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CORRELATION LENGTH AS ESTIMATE OF THE DOMAIN OF INFLUENCE OF CRYSTAL GRAIN

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ABSTRACT

As a rule the continuum mechanics assumes homogeneity and isotropicity of the involved material. These assumptions are satisfactory for engineering load capability analysis and the engineering lifetime analysis of the parts that are significantly larger than the order of the material inhomogeneities and are only moderately deformed. However, the inhomogeneity of the material becomes more and more important when analyzing the initiation and propagation of cracks or load capability of the material in the vicinity of the limit strength. The inhomogeneity and anisotropicity of the material can be modeled by dividing the continuum into limited number of randomly shaped grains with variable material properties. However, this procedure is numerically quite demanding. The solution to this problem is envisioned by the development of methods that transfer the significant data on the inhomogeneity into the classical macroscopic models. The interesting method is the usage of the correlation length. The correlation length can be used to estimate the domain of influence of the individual inhomogeneities in the simulated aggregate of randomly oriented and shaped crystal grains. This article deals with several issues related to the calculation of correlation length from a 2D stress field.

1 INTRODUCTION

As a rule the continuum mechanics and rheology assumes homogeneity and isotropicity of the material involved. These assumptions are satisfactory for engineering load capability analysis and the engineering lifetime analysis of the parts that are significantly larger than the order of the material inhomogeneities and are only moderately deformed. However, the inhomogeneity of the material becomes more and more important when analyzing the initiation and propagation of cracks or load capability of the material in the vicinity of the limit strength. The stress in the vicinity of the inhomogeneity in the material is often increased. This can lead to the initialization of micro cracks that can develop into macro cracks and finally lead to the failure of the material.

The structure of steel is in general non-homogenous and anisotropic. Material properties are often anisotropic and non-homogenous. The variation of the material properties throughout the given structural element can be modeled using stochastic methods. Gaussian random process is usually used. Chakraborty [1] uses it for modeling the distribution of the Young modulus and load in a beam element. Stochastic methods are also used for modeling the geometrical imperfections in the cylindrical shells. Schenk in Schuëller [2] use Gaussian

random process in combination with the Karhunen-Loéve expansion to model these imperfections. The failure limit of the shell is later calculated using the finite element method (FEM). Zheng in Ellingwood [3] use non-Gaussian random process to evaluate the time gradient of the crack size growth.

This paper deals with estimating the domain of influence of inhomogeneties in a model of non-homogenous and anisotropical steel structure. The variation of the material properties is modeled by dividing the continuum into finite number of randomly oriented and shaped crystal grains. The stress and strain fields for the given loads and boundary conditions are then calculated using FEM method. The domain of influence of inhomogeneties is determined by calculating the correlation length from the stress field.

2 THEORY

The variation of the material properties in a model can be modeled by dividing the continuum into finite number of randomly oriented crystal grains of different size [4]. Crystal grains are generated using the Voronoi tessellation [5]. Each crystal grain is composed of certain number of finite elements, all having the same orientation within the crystal. Between the crystals the orientation of the finite elements is varying. Anisotropical elasticity material model is used for the finite elements. The macroscopic response of such a model depends on the material properties of all crystal grains with different material properties, orientation and boundary/load conditions of the model. Using this approach the non-homogenous structure of steel can be simulated. The numerical effort is however quite large. This could be reduced if only the essential inhomogenities are taken into the account. One way of estimating essential inhomogenities is to calculate the domain of influence of crystal grains. The correlation length is one of the criteria for estimating statistical dependency of stress field in certain direction and enables one to estimate the domain of influence of the individual crystal grain.

