On the Inherent Polycrystal Stress Concentration

V V Gulin *, A D Nikitin
Institute for Computer Aided Design of RAS, 19/18, 2nd Brestskaya, 123056, Moscow, Russia
E-mail: a.kornet104@gmail.com

Abstract. When analyzing the structural integrity of a material or structural part, the mechanics of continuous media is traditionally used with the concept of the homogeneity and isotropy of material properties; with this approach, the fracture criteria are related to the integral characteristics of the material and are described by the invariants of the stress tensor. However, this approach does not consider the physical aspects of the occurrence of local areas of plastic deformation, which ultimately means the impossibility of predicting the fracture, and, consequently, the resource of the structure. This is especially evident in the conditions of cyclic loading, when the material can fail at stresses well below the traditional «fatigue limit». In the current work, an approach is proposed that allows to save traditional methods of design and resource forecasting by expanding the scale of modeling. The paper introduces the concept of inherent stress concentration in any structurally heterogeneous medium as its inherent attribute. A universal algorithm for determining this characteristic is presented.

1. Introduction
The problem of determining the resource of a structure in a variety of operating conditions is currently moving to a new level. The development of the scientific direction «Physical Mesomechanics» is associated with the desire to master the laws that determine processes occurring in the material during the operation of the structure and lead, subsequently, to destruction. An important condition for the transition to a new level is the development of computer technologies, thanks to which a modern scientist can work with complex systems1, which, among other things, are not directly analytically described.

To date, a lot of works [1-3] have been carried out to study the mesomechanical response of a polycrystal to an external action. However, the authors of current paper have not found a study that would offer the most universal approach to the issue. The idea that the inhomogeneity of the stress-strain state is determined entirely by the structural features of the polycrystal eluded the scientific teams. In fact, if one is modeling on a polycrystalline scale level, it is necessary to deal with an additional property that a polycrystal acquires when it is composed of anisotropic crystallites.

In the current work, we propose to understand the essence of the elastic response of a polycrystal to mechanical impact. And thus, draw the line in modeling a polycrystal at the level of a continuous medium in an elastic formulation. An algorithm is proposed that allows one to determine the value of inherent stress concentration in a polycrystal, as an intrinsic attribute (characteristic) of a polycrystal, which is determined by its structure and at the same time turns out to be invariant with respect to the choice of the mechanical impact.

1 A complex system is understood as a system consisting of many interacting components, as a result of which it acquires new properties that are absent at the subsystem level and cannot be reduced to the properties of the subsystem level.
2. The crisis in the traditional approach to the strength of materials

Currently, in determining the resource of a particular structure, it is considered a generally accepted approach that uses CAE (Computer Aided Engineering) software packages. This approach is based on the following steps:

- Geometry creation
- Selection of the material properties
- Determination of the type of mechanical load
- Determination of initial and boundary conditions
- Subdivision of structure geometry into finite element mesh
- Solving the problem with the subsequent determination of certain parameters of interest (maximum deformations, principle stresses, etc.)
- Using the obtained parameter values as arguments in failure criteria

This approach has a number of advantages, thanks to which it became possible to create and use in practice intricate and resource-intensive structures.

At the same time, in practice, we had to face the fact [4-6] that the models that try to estimate the fatigue life are unsatisfactory, and the best of them are empirical ones, that is, those that use the limited experimental conditions as an argument in determining behavior under real impact conditions. Or, attempts are being made to formulate the fracture process at the macroscopic scale – the level of a continuous homogeneous isotropic medium [7], thus the cause of fracture is excluded from the modeling, so the question of crack initiation cannot be formulated neither physically or logically.

3. Algorithm for determining the value of inherent stress concentration

It should be emphasized that in the context of the current work, modeling is carried out on the basis of a physical and mathematical model of a continuous elastic medium. This allows, on the one hand, to consider the most universal behavior that occurs with any deformable solid, and on the other hand, it is the boundary for the next stage of deformation associated with the occurrence of plastic deformation. This is a fundamental point, since it is precisely this circumstance that determines the limits of applicability of the results obtained in this approach. Elastic formulation (1), on the one hand, is significantly limited in the possibilities of modeling behavior, but, on the other hand, it is completely universal in the context of any model of deformation of a continuous medium.

$$\sigma_{ij} = C_{ijkl} \varepsilon_{kl}, \quad i, j, k, l = 1, 2, 3$$ (1)

Generalized Hooke’s law relating the components of the stress $\sigma_{ij}$ and strain $\varepsilon_{kl}$ tensors through the matrix of elastic constants $C_{ijkl}$.

