Optimization of Material Properties Using Genetic Algorithms

The genetic algorithms method (GAM) was originally based on ideas taken from biological **evolution theory**.

Now, GAM is a modern computer technique widely used in different fields of **science and technology**.

Basic elements of GAM

In GAM it is not necessary to know a priori a general scheme of solution of a given problem.

It is important to have a procedure estimating the quality of a solution, ie. : ***accommodation function***

Each possible solution *I* of a studied problem is called an *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 an initial random set of solutions:
$I_1, I_2, \ldots I_N$:

$$I_1 (p_{11}, \ldots, p_{12}, p_{13}, \ldots, p_{1M})$$
$$I_2 (p_{21}, \ldots, p_{22}, p_{23}, \ldots, p_{2M})$$
$$\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots$$
$$I_N (p_{N1}, \ldots, p_{N2}, p_{N3}, \ldots, p_{NM})$$

The set of solutions is called *population* ***P***

In consecutive iterations we perform:
reproduction, mutation and ***crossover***

* 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.

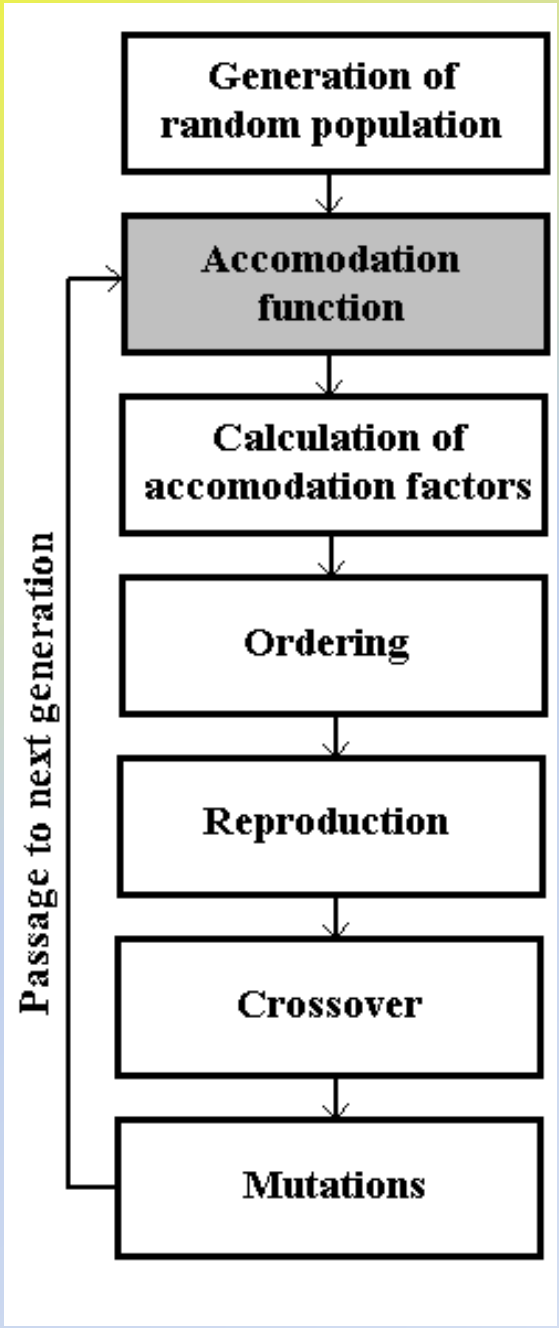
$I_x\ (p_{x1}, \ldots, p_{xr}, p_{x(r+1)}, \ldots, p_{xM})$
$I_y\ (p_{y1}, \ldots, p_{yr}, p_{y(r+1)}, \ldots, p_{yM})$