2.1 Correlation length

The autocorrelation function $R_{xx}(t_1,t_2)$ of a random process $x(t)$ is defined with the expression (1), where E represents mathematical expectation and $f_{x(t_1)x(t_2)}$ joint probability density function [6]. The covariance function $K_{xx}(t_1,t_2)$ of a random process $x(t)$ is defined with the equation (2) and can be expressed using the autocorrelation function, equation (3).

$$R_{xx}(t_1,t_2) = E[x(t_1)\cdot x(t_2)] = \int\int x_1 \cdot x_2 \cdot f_{x(t_1)x(t_2)}(x_1,x_2)\cdot dx_1 \cdot dx_2 \qquad (1)$$

$$K_{xx}(t_1,t_2) = E[\ (\ x(t_1) - E[x(t_1)]\ )\cdot(\ x(t_2) - E[x(t_2)]\ )\ ] \qquad (2)$$

$$K_{xx}(t_1,t_2) = R_{xx}(t_1,t_2) - E[x(t_1)]\cdot E[x(t_2)] \qquad (3)$$

For stationary random processes the joint probability density function $f_{x(t_1)x(t_2)}$ depends only upon the difference t_2-t_1. Consequently, the autocorrelation and covariance functions also only depend upon the difference t_2-t_1. If in addition to the stationarity, the average value of the random process is zero, then the autocorrelation and covariance functions of the process involved are equal, expressions (4) and (5).

$$R_{xx}(t_1,t_2) = R_{xx}(0,t_2-t_1) = R_{xx}(t_2-t_1) = R_{xx}(t), \qquad t = t_2 - t_1 \quad (4)$$

$$K_{xx}(t) = K_{xx}(t_2-t_1) = R_{xx}(t) - \underbrace{E[x(0)]}_{=0}\cdot\underbrace{E[x(t_2-t_1)]}_{=0} = R_{xx}(t) \qquad (5)$$

For covariance functions of the form given by the equation (6), the correlation time τ can be defined as the value of the parameter t for which the envelope of the covariance

function falls to the $K_{xx}(0)/e$, Figure 1. In cases where parameter t represents length, the correlation time is referred to as correlation length and symbol λ is used for it.

$$K_{xx}(t) = K_{xx}(0) \cdot e^{-|t|/\tau} \cdot \cos(\omega \cdot t) \qquad (6)$$

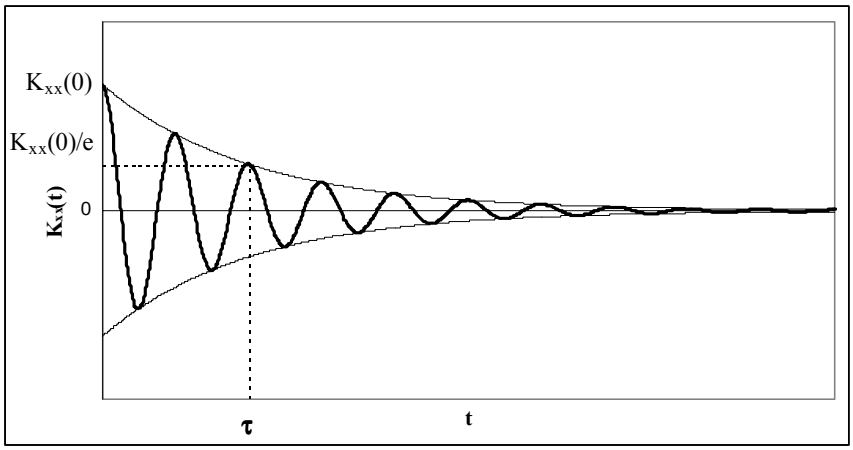

Figure 1: Correlation time definition

Let us assume that we have a vector of data **g** for which we want do determine the correlation length. First the autocorrelation function is estimated using discrete correlation theorem, expression (7). In expression (7) symbol G_k presents discrete Fourier transformaction of vector **g** and symbol * stands for complex conjugation. First we calculate the discrete Fourier transform of vector **g** to obtain G_k. Next we multiply, index by index, the vector G_k with the G_k^*. Finally we calculate the inverse Fourier transform of the product $G_k G_k^*$ to determine autocorrelation function. Correlation length is calculated from the envelope of the autocorrelation function. Instantaneous envelope of function *f(t)* is defined with the expression (8), where *H(t)* presents the Hilbert transform of function *f(t)*, expression (9).

