MATHEMATICAL MODELS OF ULTRA-FINE GRAINED MATERIALS BASED ON DISSIPATION NORMAL FORM

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Abstract

Dissipation normal form (DNF) is a special system structure which originally came from the signal and system theory. It was derived from natural requirements of some form of an abstract energy conservation law validity. Strong nonlinearities brought into the DNF parameters can cause complex irregular oscillations of the system. Such a system is used as a generator of numerical sequencies whose properties are useful for mathematical modelling of irregularities in real fine and ultra-fine grained metal microstructures. The particular metal grains are modelled as the Gaussian curve with a 2-dimensional domain and their partial properties such as their height, width, position in the surface, elongation in a certain direction etc. can be chaotically modified. A certain part of grains can be modified separately by irregular splitting their area etc. It allows to define the individual components surface percentage to meet important statistical properties of the real material with complicated structure. In the contribution there it is shown that the presented mathematical model approximates real multiphase microstructure quite well and using DNF with strong nonlinearities represents approach with good prospects to mathematical modelling of metal microstructures including complex ones.

Key words

Chaotic systems, microstructure of metals, ultra-fine grained metal, mathematical modelling

1 INTRODUCTION

During last decades, the chaos theory evolved into a discipline which intervenes in many branches. Among others, chaotic oscillations can be found in fluid flows, nonlinear electronic circuits or dynamics of populations. Vibrations in nonlinear mechanic systems can have chaotic character as well. [1] Chaotic signals are deterministic but their time behaviour is unpredictable in the long term. It is impossible to find any periodicity in the chaotic oscillations. From that point of view they are indistinguishable from stochastic signals. It can be very useful for mathematical modelling. It is paradoxical that chaotic signals are unpredictable but they can be controlled and even synchronized [2]. Chaotic signals can be generated both continuous- and discrete-time systems. In linear systems chaotic oscillations are impossible. In case of discrete-time domain, we can generate chaotic sequence using autonomous system of the second order with suitable nonlinearity. For applications it is convenient to work with systems of higher orders.

2 DISCRETE-TIME CHAOS SYNTHESIS

Systematic methods of chaotic systems synthesis were recently developed. The method is based on introducing suitable nonlinearities in a special system structure which is called „dissipation normal form“ [3], [4]. In following we briefly describe derivation of this structure in discrete-time domain and show how to synthetize chaotic systems of arbitrarily high finite order.
2.1 Dissipation normal form in discrete-time domain

Consider a state representation of linear, strictly causal \( n \)-order system with scalar input and scalar output:

\[
x(k + 1) = Ax(k) + Bu(k)
\]

\[
y(k) = Cx(k)
\]

\[
\text{dim } A = n \times n \quad \text{dim } B = n \times 1 \quad \text{dim } C = 1 \times n
\]

Some form of energy conservation law should hold in every real system. When we come from the signal theory, we can define an abstract system energy \( E(x,k) \) and the output signal power \( P(k) \) as well:

\[
E(x,k) = \frac{1}{2} \| x(k) \|^2 \quad P(k) = -\| y(k) \|^2
\]

It is assumed that the system is dissipative. Considering zero input \( u(k) = 0 \) we can write an equation expressing a power balance condition:

\[
\Delta E = E(x,k + 1) - E(x,k) = \frac{1}{2} \| x(k + 1) \|^2 - \| x(k) \|^2 = -P(k) = -\| y(k) \|^2
\]

We can substitute (1) into (3) and after some manipulations we obtain that it must hold

\[
[A^T A - I] = -C^T C
\]