solutions I_x and I_y before crossover

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

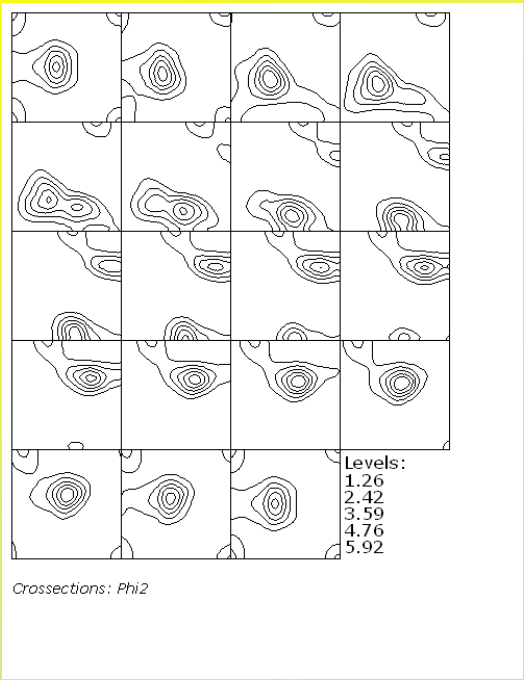
solutions I_x and I_y after crossover

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

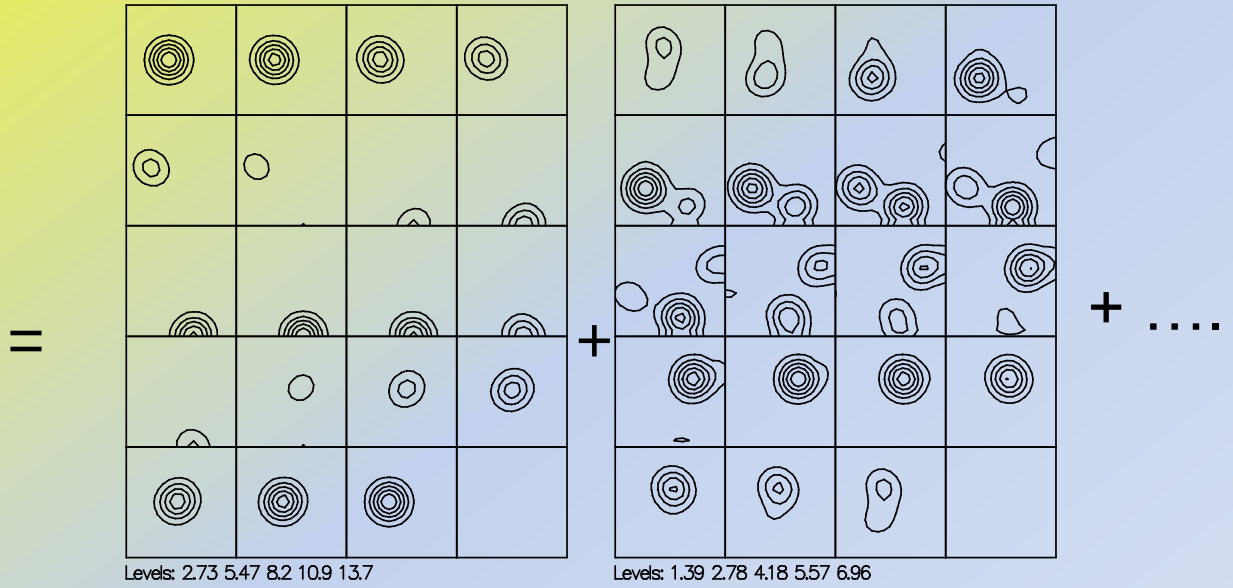

Generation of random population
Accomodation function
Calculation of accomodation factors
Ordering
Reproduction
Crossover
Mutations
Passage to next generation

Idea of texture decomposition .....

Rolling copper texture



Exemple standard functions



B component: $(35^0,45^0,90^0)$ **S** component: $(59^0,37^0,63^0)$

Component	Component symbol	φ_1	ϕ	φ_2
{112}<111>	Copper, C	90	35	45
{123}<634>	S	59	37	63
{011}<100>	Goss, G	0	45	90
{011}<211>	Brass, B	35	45	90
{4,4,11}<11,11,8>	Dillamore, D	90	27	45
{001}<100>	Cubic	0	0	0

Texture components in rolled FCC metals

Idea of texture decomposition .....

