Correlation Length Estimation in a Polycrystalline Material Model

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ABSTRACT

This paper deals with the correlation length estimated from a mesoscopic model of a polycrystalline material. The correlation length can be used in some macroscopic material models as a material parameter that describes the internal length. It can be estimated directly from the strain and stress fields calculated from a finite-element model, which explicitly accounts for the selected mesoscopic features such as the random orientation, shape and size of the grains. A crystal plasticity material model was applied in the finite-element analysis.

Different correlation lengths were obtained depending on the used set of crystallographic orientations. We determined that the different sets of crystallographic orientations affect the general level of the correlation length, however, as the external load is increased the behaviour of correlation length is similar in all the analyzed cases. The correlation lengths also changed with the macroscopic load. If the load is below the yield strength the correlation lengths are constant, and are slightly higher than the average grain size. The correlation length can therefore be considered as an indicator of first plastic deformations in the material. Increasing the load above the yield strength creates shear bands that temporarily increase the values of the correlation lengths calculated from the strain fields. With a further load increase the correlation lengths decrease slightly but stay above the average grain size.

1 INTRODUCTION

In state-of-the-art structural and stress analyses it is normal to assume that the materials under test are homogeneous and isotropic. Such assumptions are valid for the load-carrying capacities and lifetime analyses of moderately deformed parts that are significantly larger than the inhomogeneities, such as grains, voids or inclusions, which constitute the material. The grains in metals, for example, are typically of the order of $10^{-5}$ m. Material inhomogeneities may, however, become important when analyzing the following: small parts with sizes similar to the inhomogeneities [1, 2, 3, 4], parts subject to a load approaching their strength limit [2, 5, 6, 7] and the initiation and propagation of short cracks [8, 9, 10]. In such cases the localized stress and strain peaks caused by the inhomogeneities usually dominate the response of the
material and this may severely limit the applicability of state-of-the-art engineering structural
and stress analyses.

A number of attempts to include the inhomogeneities in the models used to describe materi-
als can be found in the literature. In this paper we have defined two, somewhat arbitrary, classes
of models: (1) Advanced macroscopic material models. This group includes, among others,
gradient theories [11, 12, 13], continuum damage models [14, 15] and stochastic finite-element
approaches. A common feature of these models is that a more or less explicit model of the in-
homogeneities is employed to predict the behavior at the macroscopic (engineering) level. This
again requires assumptions that lead to the additional material parameters, which may require
a number of expensive additional tests. Typically, the internal length representing the size of
the inhomogeneities is one of the most important material parameters. (2) Multi-scale mod-
els. These explicitly model at least the mesoscopic inhomogeneities (e.g., grain structure, for a
review see [16]). While very general and relatively free of assumptions about homogeneities,
they are computationally very demanding and not yet suitable for routine engineering analyses.

The most efficient way to improve engineering analyses is, therefore, a combination of both
these approaches. A very promising way seems to be to employ a multiscale approach in the
first step, in order to derive mesoscopic (i.e. on the scale of the grains in the material) stress
and strain fields. A statistical analysis of such fields is then used in the second step to derive the
correlation lengths. Correlation length is here defined as a distance where the initial value of the
envelope of the covariance function decreases by a factor of $e$. Calculated correlation lengths
may be used as a direct input for a stochastic finite-element analysis, which represents the third
step. A number of authors have dealt with the third step: see, for example, [17, 18, 19, 20, 21].

The main goal of this paper is, therefore, an estimation of the correlation lengths within the
stress and strain fields of a mesoscopic model of a non-homogenous and anisotropic steel struc-
ture. The first part of the paper briefly explains the basic ideas of the mesoscopic model and the
procedure employed to derive the correlation lengths. This is followed by a numerical example,
which outlines and discusses the most important results - the changes in the correlation lengths
with the increase of the remote load for several sets of grains’ crystallographic orientations -
and the conclusions.

