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# Multilevel modeling of damage accumulation processes in metals

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**Abstract.** To predict the behavior of components and constructions it is necessary to develop the methods and mathematical models which take into account the self-organization of microstructural processes and the strain localization. The damage accumulation processes and the evolution of material properties during deformation are important to take into account. The heterogeneity of the process of damage accumulation is due to the appropriate physical mechanisms at the scale levels, which are lower than the macro-level. The purpose of this work is to develop a mathematical model for analyzing the behavior of polycrystalline materials that allows describing the damage accumulation processes. Fracture is the multistage and multiscale process of the build-up of micro- and mesodefects over the wide range of loading rates. The formation of microcracks by mechanisms is caused by the interactions of the dislocations of different slip systems, barriers, boundaries and the inclusions of the secondary phase. This paper provides the description of some of the most well-known models of crack nucleation and also suggests the structure of a mathematical model based on crystal plasticity and dislocation models of crack nucleation.

## 1. Introduction

The increase of the lifetime of components and constructions is one of the most important problems of mechanics and material science, which has been standing for many decades. In this regard, the development of reliable methods and models for predicting the material behavior up to the point of destruction is required. The one of the most perspective directions to solve this problem is the construction of multilevel models based on crystal elastic-visco-plasticity.

A huge number of scientific publications are devoted to the study of damage accumulation processes. The purpose of this work is to develop a mathematical model to analyze the behavior of polycrystalline materials with the description of the damage accumulation processes and fracture in the wide range of thermomechanical effects. By fracture we mean is the multistage and multiscale process of the build-up of micro- and mesodefects. The structure of the model for describing the destruction of polycrystalline materials without a certain (“imposed” a priori) macrolevel damage mode is considered. Herewith, the diffusion and dislocation processes of the nucleation of micropores and microcracks are necessary to include. Then their number and size increases (damage accumulation). The final stage is the coalescence of microdamages and growth of the macroscopic crack.

## 2. Some dislocation mechanisms of crack nucleation

The dislocation theory of fracture assumes that plastic deformation plays a decisive role and includes the force criterions of crack nucleation and propagation. This area includes the well-known dislocation models of crack nucleation by Zener, Stroh, Cottrell [1]. The following theoretical directions for the construction of such theory can be specified: 1) models based on the concept of the dislocation pile-up in separate slip planes in front of impediments such as the boundaries of twins, inclusions, etc.; 2) models with the occurrence of cracks related with the interaction of the dislocations located in intersecting slip systems; and 3) models which are not based on locks ("barrier-free models").

The purpose of the current stage of our research is the physical analysis of damage accumulation mechanisms in metals and their mathematical description. We intend to use an explicit description for the changes in the internal structure of material defects in the manufacturing and operating processes. The approach based on the introduction of internal variables is used to construct constitutive models. The models of such class allow, firstly, to analyze deformation processes at various scales and, secondly, to take into account microstructure evolution and damage accumulation.

Let us focus on the description of several well-known crack nucleation models. Microcracks nucleation is the collective effect of dislocation interactions, which is related to their reconstruction accompanied by the conversion of the stored energy into the surface energy. The model of a crack nucleation near a flat dislocation pile-up, the mathematical description of which is given by Stroh [2] will be considered in more detail. The idea of this model is based on the physically reasonable assumption about a occurrence of high local stresses due to a hindered shear, the particular case of which is the pile-up of the $n$ same-sign dislocations as shown in figure 1. Herewith the stresses between the two head dislocations of the pile-up are $\sigma \approx n\tau$, where $\tau$ is the stress in the shear plane. The criterion for the formation of a crack is the fulfillment of the condition (1), where $\gamma$ is the surface energy of the material, $G$ is the shear modulus, $\nu$ is the Poisson's ratio, $L$ is the length of the dislocation pile-up which is determined by the relation (2).