In order not to face the problem of modeling the entire designed structure on a polycrystalline scale, the following chain of actions is proposed:
Perform traditional strength analysis using traditional material properties (as described in section 2, with the possible exception of the last point);

- Determine the area of greatest stress, for example, equivalent tensile stress. Extract the stress tensor in this area and convert it to a diagonal form;
- Use the obtained principal stresses to the polycrystalline volume as a boundary condition;
- Evaluate stress concentration as the ratio of the maximum occurred stress in the polycrystal to the nominally applied stress:

\[
SMX = \frac{\sigma_{\text{effective}}^\text{Mises}}{\sigma_{\text{nominal}}^\text{Mises}}
\]

(2)

\[
TNMX = \frac{\tau_{\text{max}}^\text{effective}}{\tau_{\text{max}}^\text{nominal}}
\]

(3)

where the index «effective» corresponds to the effective, occurred value of the characteristic, and «nominal» corresponds to the value determined for a physically infinitely small volume;

- Use the knowledge gained to work at other scale levels and for use in more advanced failure criteria.

In this paper, the concentration of maximum shear stress (3) and the concentration of equivalent tensile stress (von Mises stress) (2) will be considered.

3.1. Geometry creation

Assuming that the traditional approach had been carried out, then it is necessary to create a grain geometry that reflects the real structure of the polycrystal. That is, it is necessary to split the representative volume of the material (cube) into areas – grains. For this, the DREAM.3D [9] software package was used. It implements the procedure for generating a structure (based on Voronoi diagrams) and it is possible to fine-tune the geometric parameters of grains, such as: average size, range and frequency of grain size, the presence of precipitation phases, proportions between grain axes, etc. It is also possible to import geometric parameters based on EBSD images, which in general open up the possibility of carrying out joint field and computer experiments.

The mentioned software package allows one to obtain an array of voxel (voxel – volumetric pixel) data with information about their belonging to a particular grain. The easiest way to get geometry suitable for importing into a CAE system is to use cubic voxels.

For physical simulations, the ANSYS software package was used. Voxel geometry was imported by converting it into finite elements of the SOLID185 type.

In this study throughout all experiments, a 100x100x100 voxel-element cube is considered.

The role of convergence analysis was performed by studying the grain size influence on the parameters that determine the stress concentration. As will be shown below (Table 2), a decrease in the number of grains in the volume (equivalent to smoothing the shape of the boundaries) at a qualitative level affects only the standard deviation of the parameters. Note that in the future, a similar study should be performed with a finite element model, in which the regions boundary will consist of a different type of finite elements, providing a non-raster boundary structure.
3.2. Boundary conditions

In contrast to an isotropic medium, when a symmetric load is applied to an anisotropic medium filling a cube, the latter, in general case, does not come to equilibrium. In it arises uncompensated torque, which lead to rotations of the solid. Therefore, it is necessary to limit the degrees of freedom. However, it is forbidden to apply a constraint that is noticeable in magnitude, since this fundamentally distorts the boundary conditions determined by the traditional approach.

To solve this difficulty, it is proposed to use six springs of low stiffness, located along the vertices of the cube in such a way as to limit all degrees of freedom on the one hand and, on the other hand, to influence the stress-strain state in an insignificant decimal place.

Fig. 4 (a) shows the arrangement of the springs along the six vertices of the cube and also a unite uniaxial tensile load can be seen. And in Fig 4 (b) one can see particular position of equilibrium that cube takes if its entire volume is uniformly filled with anisotropic material. The diagram shows von Mises stress, which in the homogeneous isotropic case with a single uniaxial tension should be equal to one.

The fact that an anisotropic medium in the aforementioned boundary conditions tends to reduce the arising stresses as much as possible is taken as a verifying circumstance. In this way, any stresses that could arise due to the limitation of the body are excluded, while the equilibrium condition of the finite element model is satisfied.

The situation is different if the cube consists of more than one grain. In this case, if the directions of their crystallographic axes are not parallel, then each of them would tend to make its own unique combination of rotations. But the presence of an inextricable connection between them leads to a contradiction in the relaxation of the external load and is expressed in an increase in the value of the effective stress (Fig 4 (c, d)).