2 MODEL DESCRIPTION

The estimation of the correlation lengths is based on a mesoscopic material model [22]
that includes grains of random size, shape and orientation, see Figure 1. Grain boundaries are
plotted with blue colour while red colour is used for finite elements. Random grain structure
is generated with Voronoi tessellation [23], using code VorTESS [24]. A Voronoi tessellation
represents a cell structure constructed from Poisson points by introducing planar cell walls
perpendicular to the lines connecting neighboring Poisson points. This results in a set of convex
polygons embedding the Poisson points.

Each grain is assumed to behave as a randomly oriented continuum described by the anisotropic
elasticity and crystal plasticity model outlined in the following section. A random generator
with a uniform distribution and range 0 to $2\pi$ is used to generate an angle $\alpha$ for which crystal-
lographic orientation of a given grain is rotated around the Z axis (see Figure 2) in the counter
clock-wise direction from its initial position shown in Figure 2. In the analysis plane strain will
be assumed with a model placed into the XY-plane. Each grain is subdivided into 8-noded,
reduced-integration, plane strain finite elements. The finite-element method [25] is employed
to determine the strain and stress fields resulting from a remote load. Stress field is then used
for the estimation of the correlation lengths.

Figure 1: The finite element model, indicating the boundary conditions and remote applied load.

Figure 2: Relation between the slip planes of a face centered cubic material and the crack for $\alpha = 0^\circ$.

2.1 Constitutive model

The elastic deformation at the monocrystal level is generally anisotropic and is governed by the generalized Hooke’s law, $\sigma_{ij} = C_{ijkl}\epsilon_{kl}$, where $\sigma_{ij}$ represents the second-rank stress tensor, $C_{ijkl}$ the fourth-rank stiffness tensor and $\epsilon_{kl}$ the second-rank strain tensor. The number of independent elastic constants for a cubic crystal system (BCC and FCC) is 3.

Crystal plasticity theory is used [26, 27] to describe the material’s plastic behaviour at the grain level. Crystal plasticity assumes that the plastic deformation in monocrystals takes place via a simple shear on a specific set of planes, see Figure 2. Deformation by other mechanisms
such as for example diffusion, twinning and grain boundary sliding is currently not taken into the account. Details of the implemented crystal plasticity constitutive model are given in [16, 28, 29].

The combination of a slip plane, denoted by its normal $m_i^\alpha$, and a slip direction, $s_i^\alpha$, is called a slip system, $(\alpha)$. The plastic velocity gradient, $\dot{u}_{ij}^p$, due to a crystallographic slip can be written as [30],

$$\dot{u}_{ij}^p = \sum_\alpha \dot{\gamma}^{(\alpha)} s_i^{(\alpha)} m_j^{(\alpha)},$$  

(1)

where the summation is performed over all active slip systems, $(\alpha)$, while $\dot{\gamma}^{(\alpha)}$ represents the shear rate. The cumulative slip, $\gamma$, is defined as,

$$\gamma = \sum_\alpha \int_0^t \dot{\gamma}^{(\alpha)} \, dt.$$  

(2)

The constitutive relation of the elastic-plastic monocrystal can be given in terms of stress and strain rates as

$$\dot{s}_{ij} = C_{ijkl} \left( \varepsilon_{kl} - \varepsilon_{ij} \right).$$  

(3)

This is a reasonable approximation at room temperature and for ordinary strain rates and pressures [30]. The Schmid resolved shear stress for a given slip system is given by eq. (4).

$$\tau^{(\alpha)} = s_i^{(\alpha)} \sigma_{ij} m_j^{(\alpha)}$$  

(4)

where $s_i^{(\alpha)}$ and $\sigma_{ij}$ are the slip-hardening moduli defined by the adopted hardening law. In this work Peirce et al. hardening law is used [31], where self-hardening moduli $h_{\alpha\alpha}$ are defined by:

$$h_{\alpha\alpha} = h(\gamma) = h_0 \text{sech}^2 \left( \frac{h_0 \gamma}{\tau_s - \tau_0} \right).$$  

(5)

The latent-hardening moduli $h_{\alpha\beta}$ are given by,

$$h_{\alpha\beta} = q h(\gamma), \quad (\alpha \neq \beta),$$  

(6)

where $q$ is a hardening factor. This model was implemented as a user-subroutine into the finite element code ABAQUS [25]. Further details on its theory and implementation can be found in [32, 16].