$$\tau^2 = \frac{2\pi\gamma G}{8(1-\nu)L} \tag{1}$$

$$L = \frac{Gbn}{\pi(1-\nu)\tau} \tag{2}$$

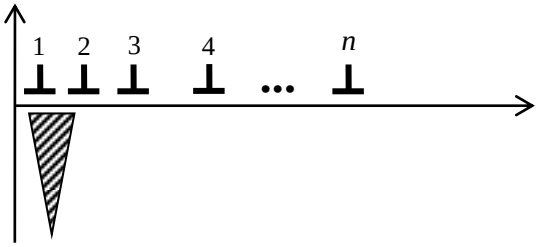


**Figure 1.** The fracture nucleation scheme in the Stroh's model.

Nevertheless, the original Stroh's model of crack nucleation has several disadvantages. Firstly, according to this model, $10^2 \div 10^3$ dislocations are required, but no such pile-ups are experimentally observed. Secondly, the strong obstacle during the inhibition of such pile-up is necessary. Thirdly, during the evaluation of the energy advantage for a crack nucleation, only the relaxation energy of the already existing stresses is taken into account unlike the work of external forces and the energy of dislocation nuclei. Despite this, the model demonstrates the possibility to describe the nucleation of a crack due to the coalescence of dislocations held in front of a barrier. The mentioned above disadvantages can be overcome by modifying the model [3].

Another crack nucleation model is the mechanism proposed by Gilman and Rozhansky [4], which describes the opening of a crack in the slip plane of dislocations, as it, is typical for HCP metals.

According to this mechanism, the crack nucleation in the slip plane occurs due to the curvature of atomic planes in the head of a blocked pile-up. The entire area above the pile-up plane lies in the region of compressive stresses while the rest area lies in the region of the tensile stresses; this stress state is similar to the state of a bent beam. Shear along curved planes should cause normal stresses leading to the separation of slip planes. The formation of a microcrack indicates emerging of new free surfaces and, as a consequence, the relaxation of internal stresses near the head dislocation of pile-up. For HCP metals, the value of the specific surface energy is the smallest in the basis plane and it probably plays a decisive role for the nucleation of cracks in this plane. This mechanism was experimentally observed.

Another well-known scheme of crack nucleation is the Cottrell's model of intersecting dislocation pile-ups which is typical for BCC metals [4]. In this scheme, there are no external barriers against slip and the formation of a barrier is caused by the interaction of the head dislocations of the pile-ups with the formation of a sessile dislocation. The realization of the Cottrell mechanism was not experimentally observed.

The scheme of the annihilation model of crack nucleation can be referred to the barrier-free model with the pile-ups of different signs as shown in figure 2 [3]. It is assumed that if the head dislocations of a pile-ups pass one above the other at the distance of (5÷7)*b* then they annihilate with the formation of vacancies. New vacancies appear by the further inflow and the annihilation of dislocations. The annihilation of a dislocations sequence (*n=5÷10*) forms the sufficient number of vacancies to form a microcrack. In Section 3.3, the criterion of crack nucleation based on the Stroh's model is provided.

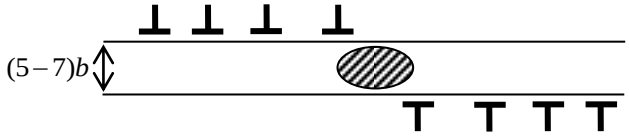


**Figure 2.** Crack nucleation scheme in the case of opposite dislocation pile-ups.

## 3. The mathematical formulation

The crystal plasticity based model allows describing the evolution of the internal structure of a material and the build-up of defects of various natures. The destruction research of components and constructions in the manufacture and operation process without the creation of appropriate mathematical models is impossible. The models must take into account the physical causes of the evolution of the material internal structure and damage accumulation at large deformations.

To describe the physical mechanisms of plastic deformation and fracture it is necessary to study the behavior of the material at a lower than macro scale levels. There are various physical mechanisms of damage accumulation (formation of embryonic cracks, their stabilization and growth the formation of the macroscopic crack) at each scale level. A complete description of deformation and fracture requires an approach that takes into account the multistage processes occurring in the material.

There are macro-, meso-I and mesolevel-II in the structure of the developed model. The macrolevel representative volume element is a polycrystalline aggregate of a large (at least 400) number of crystallites (grains, subgrains), each of which is considered as a mesolevel-I representative volume element. Parts of the grains and subgrains are considered at mesolevel-II. Different types of dislocations densities are evenly distributed within this level. At the macrolevel, the deformation of the material is described using an asymmetric indifferent strain rate [5]. Mesolevel-I is used to describe processes of plastic deformation in terms of shear in the slip systems of a crystallite and hardening. Description of damage accumulation and evolution of dislocation densities are given at the mesolevel-II. In addition, for an adequate description of the damage accumulation process is analyzed the dislocation interaction of various slip planes.

