high- and gigacyclic fatigue we develop a generalization of statistical model of microcrack evolution. The statistical model combined with a stochastic description of damage accumulation process allows us to describe the interaction of microplasticity and damage (submicrocracks) under cyclic deformation and propose a model of fatigue crack initiation. Considering a fatigue crack initiation as a blow-up regime of damage accumulation we propose a method for prediction of SN-curves of materials. The SN-curve has dual form caused by shift the location of crack initiation from surface to the bulk of specimen.

Keywords statistical model of defects, gigacyclic fatigue, dual Woller curve

1. Introduction

It is now well known that real metals have complex structure, which is a hierarchy of different levels. Under deformation process the structural evolution observed at all scale levels and leads to irreversible deformation and destruction. The most interesting situation observed under gigacyclic fatigue when the stress amplitude is less than the yield stress of materials and fracture emergence under macroscopic “pure” elastic conditions. One of most critical issue of the gigacyclic fatigue is the location of fatigue crack initiation. The decreasing of stress amplitude leads to the shift of crack initiation from specimen surface to the bulk.

To develop a model of defect evolution under small stress amplitude we have to choice of the basic physical level of description of the material microstructure and describe the geometry of the elementary defects. Analysis of the experimental results of the study of structural levels of plastic deformation and fracture [1,2] and resent experimental investigation of damage evolution of fine grain metals can hypothesize that scale level with the size of submicrocracks 0.1-0.3 mm plays a key role in this process [3]. The failure process includes both the nucleation of new microcracks and their development. The contribution of these processes in the failure varies depending on the structure of the material conditions of its loading.

The defect kinetics is different near specimen surface and in the bulk. The rate of microcracks nucleus initiation in the surface layers of one to three orders of magnitude higher than in the bulk material. It is also well known that for high concentration the defect ensemble exhibits both collective and nonlocal effects.

One of the possible descriptions of defect kinetics is the statistical model of defect ensample. This model has to take into account the stochastically properties of defect initiation, their nonlinear integration and link between micropalsticity and damage accumulation.

This work is devoted to the development of such model in the application to cyclic loading of metals. The paper is organized as follow. The first part is devoted to the statistical description of submicrocrack ensemble. The statistical description was developed based on the mean field approximation of defect interaction and allows us to investigate the effect of initial nucleus concentration of defect evolution process and determine the equilibrium state of materials with

defects.

The second part of the paper devoted to the thermodynamic description of deformation process. Based on the results of solution of the statistical problem we introduce a new thermodynamic variable and derive the constitutive equation for metals with submicrocracks.

In the last part the proposed constitutive equation applied for the description of defect kinetics near specimen surface and in the bulk. The model allows us to describe the shift of crack initiation location from the specimen surface to the bulk and numerically obtain dual S-N curve for 2023 T3 aluminum alloys.

The discusses about physics of the investigated process and proposition for father experimental verification of the model presented in conclusion.

2. Statistical description of damage accumulation in metals

The data obtained from systematic studies of defects evolution, carried out at Physical technical institute named after A.F. Ioffe RAS shows that the volume defects (submicrocracks with characteristic size about 0.1 mkm) play the important role in deformation process [3]. These defects emerge at the early stage of deformation and effect on the microplasticity and failure processes. The same situation could be observed under cyclic loading. The best materials for the experimental proofing of this hypothesis are the fine grain metals which contained the high concentration of volumes defects (micropores) after manufacturing procedures (equals channel pressing).

The value, geometrically representing the real microcracks with allowance made for a variety of their shapes, sizes and arbitrary orientations as well as or the crack initiated material loosening, can be introduced in terms of the dislocation theory [4].

The dislocation loop D , bounding the surface S , where the displacement vector undergoes a finite increment equal the Burgers vector b , is characterized by the tensor of the dislocation moment $S v_i b_k$. The sum of N dislocation loops, which is equivalent to a microcrack, introduces the tensor of dislocation moment of a microcrack:

$$s_{ik} = \sum_{l=1}^N S^l v_i^l b_k^l, \quad (1)$$

where \vec{v}^l is the vector of a normal to the surface S of the 1-th loop. Small sizes and multiple character of microcrack nucleation as well as size and orientation distributions of microcracks permit averaging of their parameters over elementary volume to obtain the macroscopic tensor

$$p_{ik} = n \langle s_{ik} \rangle, \quad (2)$$

where n is a concentration of microcracks.