$$\text{Autocorr}(\mathbf{g},\mathbf{g})_j \Leftrightarrow G_k G_k^*, \qquad k = 0,1,2,\ldots length(G)-1 \qquad (7)$$

$$A(t) = \sqrt{(f(t))^2 + (H(t))^2} \qquad (8)$$

$$H(t) = \int_{-\infty}^{+\infty} \frac{1}{\pi \cdot (t-\tau)} \cdot f(\tau) \cdot d\tau \qquad (9)$$

3 ESTIMATING CORRELATION LENGTH OF A STRESS FIELD

The 0.4 by 0.28 [mm] size finite element model is loaded with p_1=800 [MPa] and p_2=100 [MPa] as shown in Figure 2 (left). The model is composed out of 212 randomly oriented and sized crystal grains, Figure 2 (right), obtained by using Voronoi tessellation [7]. The stress and strain fields are calculated using FEM. Anisotropical elasticity material model is used. The material properties for the reactor pressure vessel 22 NiMoCr 3 7 with bainitic microstructure and b.c.c. crystal lattice have been applied in the FEM model and are given in [7].

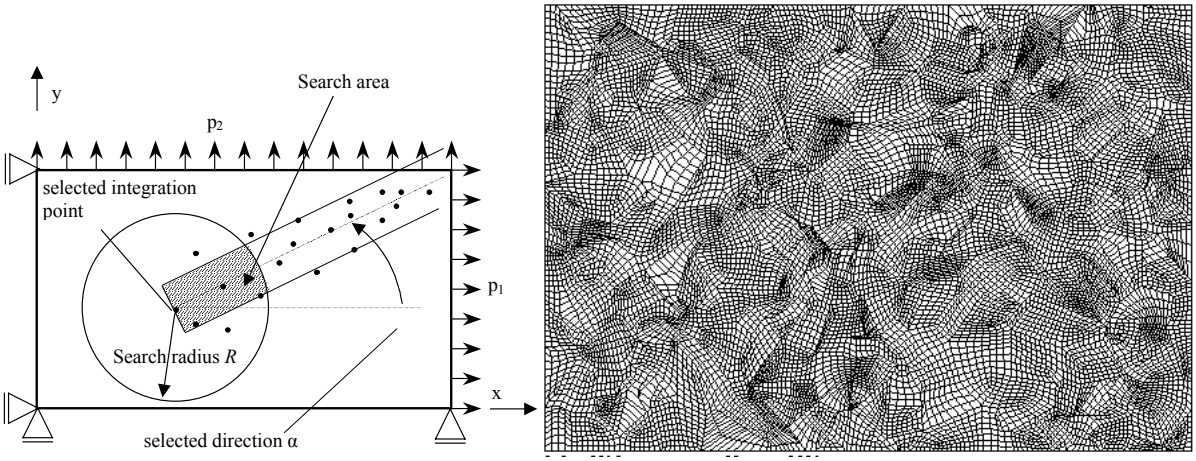

Figure 2: Boundary/load conditions (left), the crystal grains with finite element mesh (right)

Correlation length is calculated from the von Mises stress field σ_{Mises} that is determined for every Gaussian integration point of the finite element, equation (10). In the equation (10) the s_{ij} presents the deviator stress tensor while δ_{ij} stands for the Cronecker δ tensor. The calculated von Mises stress field is shown in Figure 3. For the correlation length calculation the von Mises stress is assumed to be a random variable.

$$\sigma_{Mises} = \sqrt{\frac{3}{2} \cdot s_{ij} \cdot s_{ij}}, \qquad s_{ij} = \sigma_{ij} - \frac{\sigma_{kk}}{3} \cdot \delta_{ij}, \qquad \delta_{ij} = \begin{cases} 1, & i = j \\ 0, & i \neq j \end{cases} \qquad (10)$$