Definition of STANDARD function (Gauss-shaped function; Matthies, 1987):

$$f(S, \varpi) = N(S)\, exp\, S\, cos\, \varpi)$$

where:

$\varpi = \varpi(g_o, g)$ - is the angular distance between orientations g_o and g $(0 \leq \varpi \leq \pi)$,

S - is connected with the peak width: $S = \frac{ln2}{2\,[\sin(\frac{b}{4})]^2}$ with $b \leq 2\pi$,

$N(S)$ - is the normalization constant.

Use of GAM in texture decomposition

$$f(g) = \sum_{m=1}^{M} a_m f_m\left(b_m, g_{0(m)}\right)$$

Each solution for $f(g)$, i.e.: $\boldsymbol{I_n}$ contains

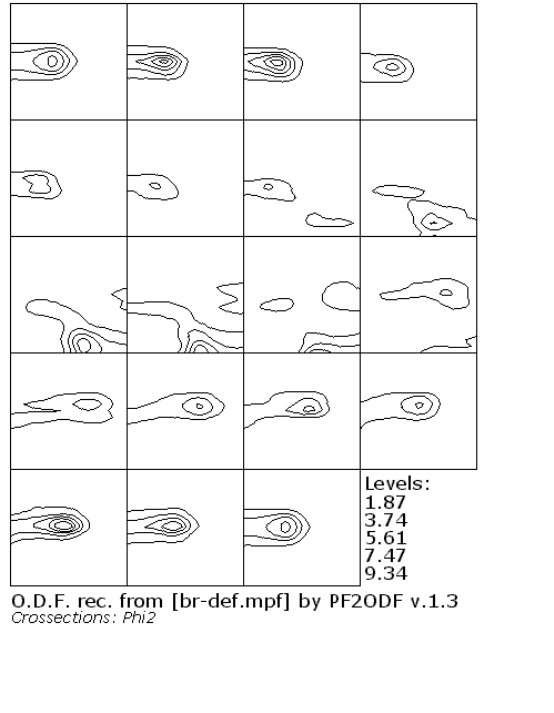
- share coefficients (a_m) and widths (b_m) of gaussian functions, and
- three Euler angles defining the centers of the Gauss functions:

  $g_{0(m)} = g_0\,(\varphi_{1(m)}, \Phi_{(m)}, \varphi_{2(m)})$:

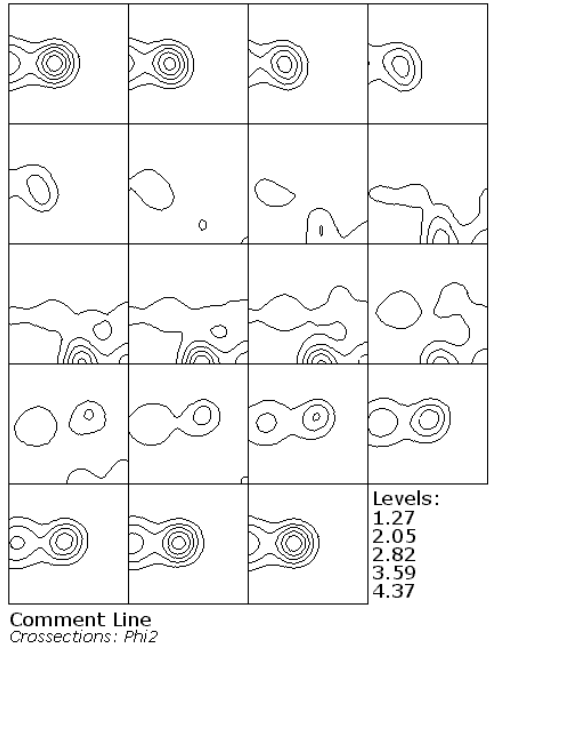
$$I_n\,(\,a_1, b_1, \varphi_{1(1)}, \Phi_{(1)}, \varphi_{2(1)},\ a_2, b_2, \varphi_{1(2)}, \Phi_{(2)}, \varphi_{2(2)}, \ldots\ldots,\ a_M, b_M, \varphi_{1(M)}, \Phi_{(M)}, \varphi_{2(M)}\,)$$

The **accommodation condition** is:
the sum of standard functions has to be as close as possible to the analysed ODF
(χ^2 test is used).

