A R C H I V E S O F M E T A L L U R G Y A N D M A T E R I A L S
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USE OF GENETIC ALGORITHMS FOR OPTIMISATION OF MATERIALS PROPERTIES

ZASTOSOWANIE ALGORYTMÓW GENETYCZNYCH DO OTYMALIZACJI WŁASNOŚCI MATERIAŁÓW

The genetic algorithm method was applied in order to decompose the texture function and to optimize elastic constants by an approprite choice of texture function. These example applications of genetic algorithm method show its potential in the field of material engineering.

Metodę algorytmów genetycznych zastosowano do analizy tekstury oraz do optymalizacji stałych sprężystych poprzez dobór odpowiedniej tekstury. Te przykładowe zastosowania metody pokazują jej potencjalne możliwości w dziedzinie inżynierii materiałowej.

1. Introduction

The genetic algorithms method (GAM) is a modern computer technique based on some ideas taken from the evolution theory [1,2]. GAM is particularly useful for a study of problems being not completely determined. These are, e.g., problems having a few but not very different solutions or problems without an exact solution. The last situation may occur if it is enough to find a good solution but not necessarily the best one. In GAM approach it is not necessary to know a priori a general scheme of solving a given problem; however, it is important to have a procedure estimating the quality of a solution. This procedure is used to eliminate some solutions and to accept another. In last years GAM was applied with success in different areas of science, e.g., in: sociology, construction engineering, artificial intelligence and many others. The present authors have already used it in the field of texture analysis [3-5]. This work reports the application of GAM for optimisation of elastic constants of a polycrystalline material. This is obtained by finding a respective crystallographic texture which leads to a given property.

2. Genetic algorithm method

In GAM it is not necessary to know a priori a general scheme of solution of a given problem but it is important to have a procedure (*accommodation function*) estimating the quality of a solution. Each possible solution I is called *individual* and is defined as a string of coefficients (*coding procedure*), e.g:
$I(p_1, \ldots, p_2, p_3, \ldots, p_M)$.
The algorithm starts with initial, random set of solutions:
I_1, I_2, ... I_N :
$I_1(p_{11}, \ldots, p_{12}, p_{13}, \ldots, p_{2M})$
$I_2(p_{21}, \ldots, p_{22}, p_{23}, \ldots, p_{1M})$
.....
$I_N(p_{N1}, \ldots, p_{N2}, p_{N3}, \ldots, p_{NM})$

The set of solutions is called population P. Consecutive iterations are done next; in each iteration three basic numerical operations are performed on solutions: *reproduction, mutation and crossover* [1,2].

– During *reproduction* each solution I_n from the population P_k gets some number of copies, proportional to its accommodation factor. The solutions with accommodation factor below a mean value for the population are removed.
– During *crossover* some (randomly chosen) pairs of solutions are retained. Next, some parts of their coefficient strings are cut in the same point and are interchanged. In the example below, the crossover for the solutions I_x and I_y is shown. The parts of coefficient strings (with indices from *1* to *r*) were cut and interchanged.

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$I_x(p_{x1}, \ldots, p_{xr}, p_{x(r+1)}, \ldots, p_{xM})$ $\quad$ $I_x(p_{y1}, \ldots, p_{yr}, p_{x(r+1)}, \ldots, p_{xM}$

$I_y(p_{y1}, \ldots, p_{yr}, p_{y(r+1)}, \ldots, p_{yM})$ $\quad$ $I_y(p_{x1}, \ldots, p_{xr}, p_{y(r+1)}, \ldots, p_{yM}$

Solutions I_x and I_y before crossover $\quad$ Solutions I_x and I_y after crossover

– During *mutation* some coefficients in some solutions are randomly changed,

After carrying out these operations on the population, P_k one gets the population P_{k+1} (starting population for the next iteration). The quality of the best solutions increases systematically with the number of iterations (populations). Calculations are stopped when the quality of the best solution is satisfactory.