Dissipation normal form is the system structure which corresponds to the equation (4). Hence it can be derived that the \( A, B \) and \( C \) matrices have following structure (for a 4th-order system):

\[
A = \begin{bmatrix}
-\Delta_3 \Delta_4 & \delta_3 & 0 & 0 \\
-\Delta_2 \delta_3 \Delta_4 & -\Delta_2 \Delta_3 & \delta_2 & 0 \\
-\delta_1 \delta_2 \delta_3 \Delta_4 & -\Delta_1 \delta_2 \Delta_3 & -\Delta_1 \Delta_2 & \delta_1 \\
\delta_1 \delta_2 \delta_3 \Delta_4 & \delta_1 \delta_2 \Delta_3 & \delta_1 \Delta_2 & \delta_1
\end{bmatrix}
\]

\[
B = [\beta_1 \beta_2 \beta_3 \beta_4]^T
\]

\[
C = [\gamma \ 0 \ 0 \ 0]
\]

For parameters in the \( B \) and \( C \) matrices it holds:

\[
\gamma = \delta_n \neq 0 \quad \beta_i \neq 0, \quad i \in \{1,2,\ldots,n\}
\]

Following conditions are related to the system stability and the system structural minimality as well. Parameters \( \delta_i \) and their complements \( \Delta_i \) in the \( A \) matrix must satisfy:

\[
\forall i, i \in \{1,2,\ldots,n\}: \quad 0 < \delta_i \leq 1, \quad \delta_i^2 + \Delta_i^2 = 1
\]

Necessary condition of the system asymptotic stability is

\[
\forall i, i \in \{1,2,\ldots,n\}: \quad |\Delta_i| < 1
\]

Physical interpretation of all the parameters and their measure depend on application (e.g. physical qualities formed in the state vector \( x(k) \)).

2.2 Autonomous discrete-time chaotic systems based on dissipation normal form

Dissipation normal form can be successfully used for design of nonlinear oscillating systems including systems with complex behaviour and high order [2], [5]. The structure derived above is linear. Bringing suitable nonlinearities into the system parameters can radically change its behaviour and lead to chaotic oscillations occurrence. Parametrization of dissipation normal form requires validity of expressions (9) and
If we break those conditions and absolute value of some $\Delta_i$ parameter is greater than one, the system will be unstable, because those parameters represent a local feedback in the structure. If, however, was some $\Delta_i$ parameter zero, no instability could occur in relevant part of the structure. Suitably chosen nonlinearity can cause changing intervals of stability and instability by increase and decrease in value of some $\Delta_i$ parameter. For suitable parametrization the arised oscillations can be chaotic.

Another interesting class of systems which can exhibit complex behaviour is the class of systems with linear parameters where the nonlinearity is present in switching of some parameters sign [5]. The system is designed as conservative, i.e. $\Delta n = 1$, and its energy (eq. (2)) is constant. The state vector moves along the $n$-dimensional hypersphere which radius is given by initial conditions. After several iterations (time steps) the sign of some parameters is changed to opposite. The system energy stays constant.

As an example let us introduce the following system of 4th order. Its structure is given by equation (5) and its parametrization is

$$\begin{align*}
\Delta_1 &= \pm 0.9, \\
\delta_1 &= \sqrt{1 - \Delta_1^2}, \\
\Delta_2 &= \Delta_3 = c, \\
\delta_2 &= \delta_3 = \sqrt{1 - \Delta_2^2} = \sqrt{1 - \Delta_3^2}, \\
\Delta_4 &= 1, \\
\delta_4 &= 0
\end{align*}$$

The sign of the $\Delta_1$ parameter is switched after 15 iterations. The $\Delta_2$ and $\Delta_3$ parameters are used as the control ones. Their value affects particular sequence generated by the system. Histograms of chaotic sequences generated by this system are depicted at the Fig. (1). This system was used for modelling of metal microstructures in following numerical experiments.

![Fig. 1: Histograms of sequences generated by the chaotic system with control $\Delta_2 = \Delta_3 = 0.99$. These sequences were used for replacement of grains in the mathematical model described below.](image)

### 3 MODELLING OF METAL MICROSTRUCTURE

Chaotic sequences which are generated by the system described above can be used for mathematical modelling of irregularities in polycrystalline metals microstructures [6] or multiphase microstructures. Some sequences are used for modelling of grain position, another ones modify parameters like distribution of the phases in the multiphase microstructure.