A solution of equation (2) was presented in [4]. The solution depends on structural parameter δ and defect concentration n . Figure 1 presents two solutions of the equation (2) for $\delta = 1.1$ and different values of initial defect concentration (curves 1,2).

To describe a real deformation process which characterized by the growth of defect concentration we propose that the representative material volume V_r contains $n_0 V_r$ defects

nucleuses. Following [5] we propose that the applied stress activates the defects and this process can be described as a stochastic Poisson point process with intensity function $n(\Sigma)$.

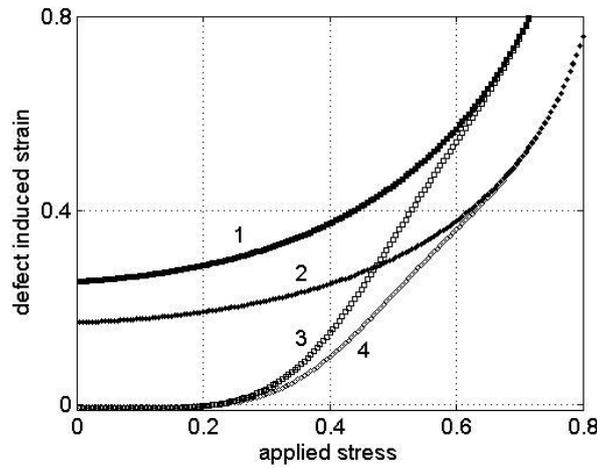


Figure 1. Equilibrium defect induced strain versus applied stress for different values of initial defect concentration (curves 1,2) and the mean values of defect induced strain during deformation process (curves 3,4).

Intensity function describes both the growth of active defects (which contribute to the defect induced strain) and growth defect nucleuses. Following the experimental data [5] about evolution of microcrack concentration we can assume the following approximation for intensity function

$$n(\Sigma) = \frac{\alpha_0}{2} \left(1 + \text{Erf} \left(\frac{\Sigma - \Sigma_0}{\Sigma_1} \right) \right) (n_0 + \alpha_1 \Sigma), \quad (3)$$

where $\alpha_0, \alpha_1, \Sigma_0, \Sigma_1$ - material constants.

The probability of find N active defects in representative material volume is

$$P(N) = \frac{n(\Sigma)^N \text{Exp}(-n(\Sigma))}{N!}.$$

The stochastic consideration of defect evolution process change the self-consistency equation for defect induced deformation. The solution of equation (2,3) is presented in figure 1 (curves 3,4). For small stress values we observe a pure elasticity which passes to the plastic deformation with different intensity. The intensity of plastic deformation and damage accumulation depends on the initial concentration of defect nucleuses.

3. Thermodynamics of metals with defects

A thermomechanical process of plastic deformation obeys the momentum balance equation and the first and second laws of thermodynamics. In the case of small deformation, these equations involve the following thermodynamic quantities: volumetric mass ρ , specific internal energy e , strain and stress tensors ε_{ik} and σ_{ik} , heat supply r , heat flux vector \vec{q} , specific Helmholtz free

energy F , and specific entropy η . The energy balance and the entropy can be written as

$$\dot{e} \equiv (\dot{F} + \eta\dot{T} + \dot{\eta}T) = \frac{1}{\rho} \sigma_{ik} : \dot{\varepsilon}_{ik} + r - \bar{\nabla} \cdot \bar{q}, \quad (4)$$

$$\dot{\eta} - \bar{\nabla} \cdot \left(\frac{\bar{q}}{T} \right) - r' \geq 0,$$

where $\bar{\nabla} = \left(\frac{\partial}{\partial x_1}, \frac{\partial}{\partial x_2}, \frac{\partial}{\partial x_3} \right)$, the superposed dot stands for the material time derivative.