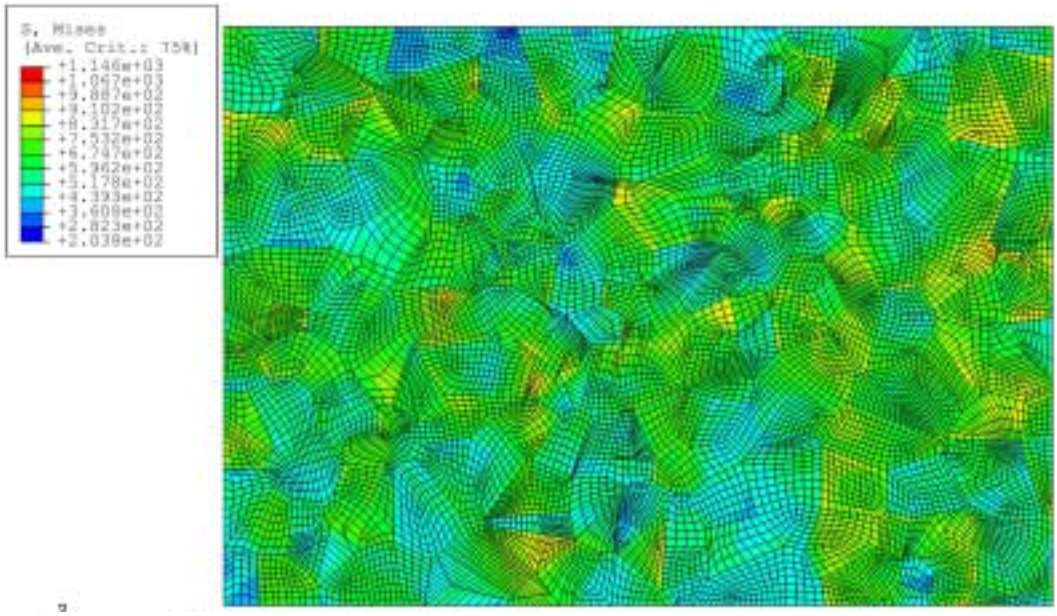

Figure 3: Von Mises stress field

Since stress is a 2D variable, the vector of suitable data for the correlation length calculation has to be extracted. This can be done in the following way, Figure 2: i) an integration point for which the correlation length is to be calculated is selected, ii) a direction for searching integration points is chosen, iii) interpolation is applied to obtain the equally spaced vector from the points found, iv) the correlation length is calculated for the selected direction, v) the procedure is applied for other directions and finally the correlation length is determined as the average value of correlation lengths for the selected directions. In the presented work 12 predefined directions were used: from 0 [^{o}] up to 360 [^{o}] in the intervals of 30 [^{o}].