#### 3.1 Model of grain and metal microstructure

Particular grains are represented by the Gaussian bell curve with a two-dimensional domain. In this particular example, all the grains have the same weight and height. Their final position on the surface is not regular but re-defined by chaotic sequence. At the figure (2) there is an illustrative example of several such grains with originally regular placement and after re-placement. The basic model comes from 2D-view and from marking boundary lines between adjacent grains. Described procedure can be used for modelling of some fine-grained structures [6].
3.2 Mathematical model of multiphase microstructure

For modelling of complicated metal structures such as TRIP steel we must provide another series of modification to meet the real specimen properties. In following we describe the development of the multiphase microstructure (ferrite, bainite, austenite) mathematical model.

Fig. 3: a) advanced mathematical model b), c) several grains are assigned to ferrite and removed, the remaining grains are splitted d) chaotically distributed “austenite” particles
We come from the basic model described above, see fig. (2 d). The next step is searching for points where three grains make contact. Coordinates of these points are used for another smaller grains placement. This procedure does not use chaotic sequence and provides results depicted at the figure (3 a).

Now we have structure with grains of various size. The biggest grains of the modelled multiphase microstructure are assigned to ferrite and excluded from subsequent modification of the mathematical model, see fig. (3 b).

Searching for unoccupied grains and their splitting into smaller pieces follows. The splitting is solved by the same procedure as the splitting of the basic model original area. New grains are placed at the splitted grain area and their new boundaries are found. The situation is depicted at the fig. (3 b,c). The procedure is repeated twice. A number of grains is assigned to the particular phase (ferrite) of the modelled metal microstructure to capture the main statistical properties of the real specimen.

The remaining grains are used for modelling of the austenite grains. The austenite is represented by white color and it is chaotically distributed over the remaining small particles. The rest of the picture is black. The small white adjacent grains are put together to represent bigger grains with irregular shape. At this step we have a lot of white grains of various size (fig. 3 d)). It allows to choose grains with suitable surface area to meet the real specimen properties. Redundant white grains are removed (turned into black color). The grains which are not assigned to ferrite and austenite represent the third phase (bainite) of the multiphase microstructure.

Fig. 4: Comparison of the microscope photography and the mathematical model, multiphase microstructure (ferrite, bainite, austenite). Width and height of both pictures correspond to 83 x 64 μm.

<table>
<thead>
<tr>
<th></th>
<th>Measured sample</th>
<th>Mathematical model</th>
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<tbody>
<tr>
<td></td>
<td>Ferrite</td>
<td>Austenite</td>
</tr>
<tr>
<td>Number of grains</td>
<td>543</td>
<td>85</td>
</tr>
<tr>
<td>Percentage of surface [%]</td>
<td>48,6</td>
<td>8,06</td>
</tr>
<tr>
<td>Average grain surface [μm²]</td>
<td>4,84</td>
<td>5,12</td>
</tr>
<tr>
<td>Median of grain surface [μm²]</td>
<td>1,13</td>
<td>3,77</td>
</tr>
<tr>
<td>Biggest grain surface [μm²]</td>
<td>95</td>
<td>27</td>
</tr>
</tbody>
</table>
At the figure (4 b) there is the final mathematical model. All the grains are depicted together in the final figure. Obtained mathematical model is compared with the specimen at the figure (4 a). The results are summarized in the Tab. 1.

4 CONCLUSION

Discrete-time chaotic system of 4th order with switching was synthetized and sequencies generated by the system were used for modelling of multiphase metal microstructure. It is shown that the mathematical model approximates the real microstructure very well. The main advantage of this approach is the respect to nonlinearities in the real objects. Particular grains in the mathematical model can be modified individually and modelling in several steps allows to capture the statistical properties of real materials quite accurately.

There is a wide space for another research and described methods can be evolved in several ways to meet specific properties of fine and ultra-fine grained materials.

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