We assume the following kinematical relationship for the material under study

$$\tilde{\varepsilon} = \tilde{\varepsilon}^e + \tilde{\varepsilon}^p + \tilde{p} + \tilde{\beta}(T - T'), \quad (5)$$

where ε_{ik}^e is the elastic strain tensor, $\tilde{\varepsilon}^p$ is the plastic strain tensor (related to the defect motion),

$\tilde{\beta}$ is the thermal expansion coefficient tensor, and T' is the reference temperature.

To introduce the list of independent variables for the free energy $F(\tilde{\varepsilon}^e, T, \tilde{p})$ the equations (4) give

$$-\bar{q} \cdot \frac{\bar{\nabla} T}{T} - F_{\tilde{p}} : \dot{\tilde{p}} + \frac{1}{\rho} \tilde{\sigma} : (\dot{\tilde{\varepsilon}}^p + \dot{\tilde{p}}) \geq 0, \quad (6)$$

$$c\dot{T} = \bar{\nabla} \bar{q} + r + Q^e + Q^p, \quad (7)$$

where $Q^e = TF_{T\varepsilon^e} : \dot{\tilde{\varepsilon}}^e$ - heat production due to thermoelastic effect;

$Q^p = TF_{T\tilde{p}} : \dot{\tilde{p}} + \frac{1}{\rho} \tilde{\sigma} : \dot{\tilde{\varepsilon}}^p + \left(\frac{1}{\rho} \tilde{\sigma} - F_{\tilde{p}} \right) : \dot{\tilde{p}}$ - represents the inelastic part to the heat production;

$c = -TF_{TT}$ - the specific heat capacity.

To assume the linear links between thermodynamic forces and the thermodynamics fluxes, we obtain the constitutive equations

$$\dot{\tilde{\varepsilon}}^p = l_{\varepsilon^p} F_{\tilde{\varepsilon}^e} + l_{\varepsilon^p p} (F_{\tilde{\varepsilon}^e} - F_{\tilde{p}}), \quad (8)$$

$$\dot{\tilde{p}} = l_p (F_{\tilde{\varepsilon}^e} - F_{\tilde{p}}) + l_{\varepsilon^p p} F_{\tilde{\varepsilon}^e}, \quad (9)$$

where the function F_p follows from the presentation of free energy given by the statistical model of solid with mesodefects.

The specific free energy of the system can be calculated as $F = -n_0 Q \cdot \ln Z$ or

$$F(p) = \frac{I}{2} \lambda p_{ik}^2 - n(\sigma_{ik}) Q \cdot \ln \int \exp \left\{ \left[(\gamma \sigma_{ik} + \lambda p_{ik}) s v_i v_k - \alpha s^2 \right] / Q \right\} ds d^3 \vec{v}. \quad (10)$$

The equation (10) request a determination materials constants at micro level and complex calculation. At macroscopic level the equation (10) can be approximated by corresponding function [4].

To consider the influence of diffusion processes on defect nucleation and evolution and to study the localization effects of the damage accumulation, we have introduced in the expression of the total free energy F the term describing spatially-nonuniform distribution of microcrack density tensor p_{ik}

$$F = \frac{I}{2} K \varepsilon_{ll}^e{}^2 + \mu \left(\varepsilon_{ik}^e - \frac{I}{3} \varepsilon_{ll}^e \delta_{ik} \right)^2 + F(p_{ik}) + \frac{I}{2} \kappa \left(\frac{\partial p_{ik}}{\partial r} \right)^2. \quad (11)$$

In order to evaluate tensor F_p , we have to consider the equation (11) as a functional determined for a representative material volume. For one dimension problem we can write

$$F_p = \frac{\partial F}{\partial p_{ik}} = \frac{\partial F}{\partial p_{ik}} - \frac{\partial}{\partial x_l} \left[\frac{\partial F}{\partial (\partial p_{ik} / \partial x_l)} \right]. \quad (12)$$