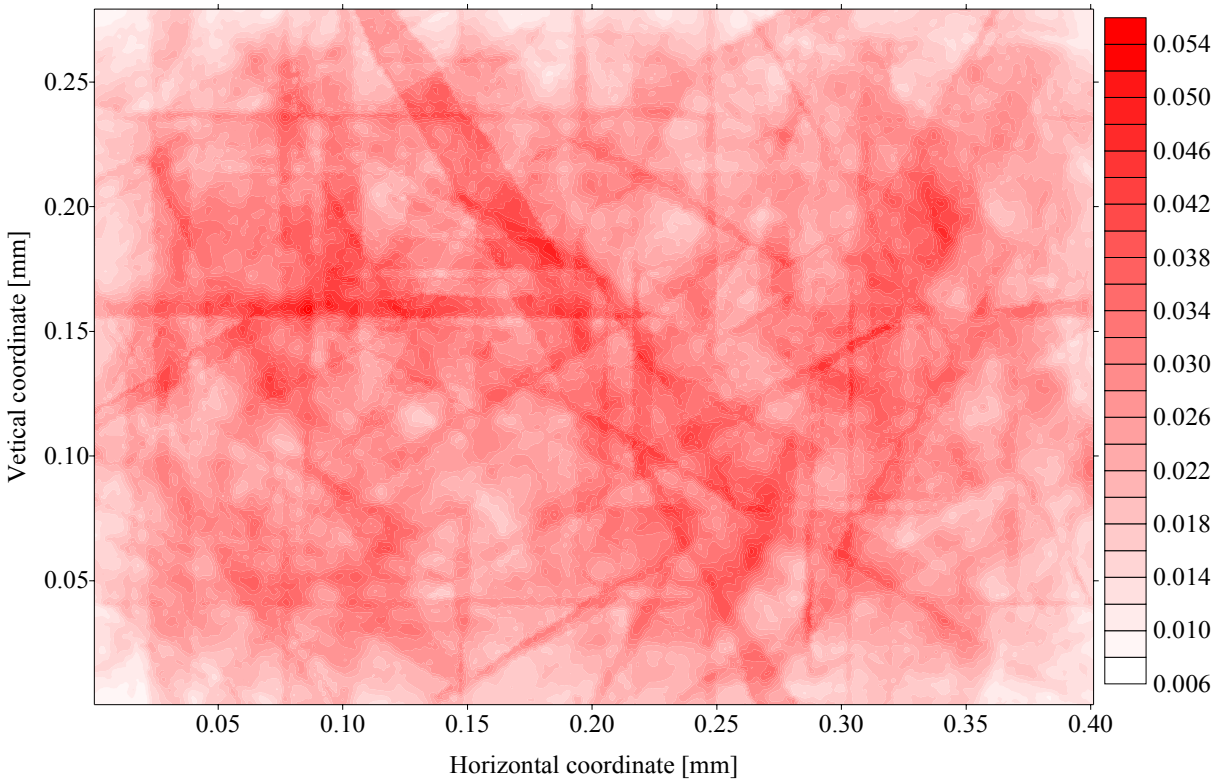

Figure 4: Correlation length

Figure 4 shows the calculated correlation length. The red color represents the highest values while the white color represents the lowest values. Red lines of high correlation length values, extending from one to the other side are clearly visible. These lines are present because the correlation function of a stationary process gives only the information on the correlation of points in the vector **g** that are separated by certain amount of distance. This information is valid for the whole vector **g**, so in a sense we do not have any local information on the correlation. The longer the extracted vector **g** is, the ever more distant crystal grains are taken into the account in the correlation length calculation, and the less information we have on the local domain of influence of a given crystal grain. One way of dealing with this deficiency is to further limit the search area when searching for the integration points for the vector **g**. We can demand that no integration point must lie outside the certain search radius R from the selected integration point, Figure 2 (left). Figure 5 shows the calculated correlation length with the search radius R=0.1 [mm] with the superimposed crystal grain boundaries. The search radius R is roughly 4 times the average size of a crystal grain (0.023 [mm]).

We can see that the red lines lengths have decreased significantly–a direct consequence of the more localized search area. The highest value of the correlation length has also decreased. The values of the correlation length are lower at the borders of the model. In these areas the number of found points in the search area for selected direction could be zero. For these instances the correlation length cannot be calculated and is set to zero. In the averaging process this reduces the calculated correlation length. The maximal correlation length value is λ_{max}=0.0457 [mm], corresponding to roughly twice the average size of a crystal grain. The average value of the correlation length is λ_{ave}=0.025 [mm], only slightly above the average crystal grain size. The correlation length histogram is very similar to the histogram of a Gaussian random process, Figure 6. If we take into the account the correlation length standard deviation 0.0059 [mm] and presume that the correlation length distribution is indeed

Gaussian, then 68 [%] of the calculated correlation lengths are larger then the average crystal grain size.