Example 1: Cold rolled brass texture



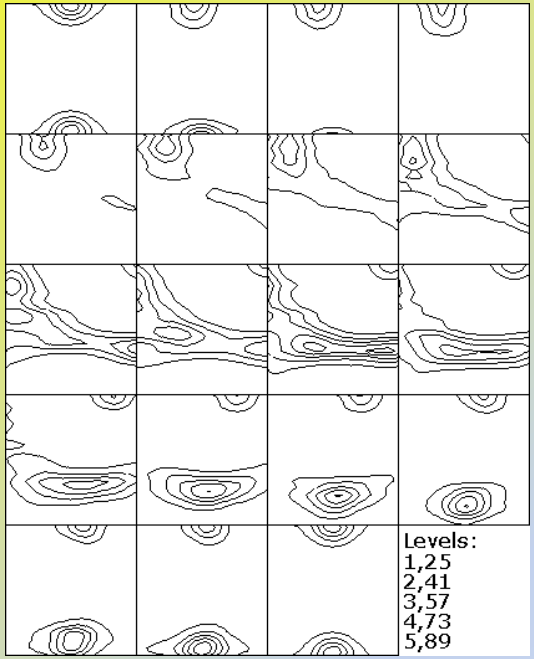
experimental texture



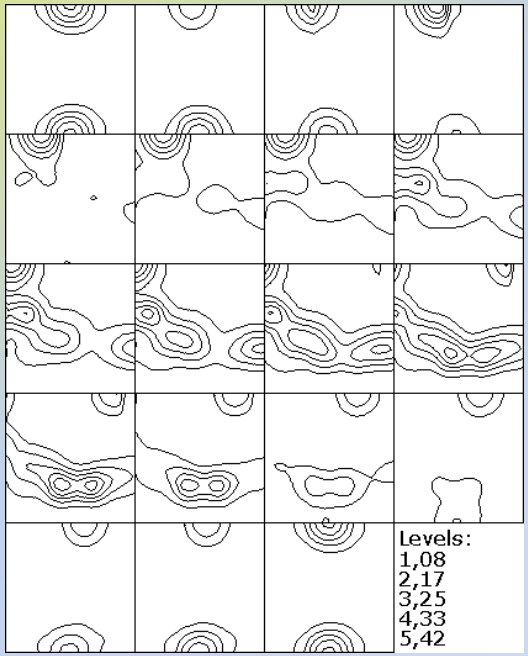
texture reproduced by GAM
(with *M*=6 standard functions)

(φ_2=const sections are shown)

Example 2: Cold rolled ferritic steel texture



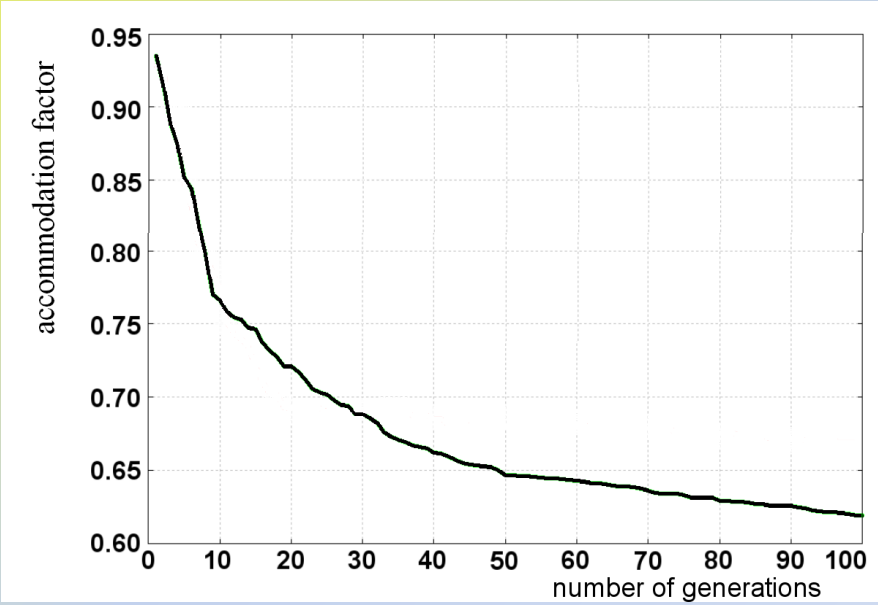
experimental texture



texture reproduced by GAM
(with *M*=5 standard functions)

(φ_2=const sections are shown)

Convergence of the method …..