The system (8)–(9) in the case of uniaxial cyclic loading ($\sigma_{zz} = \sigma$, $e_{zz} = e$, $p_{zz} = p$) takes the form

$$\dot{\varepsilon}^p = l_{\varepsilon^p} \sigma + l_{\varepsilon^p p} \left(\sigma - \frac{\partial F}{\partial p} - \frac{\partial}{\partial x} D \frac{\partial p}{\partial x} \right), \quad (13)$$

$$\dot{p} = l_p \left(\sigma - \frac{\partial F}{\partial p} - \frac{\partial}{\partial x} D \frac{\partial p}{\partial x} \right) + l_{\varepsilon^p p} \sigma, \quad (14)$$

where D is the coefficient of self-diffusion which is known to obey the Arrhenius law, $D = D_0 \exp(-E_{sd}/T)$ (E_{sd} is the activation energy of self-diffusion) and largely depends on the defect concentration.

4. Defect evolution under cyclic loading

To describe the defect evolution in bulk and near specimen surface let us to reduce the equations (13,14). Under high cyclic and gigacyclic fatigue we can propose a weak interaction of defect accumulation and microplasticity processes ($l_{\varepsilon^p p} \rightarrow 0$) and write the equation (14) in the form

$$\dot{p} = l_p \left(\sigma - \frac{\partial F}{\partial p} - \frac{\partial}{\partial x} D \frac{\partial p}{\partial x} \right). \quad (15)$$

Let us to consider two representative material volumes V_{sur} , V_{bulk} located near specimen surface (part of the surface volume coincides with specimen surface) and into specimen volume, respectively. If we introduce a mean defect induced strain in the considering volume as

$p_m = \frac{1}{V} \int_{v_i} p dv$ we can rewrite the equation (15) as

$$\dot{p}_m + \frac{h l_p}{V} p_m = l_p \left(\sigma - \frac{\partial F}{\partial p} \right)_m, \quad (16)$$

where we used the following boundary conditions

$$D \frac{\partial p}{\partial x} \Big|_{p \in S} = - \frac{h}{V} \int_{v_i} p dv. \quad (17)$$

The equation (16) requests an approximation of function $\sigma - \frac{\partial F}{\partial p}$ which determined the equilibrium states of materials with defects. Taking into account the solution of equations (2) we can propose the following approximation for defect evolution law

$$\dot{p}_m + \frac{h l_p}{V} p_m = l_p \left(\frac{n \sigma^2}{n_0 E^2} (p_m + p_0)^2 - a p_m \right), \quad (18)$$

where n is initial defect concentration, σ is mean stress for the considered volume, p_0, l_p, a are materials constants, h the constant which determine the boundary conditions for considered volumes.

To explain the different mechanisms of crack initiation on specimen surface and in the bulk we have to consider a surface as a physical object with high concentration of incomplete atomic planes and other defect of different nature. As a result we can consider the surface as negative source with infinite capacity which has a great influence on the defect evolution. This influence can be described by the value of constant h in the boundary condition (18).

There are two limiting cases for equation (18). The first case is $h \rightarrow \infty \Rightarrow p \Big|_{p \in S} = 0$. It means the surface is the sink of infinite capacity and this condition can be used for the description of defect evolution close to specimen surface (V_{sur}). The second case is $h \rightarrow 0 \Rightarrow D \frac{\partial p}{\partial x} \Big|_{p \in S} = 0$. The surface is closed for the defect diffusion. This condition can be used for the description of defect evolution in the bulk of specimen (V_{bulk}).

Let us to introduce the following dimensionless variables $\tau = t l_p a$, $n' = n/n_0$, $\Psi = \sigma/(E a)$, $h' = h/(V a)$, taking into account the fact that the initial defect (submicrocrack) concentration near specimen surface is in one or two order high then in the bulk of specimen [6] ($n'_{sur} \gg n'_{bulk}$) and the difference in boundary conditions we can write the equation (18) for V_{sur} , V_{bulk} as

$$\dot{p}_m = n'_{sur} \Psi^2 (p_m + p_0)^2 - (1 + h') p_m, \quad (19)$$

$$\dot{p}_m = n'_{bulk} \Psi^2 (p_m + p_0)^2 - p_m. \quad (20)$$

Under one dimension loading the stress is equal for both representative volumes and can be written as $\Psi = \Psi_0 \cos(\omega\tau)$. The numerical solutions of equations (19,20) are presented in figure 2.