The elastic material parameters for the 22 NiMoCr 37 steel were obtained from the literature for an $\alpha$-Fe body-centered cubic crystal [33]. The following values for monocrystals were used: $C_{iij}=230$ 000 MPa, $C_{ijij}=135$ 000 MPa, $C_{ijijij}=117$ 000 MPa, $h_0=700$ MPa, $\tau_s=15.5$ MPa, $\tau_0=155$ MPa, $n=50$, $\dot{\gamma}^{(\alpha)}=0.001$ and $q=1$.


2.2 Boundary conditions

Mixed displacement/traction type boundary conditions were applied in the analysis. The right and upper edges are loaded in uniaxial tension with zero shear traction. Maximum load at the right edge is 1400 MPa and half of that value (i.e. 700 MPa) at the top edge. Symmetry conditions were applied on the left and lower edges. The upper and the right edge were prescribed to remain straight during the deformation and parallel to the bottom/left edge. In the analysis, the models are considered to be embedded in a larger body. The constraints imposed by the straight edge requirements are a first approximation of the stiffness from the surrounding material.

3 CORRELATION LENGTH

In this section we briefly describe the correlation length which is here taken as a measure of the domain of influence of the individual grains [22]. The autocorrelation function $R_{xx}(l_1, l_2)$ of a random process $x(l)$ is defined by eq. (8), where $E[]$ represents the mathematical expectation. The covariance function $K_{xx}(l_1, l_2)$ of a random process $x(l)$ is defined by eq. (9). For a stationary process with zero average value the two functions are the same, eq. (10).

\[
R_{xx}(l_1, l_2) = E[x(l_1)x(l_2)] \tag{8}
\]

\[
K_{xx}(l_1, l_2) = R_{xx}(l_1, l_2) - E[x(l_1)]E[x(l_2)] \tag{9}
\]

\[
K_{xx}(l_1, l_2) = K_{xx}(l) = R_{xx}(l) = R_{xx}(l_1, l_2), \quad l = l_1 - l_1 \tag{10}
\]

For covariance functions of the form given by the eq. (11), the correlation length $\lambda$ can be defined as the value of the parameter $l$ for which the envelope of the covariance function falls to the value $K_{xx}(0)/e$, Figure 3.

\[
K_{xx}(l) = K_{xx}(0) \cdot e^{-\frac{|l|}{\lambda}} \cdot \cos(\omega \cdot l) \tag{11}
\]

Figure 3: Left: the definition of the correlation length $\lambda$. Right: the length (2R) and direction of the vector for calculating the correlation length.

Since strain and stress are two-dimensional variables, a vector of data for the correlation-length calculation has to be extracted. This can be done in the following way (see Figure
3): i) a point for which the correlation length is to be calculated is selected, ii) a direction for calculating the correlation length is chosen, iii) the length of the vector is determined by the search radius R, iv) a quadratic two-dimensional interpolation [34] is applied to obtain the values of Mises stress at equally spaced points on the direction line within the search radius (the bold line in Figure 3), v) the correlation length is calculated for the selected direction, vi) the procedure is applied for other directions. The final correlation length is determined as the average value of the correlation lengths for the selected directions. In this study we used six predefined directions: from $0^\circ$ up to $150^\circ$ in steps of $30^\circ$. The procedure was repeated for every Gaussian point.

4 RESULTS

In this section we take the model shown in Figure 1 and apply 10 different sets of crystallographic orientations of grains. We therefore obtain 10 models from which we calculate the strains and stresses. Mises stress is then used to calculate the correlation length and estimate its variation due to different orientation sets. Correlation length is taken as a measure of the domain of influence of the individual grains. Higher correlation length values relate to larger domain of influence. In this work we are only concerned with the variation of the correlation lengths due to different crystallographic orientations. The search radius R, boundary conditions and grain shape effects have been studied previously [35, 22]. A search radius R corresponding to twice the average grain size (0.046 mm) is used.