3.3. Determination of inherent stress concentration

Next, the ratio of the occurred stresses to the nominally applied ones should be evaluated (2, 3). In the case of an isotropic medium or anisotropic, yet filling the entire volume, this ratio would be equal to 1, which means their equality. However, in the case of a polycrystal, the body cannot relax the load by rotations, since the angles of rotation are individual for each grain. Entering into this contradiction and ensuring equilibrium in the structure in a necessary way, increased stress values occur. That is why the last circumstance should be understood as an attribute, a characteristic, that is inherent to a polycrystal, just as we assign to other bodies such properties as mass, boiling point, color, etc.

Information obtained from a sufficiently large sample of parameters of the internal boundaries of a polycrystal, as well as from a series of different mutual orientations of crystallites, should be considered representative. Each grain is assigned a local coordinate system, which is obtained by three rotations around the perpendicular axes. The amount of each rotation is an evenly distributed from 0° to 359°.

For the experimental routine, a program has been implemented that allows to perform about 500 experiments per day using the resources of a home personal computer.
Figure 4. Illustration of the boundary condition of a unite tensile load and the place of fastening of low stiffness springs (a); plots of von Mises stresses in the case of 1 grain per volume (b), 2 grains (c) and 219 grains (d)

4. Stress concentration in α-Fe polycrystal

Let us now consider a monocristalline ferrite (α-Fe) with the following elastic constants [10] (Table 1)

| T, K | C_{11} | C_{12} | C_{44} |
|------|--------|--------|--------|
| 300  | 230.37 | 134.07 | 115.87 |
| 500  | 217.69 | 130.91 | 111.64 |

Let us subject the representative volume to uniaxial unit tension. Then the principle stresses will take on the following values:

\[ \sigma_1 = 1 \]
\[ \sigma_2 = 0 \]
\[ \sigma_3 = 0 \] (4)

We will consider von Mises stress \( \sigma_{eqv} \) and the maximum tangent stress \( \tau_{max} \)

\[ \sigma_{eqv} = \frac{1}{\sqrt{2}} \sqrt{\left(\sigma_1 - \sigma_2\right)^2 + \left(\sigma_2 - \sigma_3\right)^2 + \left(\sigma_3 - \sigma_1\right)^2} \] (5)

\[ \tau_{max} = \frac{\sigma_1 - \sigma_3}{2} \] (6)

In the case of an isotropic or anisotropic medium that uniformly fills the entire representative volume according to formulas (5) and (6), we will have:
\[
\sigma_{eq} = 1, \quad \tau_{\text{max}} = 0.5 \tag{7}
\]

Let's carry out a series of computer experiments with different geometries and mutual misorientation of grains. On the basis of more than 2600 experiments grain count ranged from 19 to 223 grains per volume. With the same configurations, a parallel series of experiments with elastic constants was performed at a temperature of 500 K (Table 1).

Let's collect the stress concentration values into a diagram. The area of each diagram (Table 2) is equal to 1, so the height of the column is proportional to the probability of finding the corresponding stress concentration values (plotted horizontally).

| Table 2. Stress concentration |
|--------------------------------|
| Number of grains | Von Mises | Maximum tangent |
| ~20 |
| ~220 |

**Figure 5.** Scatter plot of stress concentration coefficients. The correlation coefficient is 0.524.

5. **Discussion and conclusions**

Automation of the numerical experiment procedure makes it possible to obtain statistical information on the stress concentration for a given class of polycrystals (for example, α-Fe for a given grain size...
distribution). The use of the approach described in the article makes it possible to refine the existing models without abandoning the traditionally established approach to determine resource of the structure. The defined characteristic of the stress concentration is completely determined by the polycrystal itself and does not depend on the type of loading, thus, it is an inherent attribute of the polycrystal. Information on stress concentration in the form of Table 2 allows to consider influence on the inhomogeneity of the stress-strain state in a polycrystal without the need to repeat modeling of the polycrystalline structure.

Based on the study of α-Fe, the authors conclude that although such factors as the number of grains in the volume and the geometry of their boundaries affect the stress concentration, when considering a large sample by combinations of mutual grain orientations, these factors take rather a secondary place.