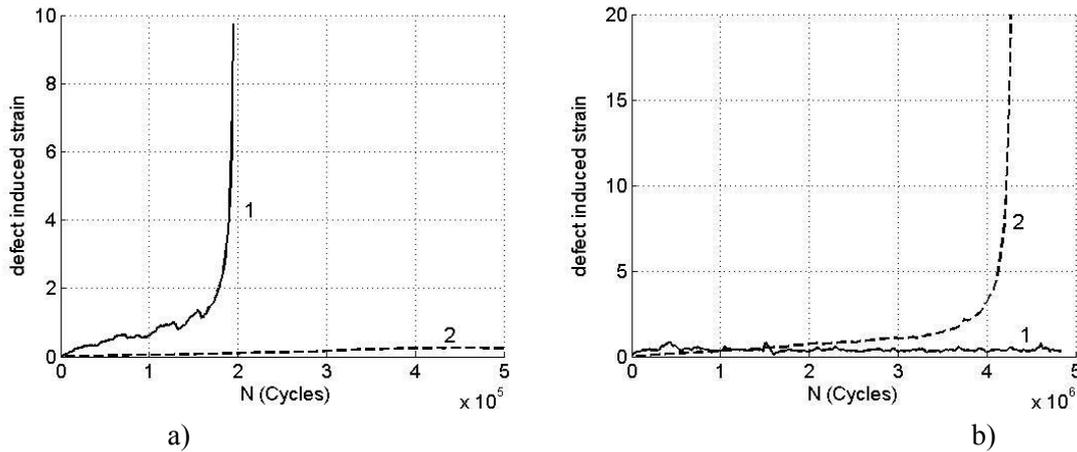


Figure 2. Defect induced strain evolution near specimen surface (1) and in the bulk of specimen (2) for high (a) and small stress amplitudes (b).

At high stress amplitude the initial defect concentration plays the main role and leads to the sharp increasing of defect density near specimen surface (Fig.2a). The blow-up regime of defect accumulation can be considered as damage to fracture transition and can manifest the emergence of macroscopic crack.

At small stress amplitude the defect diffusion and defect annihilation on specimen surface lead to the low defect growth near specimen surface and blow-up regime of defect accumulation can be observed in the bulk of specimen (Fig. 2b).

The calculation of critical times corresponding the blow-up of defect accumulation allows us to determine the S-N of the material which describes the two possibilities of fatigue crack initiation. The materials constants l_p, a, p_0, n_0, h, V were selected to describe the two stage S-N curve experimentally obtained by C. Bathias and P. Paris for 2023-T3 aluminum alloy [6]. The numerical result presented in figure 3.

The S-N curve has dual form. First branch describes the ordinary surface fatigue crack

initiation. The second part has high fracture times and describe the volume fatigue crack initiation.

The equation (19,20) allows as to propose the analytical representation for S-N curve of material. To obtain the upper bound for life time we can take into account the stress amplitude, only.

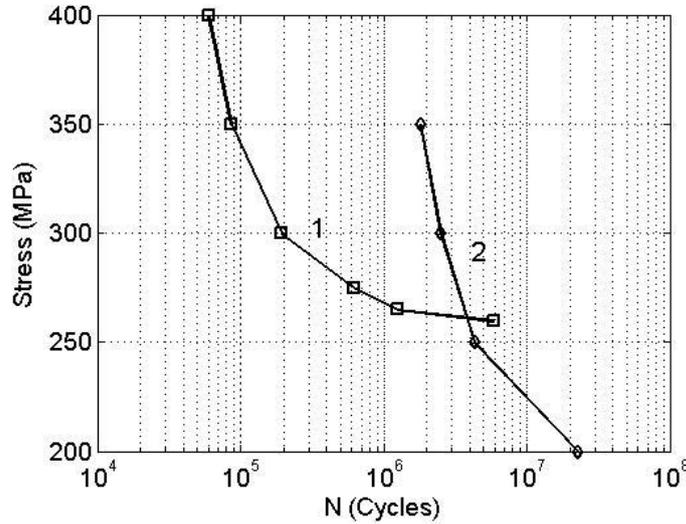


Figure 3. S-N curve for aluminum alloy 2024-T3. Failure caused by surface crack initiation (1), failure caused by under surface crack initiation (2).