3. Use of GAM in texture decomposition

The crystallographic texture is one of basic characteristics of materials. Using texture, it is possible to evaluate a macroscopic property of a material if the same quantity (and its anisotropy) is known at the crystal scale. A strict quantitative representation of texture is given by the orientation distribution function (ODF). This function gives a unique characteristic of the distribution of crystal orientations. On the other hand it enables the calculation of average physical properties for a polycrystalline material. ODF is generally calculated from a set of experimental pole figures, determined by X-ray or neutron diffraction. There exist a number of methods for this calculation (see e.g., 6-12). Having already determined ODF, it is practical in many cases to present it as a sum of main texture components, i.e., as a sum of Gauss type functions centred on selected ideal orientations. Such the decomposition enables a quick texture analysis or a simplified calculation of a sample property. This decomposition can be done using classical numerical methods (e.g., Minuit algorithm) but the calculation time becomes very long with increasing number of used texture components. Therefore, the method proposed in this work is based on the texture decomposition into Gauss type model functions [13], where their parameters and weight coefficients are found by GAM.

GAM can be also used to find optimal textures for selected material properties. Calculation of elastic constants (EC) or diffraction elastic constants (DEC) is a good example of ODF application to find macroscopic properties from crystalline ones. These constants are used in the interpretation of internal stress measurements by diffraction techniques. Two elements are necessary to calculate EC or DEC: elastic constants of single crystal (S_{ijkl} or C_{ijkl}) and numerical values of ODF. Generally, ODF is represented by its values in a set of points (forming a regular grid) in the Euler space. Each point in the Euler space defines the crystal orientation g with respect to the sample reference frame and it is expressed by φ_1, ϕ, φ_2 angles [6]. Hence, the crystal orientation can be characterized directly by three Euler angles $g = \{\varphi_1, \phi, \varphi_2\}$ or by the orientation matrix g calculated using these angles [6]. In the most frequent case of cubic crystal symmetry and orthorhombic sample symmetry, φ_1, ϕ, φ_2 vary in [0°, 90°] range, and $\Delta\varphi_1 = \Delta\phi = \Delta\varphi_2 = 5°$ steps are used for discretization; consequently ODF is presented by 19*19*19=6859 values. Stocking a huge amount of ODFs can create the computer memory problems. This difficulty is avoided if ODF is decomposed into Gauss peaks (typically of the order of ten); only a few parameters have to be recorded to define a peak (location, width and volume). This provides a tool of simplified (but sufficient for many practical purposes) texture analysis. Another advantage coming from the proposed analysis is the possibility of simplified DECs calculation using only a few texture components (ideal orientations). In this approach a property of the textured material can be approached as an average property for a few single crystals with different orientations.

The basic idea of the proposed ODF representation is to express it as a sum of Gauss-shaped functions. Special standard functions of this type, adapted to texture analysis and defined by Matthies [13], were used. These standard functions are defined by the following expression:

$$f(S, \varpi) = N(S)\exp(S\cos\varpi), \tag{1}$$

where $\varpi = \varpi(g_o, g)$ is the angular distance between the orientations g_o and g (g_o is the orientation of the peak centre and g is any orientation; $0 \leqslant \varpi \leqslant \pi$) and S is the parameter connected with the peak width: $S=\ln 2/[2\sin^2(b/4)]$ with $b \leqslant 2\pi$. The factor N(S) is the normalization constant $(N(S)=[I_o(S)-I_1(S)]^{-1}$, where I_k are modified Bessel functions [13]); it may be shown that for reasonably narrow Gauss-shaped functions ($\varpi << \pi$), an approximated formula can be used: $N(S) \approx e^{-S}\sqrt{8\pi S^3}$. Each standard function is normalized:

$$\int_G f(S, \varpi)dg = 8\pi^2, \tag{2}$$

where G denotes the orientation space.