General results:

- In the current study, it has been shown that in any mechanically inhomogeneous body there is an inherent stress concentration. Thus, the use of any failure criteria (applied in the framework of continuum mechanics) must take this concentration into account when determining the limiting states.
- Inherent stress concentration is a dimensionless characteristic of a polycrystal and is a function of: a) geometric parameters of the grains; b) temperature; c) crystallographic system type; d) values of elastic constants.
- It is noted that the main factor determining the value of inherent stress concentration is the ratio between the elastic constants. While the geometric parameters (size and shape) of the grains play a secondary role. At the same time, the authors believe this to be a consequence of the elastic formulation and admit that when using plasticity models, the influence of geometric parameters will take on a significant role.
- The range of inherent stress concentration values for α-Fe based on more than 2600 experiments with different grain geometries and their mutual orientation turned out to be [1.52, 3.11]. The average for stress concentration is 1.89 and 2.10 for von Mises and maximum tangent stress, respectively. The magnitude of the stress concentration makes it necessary to take into account its value when determining the limiting state of the material. Thus, for example, critical plane approach in multiaxial fatigue failure criteria [11-13] must now consider this phenomenon, since the object that reaches the limiting state differs from a continuous isotropic medium and the deformation and/or fracture energy differs accordingly.
- The categorical nature of the elastic formulation and the discovered property of a polycrystal to concentrate stress makes it possible to reconsider the conditions for the initiation of fracture without abandoning the traditional approach of a continuous isotropic medium. Since the abundance of information about possible statistical distributions of grain parameters is expressed in a single scalar parameter. Using the maximum value of this parameter can guarantee preparedness for the worst-case scenario and does not require re-referring to the mesoscale level.
- Information about the stress-strain state of a polycrystalline body can be used as a boundary and/or initial condition for models of a different scale level (polycrystalline plasticity, dislocation dynamics, etc.).

Acknowledgements
This work was financially supported by RSF project № 19-19-00705.

References
[1] Ashikhmin V N and Povyyshev I A 1995 Statistical regularities of stress distribution in polycrystals PNRP Math. modeling of systems and processes 3 11–18
[2] Kamaya M, Kawamura Y and Kitamura T 2007 Three-dimensional local stress analysis on grain boundaries in polycrystalline material Int. J. Solid. Struct. 44 3267–3277
[3] McDowell D and Dunne F P E 2010 Microstructure-sensitive computational modeling of fatigue crack formation, Int. J. Fatigue 32 1521–1542
[4] Bathias C, Drouilac L and Francois P Le 2001 How and why the S-N curve does not approach a
horizontal asymptote \textit{Int. J. Fatigue} \textbf{23} 143–151

[5] Maktouf W and Sāi K 2014 An investigation of premature fatigue failures of gas turbine blade \textit{Engineering Failure Analysis} \textbf{47} 89–101

[6] Nicholas T 1999 Critical issues in high cycle fatigue \textit{Int. J. Fatigue} \textbf{21} S221–S231

[7] Burago N G, Nikitin I S, Nikitin A D and Stratula B A 2019 The assessment of fatigue durability and critical plane determination for multiaxial cyclic loading at an arbitrary shift of phases \textit{PNRPU Mechanics Bulletin} \textbf{3} 27–36

[8] Arutyunyan A R 2020 Formulation of the fatigue strength criterion for composite materials \textit{Vestnik of St. Petersburg University. Mathematics. Mechanics. Astronomy} \textbf{7} 511–517

[9] Groeber M A and Jackson M A 2014 DREAM.3D: A Digital Representation Environment for the Analysis of Microstructure in 3D \textit{Integrating Materials and Manufacturing Innovation} \textbf{3} 56–72

[10] Adams J J, Agosta D S, Leisure R G and Ledbetter H 2006 Elastic constants of monocrystal iron from 3 to 500 K. \textit{Journal of Applied Physics,} \textbf{100} 113530

[11] Karolczuk A and Macha E 2005 A review of critical plane orientations in multiaxial fatigue failure criteria of metallic materials \textit{Int. J. Fracture} \textbf{134} 267–304

[12] Wang Y and Susmel L 2015 Critical Plane Approach to Multiaxial Variable Amplitude Fatigue Loading \textit{Frattura ed Integrita Strutturale} \textbf{9} 345–356

[13] Palin-Luc T and Morel F 2005 Critical Plane Concept and Energy Approach in Multiaxial Fatigue \textit{Materials Testing} \textbf{47} 278–286