In the case of proposed approximation of equilibrium solution of (2) the critical time in the equation (19) can be estimated as follows

$$t_f = \int_0^{\infty} \frac{(1+h')p_m}{n'_{sur} \Psi^b (p_m + p_0)^b} dp. \quad (21)$$

To describe the full S-N curve we have to use several equation (19) with different values h', n' which could be connected with initial heterogeneity of materials. The equation (21) gives the traditional representation of S-N curve in Basquin form

$$\ln(N_f) = a - b \ln(\Psi), \quad (22)$$

where $a = \nu \int_0^{\infty} \frac{(1+h')p_m}{n'_{sur} (p_m + p_0)^b} dp$, ν is loading frequency.

5. Conclusion

Analysis of experimental data devoted to the study of microcracks kinetics in the bulk and surface layer of the metals allowed us to choice of scale level for description of fracture of metallic materials - the level of submicrocracks with the size of 0.1-0.3 microns. To describe the geometry of these defects, as well as their effect on the mechanical material properties were used dislocation theory.

The high initial concentration of these defects in metals and their initiation during initial stage of deformation process allows us to propose the importance of the consideration of their evolution

under cyclic loading. The high concentration of these defect experimentally observed in fine grain metals after equals channel pressing allows us to propose the fine grain metals as model materials for verification of the theoretical predictions obtained in this work.

The small size and high concentration of submicrocracks in metals, the existing of their size and orientation distributions allows us to develop a statistical description of microcrack evolution in metals under cyclic loading and introduce a new thermodynamical variable – defect induced strain. The new variable gives a natural description of thermodynamics of metals with microcracks and allows one to describe the interaction of plasticity and failure processes.

The combination of statistical description of microcrack ensemble with stochastic consideration of defect initiation process allows us to describe the effect of initial nucleus concentration of the deformation process. This model coupled with a description of nonlocal effect in the defect ensemble gives us a key parameter for the description of defect kinetics in the bulk and near specimen surface under cyclic loading.

Based on the developed model the new equation for defect kinetics in the bulk and near specimen surface have been proposed. The surface was considered as a physical object with high concentration of incomplete atomic planes and other defect of different nature. It allows us to explain the difference in the defect kinetics far and close to specimen surface and describe the damage to fracture transition both in the bulk and near specimen surface.

It was show that the stress amplitude can influence on the location of macro fatigue crack initiation. At small stress amplitude the defect induced strain reaches an equilibrium value near specimen surface due to the defect diffusion and annihilation processes. It can be considered as an infinite fatigue life but in this case there is possibility of blow-up regime of defect kinetics in the bulk of specimen. It leads to the shift of location of crack initiation from the surface to the bulk of specimen.

These two modes of crack initiation leads to dual form of S-N curve of materials. The calculated S-N curve has a good quantitative agreement with experimental data obtained by C. Bathias and P. Paris for 2023-T3 aluminum alloy [6]. Each part of the dual S-N curve has the traditional Basquin representation. The micromechanical model allows as to propose the link of macroscopic parameters a, b with defect accumulation kinetics and used the experimentally determined S-N curve for the estimation of microscale model variables.

The developed theoretical model describes the important role of specimen surface and its physical state in the process of defect accumulation under cyclic loading. This model proposes a physical mechanism of the shift of crack initiation location from specimen surface to the bulk that experimentally observed under gigacyclic fatigue (cyclic loading with small stress amplitude). It is interesting to note that the best experimental verification of the model could be carried out based on the structural investigation of microcrack accumulation in fine grain metals (materials with high concentration of initial submicrocracks) under gigacyclic fatigue.

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