Let us note that each standard function is defined by b and g_0. Our goal is to decompose an ODF (we denote it as F(g)) into a sum of standard functions:

$$F(g) = \sum_{m=1}^{M} a_m f_m(b_m, g_{0(m)}), \tag{3}$$

where M is the total number of used standard functions and a_m are weight coefficients ($0 \leqslant a_m \leqslant 1$). The standard functions are normalized (Eq.2), hence the weight coefficients give also the volume fractions of grains whose orientations are covered by a given standard function. Each standard function, with its weight coefficient a_m, is located at a specific orientation $g_{0(m)}$ (in texture nomenclature it is called an ideal orientation) and is defined by the half-width b_m, which in turn defines its S_m parameter.

The condition which has to be fulfilled during optimisation (accommodation function) is that the sum of considered standard functions has to be as close as possible to the analysed ODF (χ^2 test is used).
Each solution (I_n) contains the share coefficients (a_m), widths (b_m) and three Euler angles defining the centres of the Gauss functions: $g_{0(m)} = g_0\ (\varphi_{1(m)}, \Phi_m, \varphi_{2(m)})$:

$$I_n\ (a_1, b_1, \varphi_{1(1)}, \phi_1, \varphi_{2(1)},$$
$$a_2, b_2, \varphi_{1(2)}, \phi_2, \varphi_{2(2)}, ..., \ a_M, b_M, \varphi_{1(M)}, \Phi_M, \varphi_{2(M)}). \tag{4}$$

The example result of texture decomposition using this type of individuals is shown in Fig 1. The experimental texture function (Fig. 1a) was decomposed into sum of five standard functions (Eq. 3) and this sum is presented in Fig. 1b.

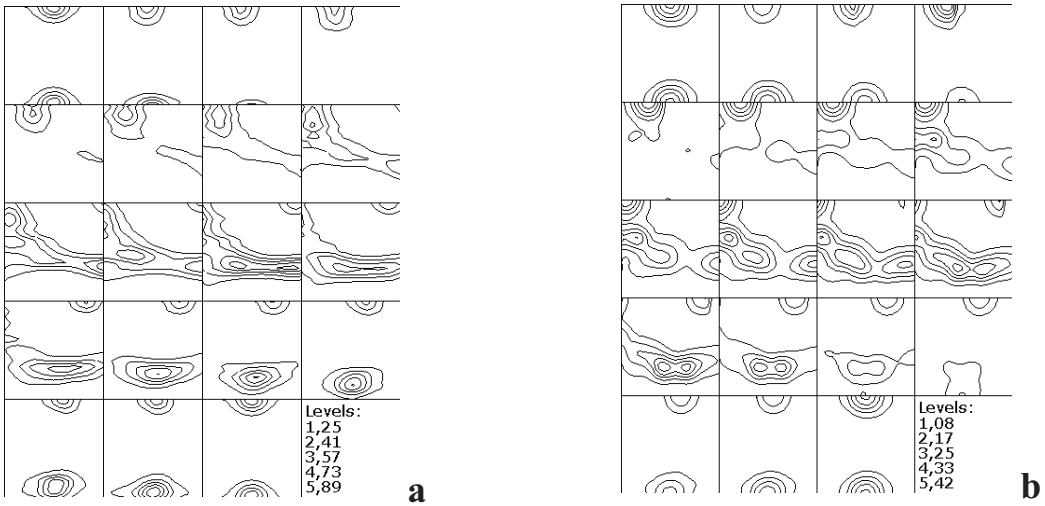

Fig. 1. Reproduction of the cold rolled steel texture: a) experimental texture, b) texture reproduced by GAM using individuals (Eq. 4) containing M=5 standard functions. φ_2=const sections are shown

The convergence of calculations, i.e. the variation of the accommodation factor vs. the number of generations is shown in Fig. 2. We note that GAM procedure is quickly convergent and after approximately hundred generations one obtains a satisfactory solution. It should be noted that in the case of M=5 used standard functions, GAM is 3-4 times faster than the classical Minuit algorithm. Moreover, this difference grows rapidly (in favor of GAM) with increasing number of Gauss standard functions.