### *3.1 Macrolevel constitutive relations*

The constitutive equation of the macrolevel is the Hooke's law in rate form (3):

$$\dot{\boldsymbol{\sigma}} + \boldsymbol{\sigma}\cdot\boldsymbol{\omega} - \boldsymbol{\omega}\cdot\boldsymbol{\sigma} = \mathbf{\Pi} : (\mathbf{z} - \mathbf{z}^{in}) \tag{3}$$

where $\boldsymbol{\omega} = \dot{\mathbf{o}}\cdot\mathbf{o}^{\mathrm{T}}$ is the spin of the movable coordinate system defined by the quasi-solid motion, $\mathbf{z} = \hat{\nabla}\mathbf{V}^{T} - \boldsymbol{\omega}$ is the asymmetric indifferent strain rate. There are elastic and plastic components of the strain rate: $\mathbf{z} = \mathbf{z}^{e} + \mathbf{z}^{in}$. The plastic component is the sum of the shear strain rates on all slip systems can be written as equation (4).

$$\mathbf{z}^{in} = \sum_{k=1}^{n} \dot{\gamma}^{(k)} \mathbf{b}^{(k)} \mathbf{n}^{(k)} \tag{4}$$

Here, $\dot{\gamma}^{(k)}$ is the shear strain rate on the *k*-th slip system, $\mathbf{b}^{(k)}$ and $\mathbf{n}^{(k)}$ are the slip direction and slip plane normal of the *k*-th slip system, respectively.

*3.2 Mesolevel-I constitutive relations*

The physical mechanisms of deformation are considered in more details at the mesolevel-I. The total dislocation density can be decomposed additively into the densities of mobile and immobile dislocations: $\rho^{(k)} = \rho_{m}^{(k)} + \rho_{im}^{(k)}$. The immobile dislocations are inhibited by the obstacles of various nature (dislocation and non-dislocation barriers, grain boundaries, etc.) while the mobile dislocations are able to slide in the case of critical resolved shear stress. Furthermore, the mobile and immobile dislocation densities can be divided into the positive and the negative parts depending on the location of the extra plane as follows:

$$\rho_{m}^{(k)} = \rho_{m+}^{(k)} + \rho_{m-}^{(k)} \tag{5}$$

$$\rho_{im}^{(k)} = \rho_{im+}^{(k)} + \rho_{im-}^{(k)} \tag{6}$$

In the reference configuration, the initial densities of positive and negative dislocations are supposed to be equal, equation (7).

$$\rho_{m+}^{(k)}\big|_{t=0} = \rho_{m-}^{(k)}\big|_{t=0} = \frac{\rho_{m}^{(k)}}{2}\Big|_{t=0} \tag{7}$$

Shear strain rate is necessary to evaluate the inelastic deformation at the macrolevel in equation (3). It is determined on each slip system by the Orowan equation with considering the separation for positive and negative dislocations density:

$$\dot{\gamma}^{(k)} = \dot{\gamma}_{+}^{(k)} + \dot{\gamma}_{-}^{(k)} = b\rho_{m+}^{(k)} v_{m+}^{(k)} + b\rho_{m-}^{(k)} v_{m-}^{(k)},$$

where *b* is the module of the Burgers vector, $v_{m\pm}^{(k)}$ is the dislocation motion velocity of mobile positive or negative dislocations.

The dislocation motion velocity depends on the temperature of the material under loading, actual and critical resolved shear stress on the slip system. Following [6] the dislocation motion velocity can be written as

$$v_{m\pm}^{(k)} = v_{0}^{(k)} \left( \frac{\tau^{(k)}}{\tau_{c\pm}^{(k)}} \right)^{m} \exp\left[ -\frac{\Delta F}{\kappa\theta} \right] \mathrm{H}(\tau^{(k)} - \tau_{c\pm}^{(k)})$$