Random crystallographic grain orientations in steel inevitable lead to variations in local strains and stresses. Macroscopic response of small specimen (smaller than representative volume element) is affected, Figure 4. Variations in macroscopic response decrease with increasing number of grains [36]. In a model with sufficiently high grain count these variations will vanish. This point is referred to representative volume element size or RVE. We can see that our model with 212 grains is below this point. The $\bullet$ in Figure 4 represents a point on the tensile curve where $<\epsilon_{eq}>=4.5\%$. At this load Mises strains and stresses are shown in Figure 5 for two selected sets of crystallographic orientations. One can see the formation of persistent slip bands on the left-hand side of the figure. The right-hand side presents Mises stresses. Different crystallographic orientations result in stress concentrations, specially on the grain boundaries. As a result, grains shapes are imprinted.

Figure 4: Variation of numerical tensile tests due to different sets of crystallographic orientations.

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Correlation lengths for two selected crystallographic orientation sets and calculated at macroscopic point shown as as dot in Figure 4 are presented in Figure 6. Elevated values of correlation lengths at the model edges are attributed to the boundary effect. Different sets of crystallographic orientation affect the correlation length considerably, however, the average values of correlation lengths are 14.6 % apart and are above the average grain size of 0.023 mm. Areas of higher correlation lengths tend to spread across several grains.

Figure 7 shows the correlation lengths dependance on external load. The behavior of the correlation length can be classified into three regions. The first region is when the specimen is stressed below the yield point. In this region the calculated correlation lengths do not change. This is in accordance with the statistical theory since the proportional change in the observed stress field (e.g. by a factor 1.1) does not change the correlation length. Using this property one can estimate how high must the macroscopic equivalent stress be for first plastic deformations to occur. For the material involved this is estimated to be between 240 and 245 MPa. In all the analyzed cases the correlation length in this region is larger than the average grain size of 0.023 mm.

The second region begins when the load is increased and the specimens are stressed above the macroscopic yield point. The correlation length initially slightly increases and later starts to decrease. The rate of decrease is approximately the same for all the analyzed cases. With increased load (this load varies due to different crystallographic sets) first shear bands start to form. In [22] authors observed that in some cases the areas of higher correlation lengths
the different sets of grains’ crystallographic orientations on the correlation length was estimated. By using the correlation length we were able to determine the length scale of the inhomogeneities. This is an important material property in advanced macroscopic material models.

A further increase in the load caused widening and elongation of the shear bands. In this (third) region the correlation lengths increased in all analyzed cases with the smallest correlation length reaching the value of 0.0258 mm and the highest value of 0.0288 mm. In the last (fourth) region the correlation lengths decrease.

5 CONCLUSION

In this study the correlation length for a mesoscopic model of a polycrystalline material has been calculated. By using the correlation length we were able to determine the length scale of the inhomogeneities. This is an important material property in advanced macroscopic material models.

The calculated stress fields were used to estimate the correlation lengths. The influence of the different sets of grains’ crystallographic orientations on the correlation length was estimated. We determined that the different sets of crystallographic orientations affect the general level of

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**Figure 6:** Correlation lengths for model with orientation set #7 (left) and set #10 (right). $<\varepsilon_{eq}> = 4.5\%$.

**Figure 7:** Variation of correlation lengths due to different sets of crystallographic orientations.
the correlation length, however, as the external load is increased the behaviour of correlation length is similar in all the analyzed cases. For elastically deformed polycrystal, the grain’s domain of influence is slightly larger than the average grain size. Increasing the macroscopic equivalent stresses between 270 MPa and 400 MPa causes some fluctuations of the domain of influence. With further increase of the macroscopic load, the correlation length calculated from the stress fields reaches its peak value and then decreases continuously. Average standard deviation of the calculated correlation lengths was 0.0011 mm.

The calculated correlation lengths were averaged over different directions. This effectively reduced their potential for detecting direction-dependant structures in an anisotropic material. This drawback may be effectively overcome by calculating a two-dimensional autocorrelation function. This represents an important goal for the future work.

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