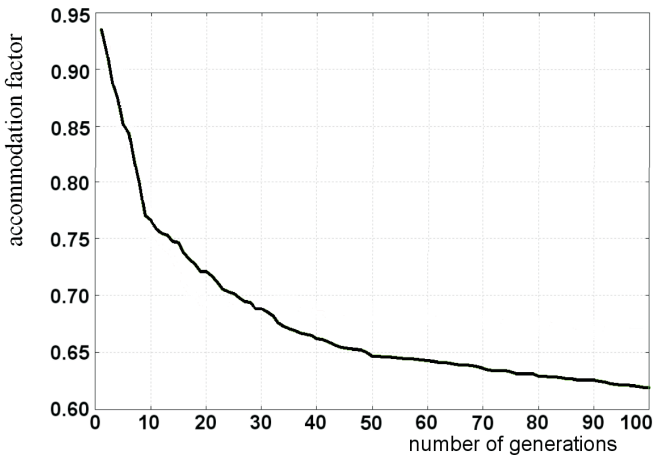

Fig. 2. Accommodation factor vs. number of generations

4. Optimization of macroscopic elastic constants

Another application of GAM, considered in this work, concerns the research of optimal elastic constants of a material. Elastic properties of crystal are described by two tensors: S_{ijkl} (compliance) and C_{ijkl} (stiffness) [14]. Calculation of the macroscopic average (i.e., sample property) will be presented for S_{ijkl} tensor. It involves two steps:

a) Single crystal tensor S_{mnop} is transformed to the sample co-ordinates system:

$$S'_{ijkl}(g) = g^T_{im} g^T_{jn} g^T_{ko} g^T_{lp} S_{mnop} \tag{5}$$

where g if the orientation matrix defining the crystal lattice orientation of a grain, generally expressed by three Euler angles: φ_1, ϕ, φ_2. This matrix relates the sample reference frame $\mathbf{K_A}$ to the crystal one $\mathbf{K_B}$, i.e.: $\mathbf{K_B}$=g $\mathbf{K_A}$, and g^T is the transposed matrix of g. Moreover, the standard repeated index summation convention is applied in Eqs. 5 and 6. The transformed elastic tensor ($S'_{ijkl}(g)$) is averaged next to obtain the mean macroscopic tensor S^M_{ijkl}'. The texture function, f(g), is the weighting parameter [6]:

$$S^M_{ijkl}{}' = \int_\Omega S'_{ijkl}{}'(g) f(g) dg = \int_\Omega g^T_{im} g^T_{jn} g^T_{ko} g^T_{lp} S_{mnop} f(g) dg \tag{6}$$

and Ω is the basic volume of the Euler angles space.

An optimal texture is often searched to produce a material with required properties. Let us perform a simple test of the presented method. The proposed example is to find a texture, which assures a minimal Young modulus (E) of the material along the $\mathbf{x_1}$ sample axis. This condition imposes the maximum value of $S^M_{11}{}' = S^M_{1111}{}'$ (because E = 1 / $S^M_{1111}{}'$).

Three independent constants (S_{11}, S_{12}, S_{44}) define elastic properties of cubic crystals [14] (standard matrix notation S_{nm} will be used for S_{ijkl} in the following text). The tensor transformation from crystal co-ordinates system to the sample one gives:

$$S^M_{11}{}' = S_{11} + \{S_{44} - 2(S_{11} - S_{12})\}(g^{T\,2}_{11} g^{T\,2}_{12} + g^{T\,2}_{12} g^{T\,2}_{13} + g^{T\,2}_{13} g^{T\,2}_{11}) \tag{7}$$

The following S_{ij} values for low carbon steel were used in the calculations: S_{11}=7,5682·10^{-6} MPa-1, S_{12}= -2.78·10^{-6} MPa-1 and S_{44}= 8,5911·10^{-6} MPa-1 [15]. Hence Eq.7, after substituting the above constants, takes form:

$$S^M_{11}{}' = 7.5682 - 12.1053(g^{T\,2}_{11} g^{T\,2}_{12} + g^{T\,2}_{12} g^{T\,2}_{13} + g^{T\,2}_{13} g^{T\,2}_{11}) \tag{7a}$$

with $S^M_{11}{}'$ expressed in MPa.

