MATHEMATICAL MODELLING OF ULTRA-FINE GRAINED MATERIAL AS A DISCRETE-TIME CHAOTIC SYSTEM

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Abstract

Strongly nonlinear dynamic systems with suitable parametrization can exhibit chaotic oscillations. These irregular oscillations have bounded amplitude but no period. Therefore it is natural to use them for modelling irregularities in microscopic structure of metals. In this work, discrete-time chaotic systems of fourth order with switching were synthetized. A sequence of numbers generated by these systems were used for definition of metal grains properties such as their size and position on the surface. Individual particles properties were modified by the chaotic system as well. Obtained mathematical model is compared with results of ultra-fine grained titanium sample observation and measuring.

Keywords: 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. Very interesting applications of the chaos theory can be found in molecular biology, chemistry, medicine, cryptography etc. [1]

Chaotic signals have several remarkable properties. They 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. That is the reason why they are described by means of statistics sometimes. It is paradoxical that chaotic signals are unpredictable but they can be controlled and even synchronized. Controlled chaos synthesis is useful for mathematical modelling.

Chaotic signals can be generated both continuous- and discrete-time systems. Considering zero input, for generation of continuous-time chaotic oscillations it is necessary to synthetize a system of at least third order with at least one strong nonlinearity. 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. To synthetize several classes of autonomous chaotic systems with different properties in both continuous-time and discrete-time domain, it is possible to come from special system structure which is called „dissipation normal form“ [2], [3]. 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:
Some form of energy conservation law should hold in every real system. When we come from the signal theory, we can define abstract system energy and the signal power as well:

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

(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:

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

(3)

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

\[ \begin{bmatrix} A^T & A - I \end{bmatrix} = -C^T C \]  

(4)

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):

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

(5)

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

(6)

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

(7)

For parameters in the B and C matrices it holds:

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

(8)

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

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

(9)

Necessary condition of the system asymptotic stability is

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

(10)

The final structure is depicted in the figure (1). The trajectory of the state vector in the state space and corresponding time evolution of the system energy are depicted in the figure (2), the example is related to a system of the second order. We can see the monotonous decrease of the system energy what characterizes dissipative systems. The derived system structure is also known as so called lattice-ladder IIR filters structure. When the \( \Delta_i \) parameters are zero, the structure turns into standard transversal FIR filters structure.
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 [4]. The structure derived above is linear. Bringing suitable nonlinearities into the system parameters can radically change its behaviour and lead to chaotic oscillations occurrence. Brief description of two different classes of chaotic systems based on this structure follows.

2.2.1 Systems with nonlinear parameters

Parametrization of dissipation normal form requires validity of expressions (9) and (10). 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. Examples you can find in [4], [5]. For suitable parametrization the arised oscillations can be chaotic.

2.2.2 Chaotic systems with switching

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. $\Delta_i = 1$, 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 $4^{th}$ order. Its structure is given by equation (5) and its parametrization is
\[ \Delta_1 = \pm 0.9 \quad \delta_1 = \sqrt{1-\Delta_1^2} \]
\[ \Delta_2 = \Delta_3 = c \quad \delta_2 = \delta_3 = \sqrt{1-\Delta_2^2} = \sqrt{1-\Delta_3^2} \quad c \in (0, 1) \]  
\[ \Delta_4 = 1 \quad \delta_4 = 0 \]  

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. 2D projection of the chaotic attractor and behaviour of the system energy are depicted at the figure (3), $\Delta_2 = \Delta_3 = 0.9$. This system was used for modelling of metal microstructures in following numerical experiments.

![Fig. 3: Projection of the chaotic attractor to the $(x_1, x_2)$ plane and the system energy time evolution](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. Depending on the control parameters value, the system generates sequences whose histograms can be very different. Some sequences are used for modelling of grain position, other ones modify parameters like: grain size, shape deformation, crystal lattice orientation, etc.

3.1 Model of grain and metal microstructure

Particular grains are represented by simple gaussian hat. Position of the grains on the surface is defined by chaotic sequence. For this purpose a sequence with normal distribution of values is suitable. Designed system generates such sequences with control parameters $\Delta_2 = \Delta_3 = 0.73$, state variables $x_3$ and $x_4$ are used. At the figure (4) there is an illustrative example of several such grains with different height and width. These properties are modified by numbers from the chaotic sequences which are generated by the same system and control parameters $\Delta_2 = \Delta_3 = 0.99$. In that case the chaotic sequence does not have the normal distribution but values around 0.8 occur with higher frequency (see fig. 5).

![Fig. 4: Illustrative example of mathematical model of metal grains – 3D view, 2D view and marked boundary lines between adjacent grains – a basic model of a metal microstructure](image)
3.2 Mathematical model of metal microstructure in comparison with measured sample

An EBSD map of grain orientation and histogram of grain size of ultra-fine grained titanium sample was chosen for evaluation of described modelling method.

Mathematical model of the metal microstructure was computed with use of 220 grains. Some of them were overlapped by other ones. One half of grains were systematically computed as higher and narrower than the other half to meet the character of the measured sample. Particular grains were colored with use of chaotic sequencies as well. Comparison of results for measured sample and for mathematical model is at the figure (6).

Statistical results for both figures are summarized in tab. (1). All the calculations including counting particles were made in MATLAB with use of Image Processing Toolbox. Grain sizes were computed in pixels. One pixel corresponds to length 0.05 μm or surface 2.5x10^{-3} μm²; the results were recalculated to meet these dimensions. Histograms of grain size for both figures (6) are at the figure (7).

Fig. 5: Histograms of sequencies generated by the chaotic system with control $\Delta_2 = \Delta_3 = 0.99$. These sequencies were used for modifying of the grains parameters (width and height).

Fig. 6: EBSD measured sample of ultra-fine grained titanium in comparison with mathematical model. Width and height of both pictures correspond to 25 x 25 μm.

Fig. 7: Histograms of grain size.
Tab.1: Measured and modelled results

<table>
<thead>
<tr>
<th></th>
<th>Measured sample</th>
<th>Mathematical model</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of grains</td>
<td>173</td>
<td>175</td>
</tr>
<tr>
<td>Average grain surface $[\mu m^2]$</td>
<td>2.71</td>
<td>2.85</td>
</tr>
<tr>
<td>Median of grain surface $[\mu m^2]$</td>
<td>1.74</td>
<td>2.32</td>
</tr>
<tr>
<td>Biggest grain surface $[\mu m^2]$</td>
<td>13.69</td>
<td>12.91</td>
</tr>
</tbody>
</table>

4 CONCLUSION

Discrete-time chaotic system of 4th order with switching was synthetized and sequences generated by the system were used for modelling of ultra-fine grained metal microstructure. It is shown that the mathematical model can approximate the real microstructure quite well. The main advantage of this approach is the respect to nonlinearities in the real objects. On the other hand, it is technically impossible to rely on principles which are valid for linear systems, e.g. principle of superposition. It makes the nonlinear models complicated but interesting as well.

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LITERATURE