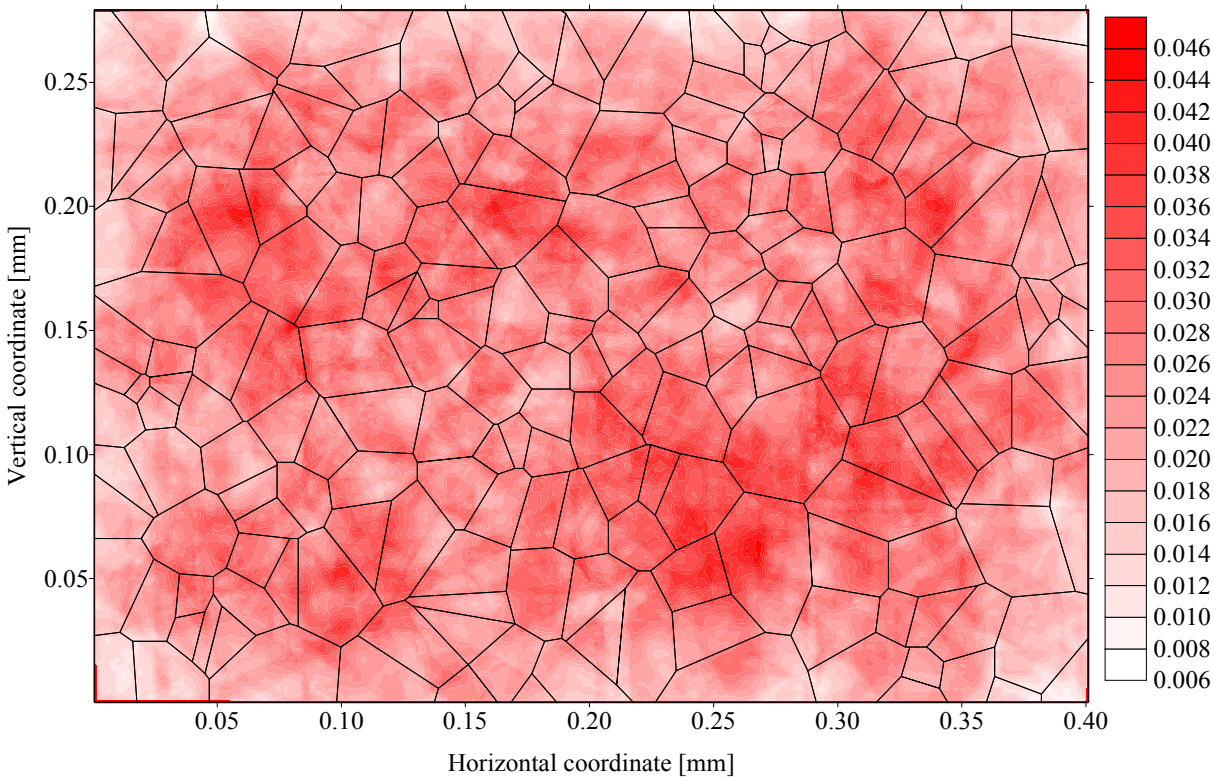

Figure 5: Correlation length, search radius R=0.1 [mm]