where $\Delta F$ is the enthalpy of dislocation movement activation, $\kappa$ is the Boltzmann constant, $\theta$ is the absolute temperature, $\mathrm{H}(\cdot)$ is the Heaviside function. The resolved shear stress on a slip system is determined by the condition, $\tau^{k} = \mathbf{n}^{(k)}\cdot\boldsymbol{\sigma}\cdot\mathbf{b}^{(k)}$. The critical resolved shear stress depends on the total

dislocation density and dislocation interactions on different slip systems and can be written in the following for:

$$\tau_c^{(k)} = \tau_{c_0}^{(k)} + Gb\left(\sum_\beta g^{(k,\beta)}\left(\rho_{m\pm}^{(\beta)} + \rho_{im\pm}^{(\beta)}\right)\right)^{1/2}$$

where $g^{(k,\beta)}$ is the dislocation interaction matrix [7].

*3.3 Mesolevel-II constitutive relations*

The model of the mesolevel-II is based on the kinetic equation for dislocation density and the relations of dislocation fracture theory. The main mechanism of inelastic deformation is the movement of edge dislocations, which interact with each other and with the lattice defects of various dimensions. Dislocation density based modeling is a universal approach to study the behavior of numerous dislocations and the various competing deformation mechanisms and their interaction. Such models allow obtaining the dependence of the dislocation density on the loading parameters and the parameters of the internal structure of a material. The advantage of these models is the ability to describe the structure, strength and plasticity of metals and alloys at the microstructural level.

The equations for describing the evolution of mobile dislocation densities can be written in the form (8) and similarly for immobile dislocation densities (9) [8].

$$\dot{\rho}_{m\pm}^{(k)} = \dot{\rho}_{nuc\pm}^{(k)} + \dot{\rho}_{mob\pm}^{(k)} - \dot{\rho}_{imm\pm}^{(k)} - \dot{\rho}_{ann(m\pm)}^{(k)} - \dot{\rho}_{ann(m\pm im\mp)}^{(k)}, \tag{8}$$

$$\dot{\rho}_{im\pm}^{(k)} = \dot{\rho}_{imm\pm}^{(k)} - \dot{\rho}_{mob\pm}^{(k)} - \dot{\rho}_{ann(m\mp im\pm)}^{(k)}. \tag{9}$$

The relations (8) and (9) take into account, that the densities of dislocations are dependent on such processes as annihilation ($\dot{\rho}_{ann(m\pm)}^{(k)}$, $\dot{\rho}_{ann(m\pm im\mp)}^{(k)}$), nucleation of new dislocations ($\dot{\rho}_{nuc\pm}^{(k)}$), mobilization ($\dot{\rho}_{mob\pm}^{(k)}$) and immobilization ($\dot{\rho}_{imm\pm}^{(k)}$).

Basic approximation, the criterion for the dislocation nucleation of microcracks, which is based on the Stroh's model described in section 2, was used. At high critical shear stress and immobile positive (or negative) dislocation densities exceeds the critical value density $\rho_{im+}^{(k)} \geq \rho^*$ (or $\rho_{im-}^{(k)} \geq \rho^*$). After that formed crack length $l_{crack} = \frac{(\rho_{im\pm}^{(k)})^2 b^5}{2}$.

## 4. Conclusion

There are the specific mechanisms of damage accumulation and fracture processes at different scale and structural levels. The properties of polycrystalline materials at the macrolevel are essentially determined by the state of the evolving meso- and microstructure of the material. In this article, we attempt to construct a multilevel mathematical model based on the crystal plasticity.

The descriptions of the basic models of dislocation crack nucleation, both the ones that take into account barriers and the ones, which are barrier-free, are given. The structure of the developed model is presented. At the macrolevel, an asymmetric indifferent strain rate is used to describe the material deformation. The mesolevel-I relations allow to describe the evolution of densities and the changes in dislocation movement velocities, shear rates, acting and critical resolved shear stresses for each slip system. The kinetic equations describing the change in the dislocation density on the slip system and the equations of dislocation fracture theory are used as a basis for the mesolevel-II model. The dislocation model developed to analyze the evolution of microstructure and deformation mechanisms includes equations for determining the densities of mobile and immobile dislocations, the density of dislocation sources and locks as well as equations for describing such processes as annihilation, etc.

The developed approach allows estimating the influence of the separated mechanisms of damage accumulation and deformation on the experimentally observed behavior features of materials.

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