Accommodation factor vs. number of generations

GAM on the research of optimal elastic constants

1) Single crystal (grain) tensor S_{mnop} transformed to the sample co-ordinates system:

$$S_{ijkl}'(g) = a_{im}^{t} a_{jn}^{t} a_{ko}^{t} a_{lp}^{t} S_{mnop}$$

where a_{ij} is the transformation matrix (from sample to crystal reference system):

2) Transformed elastic tensor is averaged (using texture function $f(g)$):

$$S_{ijkl}^{M}{}' = \int_{\Omega} S_{ijkl}'(g) f(g) dg = \int_{\Omega} a_{im}^{t} a_{jn}^{t} a_{ko}^{t} a_{lp}^{t} S_{mnop} f(g) dg$$

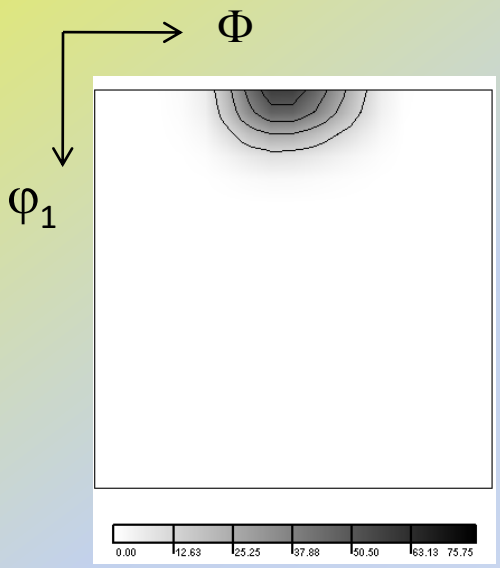
Example: **Optimization of Young modulus :**

$$E = 1/S_{1111}{}'$$

a) Find a texture, which gives a **minimal** E (along $\mathbf{x_1}$ axis).

Hence: $S_{1111}{}' = \max$

Texture found by GAM



It is the cube texture: **(001)[100]**

φ_2=45^0 section is shown

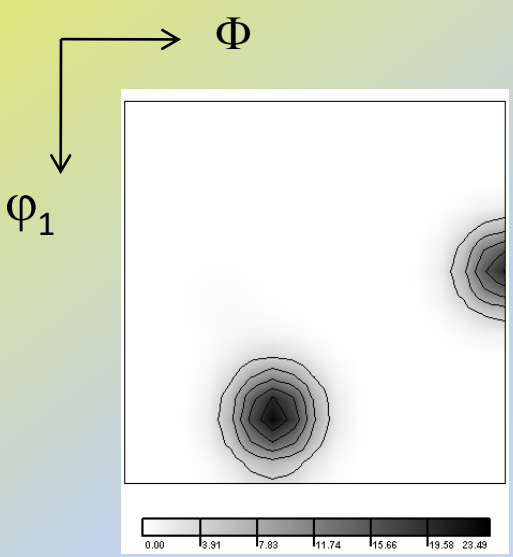
Example: **Optimization of Young modulus :**

$$E = 1/S_{1111}{}'$$

b) Find a texture, which gives a **maximal** E (along $\mathbf{x_1}$ axis).

Hence: $S_{1111}{}' = \min$

Texture found by GAM



It is superposition of

$\mathbf{(112)[\bar{1}\bar{1}1]}$ and $\mathbf{(110)[1\bar{1}\bar{1}]}$ components

φ_2=45^0 section is shown

Conclusions

GAM can be used to find material parameters which lead to optimal application properties.

It furnishes good enough 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.