The calculation of optimal elastic properties was done using the formula for texture function given by Eq. 3 (with M=5). The orthorhombic sample symmetry and cubic crystal symmetry were taken into account in the calculations. The optimal texture (ODF), giving the minimal Young modulus (which is also the accommodation function in this case), found by GAM is shown in Fig. 3a. A minimal value of Young modulus corresponds to a maximal value of $S^M_{11}{}'$, and according to Eq. 7a, it is reached for a zero value of the following factor:

$$X = g^{T\,2}_{11} g^{T\,2}_{12} + g^{T\,2}_{12} g^{T\,2}_{13} + g^{T\,2}_{13} g^{T\,2}_{11}. \tag{8}$$

The texture minimizing Young modulus (Fig. 3a), found by GAM analysis, is the cube texture (001)[100], for which X=0.

The same procedure was used to find a texture leading to the maximal Young modulus and it is shown in Fig. 3b. A simple analytical calculation shows that in this case X should take a maximal value X=1/3, which is fulfilled for {hkl}<111> texture components. The texture found by the GAM procedure (Fig.3b) is the superposition of (112)[$\bar{1}\bar{1}$1] (i.e., $\varphi_1 = 90^0$, $\phi = 35^0$, $\varphi_2 = 45^0$) and of the orientation not far from the (110)[$\bar{1}\bar{1}$1] one (i.e., $\phi_1 = 35^0$, $\phi = 90^0$, $\phi_2 = 45^0$) components.

The above example confirms that GAM procedure works correctly (in the sense of numerical solutions).

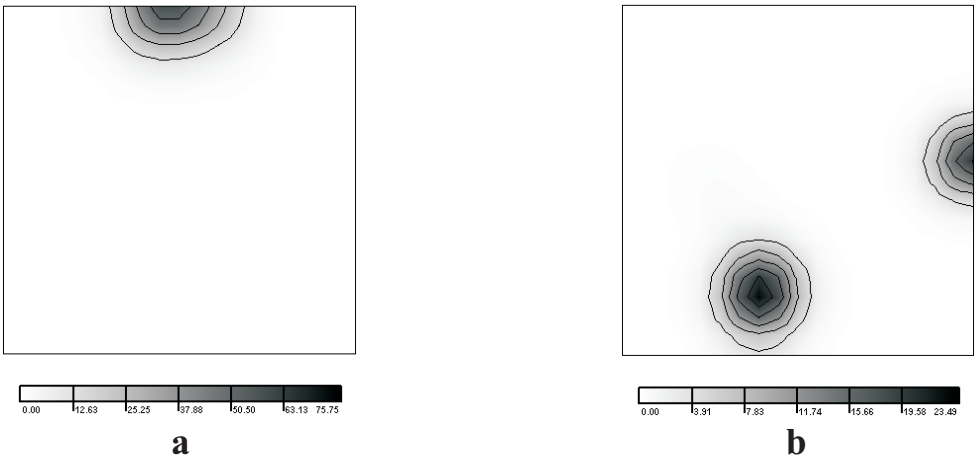

Fig. 3. Textures found by GAM leading to: a) minimal Young modulus, b) maximal Young modulus (b). $\varphi_2 = 45^0$ section is shown

5. Conclusions

GAM can be used to find material parameters which lead to optimal properties. It furnishes good results (but not necessarily the best one) verifying some imposed criteria. In each practical case a reasonable compromise between the calculation time and the solution quality has to be found. In the present work the test example of optimisation concerns the Young modulus, but the method is quite general and it can be applied to other physical properties.

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