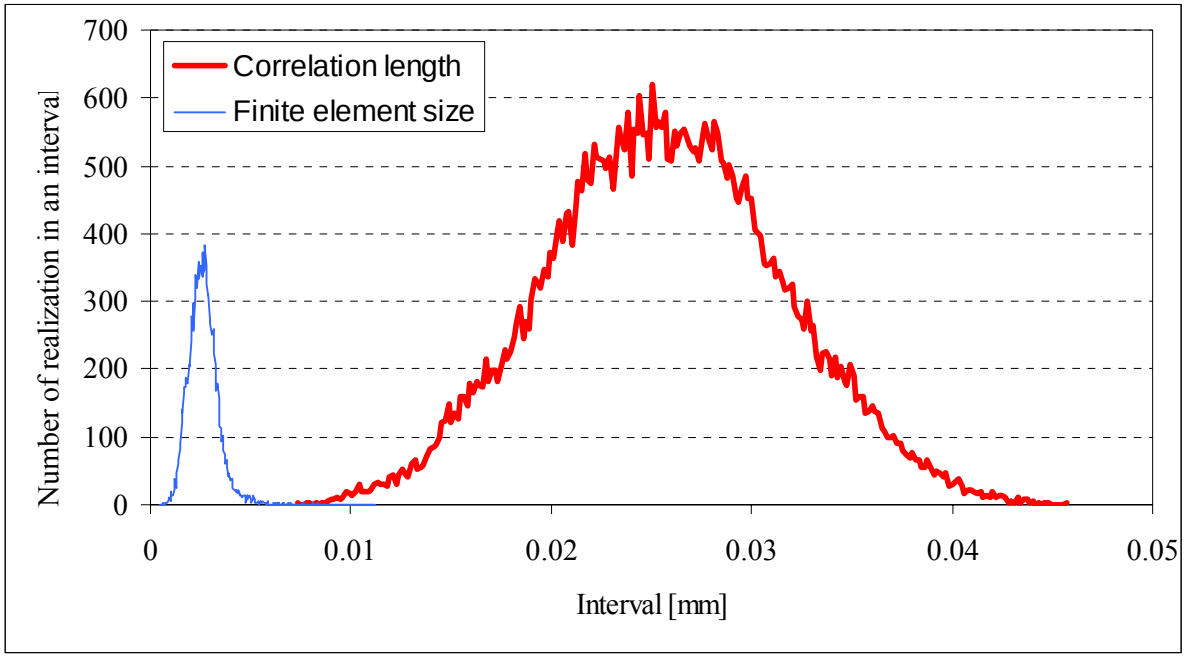

Figure 6: The correlation length and finite element size histograms

4 CONCLUSIONS

The preliminary results for estimation of a domain of influence of a crystal grain in elasticity have been presented. The domain of influence has been estimated with the calculation of a correlation length in several directions and then averaged over these directions. The correlation length is assumed to be a measure of the crystal grain domain of influence.

The correlation length is influenced by several factors. The first factor is the von Mises stress function in the selected direction. The stress distribution in the selected direction depends on the crystals, their directions and boundary/load conditions of the aggregate. If the stresses in these directions are correlated then the correlation length is large. On the other hand, if the stresses are more random, the correlation length is smaller. The tessellation process, which generates the crystal grains, therefore influences the correlation length. The second factor is the size of the search area. Since local information on the domain of influence of a single crystal grain is needed, the search area for the Gaussian integration points should be relatively small. However, if the search area is too small the number of found integration points could be too small for obtaining meaningful results. In the presented work a search radius has been introduced for limiting the size of search area. It has been shown, that this reduces the length of the highest correlation length values, see Figures 4 and 5. The alternative to this method would be calculating 2D autocorrelation function on a window of fixed size.

The results obtained show that on the average the correlation length is larger than the average crystal grain size. The maximal correlation length value is λ_{max}=0.0457 [mm], corresponding to roughly twice the average size of a crystal grain. The average value of the correlation length is λ_{ave}=0.025 [mm], only slightly above the average crystal grain size. The correlation length distribution for the whole model is very similar to the Gaussian distribution. If one takes into the account the correlation length standard deviation 0.0059 [mm] and presumes that the correlation length distribution is indeed Gaussian, then 68 [%] of the calculated correlation lengths are larger then the average crystal grain size.

The presented paper deals only with the correlation length of a model with the elasticity material model. The future work will focus on the calculation of correlation length with the crystal plasticity material model.

REFERENCES

[1] Chakraborty, S. and Dey, S.,S., “Stochastic Finite Element Method for Spatial Distribution of Material Properties and External Loading”, *Computers & Structures*, Vol. 55, No. 1, 1995, pp 41-45,.

[2] Schenk, C., A. and Schuëller, I.R., “Buckling analysis of cylindrical shells with random geometric imperfections”, *International Journal of Non-Linear Mechanics*, accepted for publication.

[3] Zheng, R. and Ellingwood, B., R., “Stochastic fatigue growth in steel structures subject to random loading”, *Structural Safety*, Vol. 20, 1998, pp. 303-323.

[4] Cizelj, L. and Riesch-Oppermann, H., “Modelling the early development of secondary side stress corrosion cracks in steam generator tubes using incomplete random tessellation”, *Nuclear Engineering and Design*, Vol. 212, 2002, pp. 21-29.

[5] Aurenhamer, Franz., "Voronoi Diagrams - A Survey of a Fundamental Geometric Data Structure", *ACM Computing Surveys*, 23(3), 1991, pp. 345-405.

[6] Grabec, I. and Gradisek, J., *Opis naključnih pojavov*, University of Ljubljana, Faculty of Mechanical Engineering, 2000.

[7] Kovač, M., Simonovski, I. and Cizelj, L., "Determination of the correlation length in stochastic material model", Kuhljevi dnevi 2002, Bled, Slovenia.

[8] Press, W.,H., Teukolsky, S.A., Vetterling, W., T. and Flannery. B. P., *Numerical Recipes in C, second edition*, Cambridge University Press, 1999.