MODELLING OF EXCITED STATES OF A CRYSTAL BASING ON THE FREQUENCY-PHASE SYNCHRONIZATION OF VIBRATIONS OF A CRYSTAL SITE LATTICE

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ABSTRACT

Model of an excited solid as a system of non-linear oscillators is considered in the work. State of the spatial dis-tribution for the system of oscillators and its limitation was shown to be a condition for transition of a solid into excited state. Mechanism responsible for structural transformations in the range of excitation is frequency-phase synchronization resulting in the formation of dynamically active cluster areas and dissipation of the energy.

1. INTRODUCTION

The presence of excited states is characteristic of a real crystal. These states appear under pulse laser illumination, cyclic disturbance or thermal or mechanical break. They are characterized by the presence of cooperative effects, steady properties, dissipation of thermal, acoustic and electromagnetic energy-Ref. 1. For the interpretation of these effects it is necessary to apply some dynamic methods such as theory of determinated chaos. In the work we present the results of modeling of appearance of the excited states in a crystal which are considered to arise due to synchronization in spatially distributed system of chaotic vibrations. When considering the effects connected with the excitation of atomic sites in a crystal lattice of a solid it is assumed that all of them form chaotic vibration system.

2. BASIC MODEL

One-dimensional chain of the bound Ressler oscillators is considered as a base model -Ref. 2. (Fig. 1).

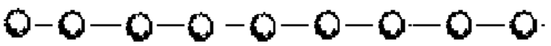

Fig. 1. Base model of one-dimensional chain of Ressler oscillators.

For j-th oscillator a system of equations can be written as follows:

$$\dot{x}_j = -\omega_j y_j - z_j$$
$$\dot{y}_j = \omega_j x_j + a\, y_j + \gamma\,(y_{j-1} - 2y_j + y_{j+1})$$
$$\dot{z}_j = b + z_j\,(x_j - c)$$

(1)

Here γ is bond parameter, a is a parameter determining chaotic character of the oscillator; b, c are oscillator parameters. Conditions of appearance of synchronization effect in dependence on chaos kind (weak chaos at the values of parameter $a \le 0.21$ and strong chaos at $0.21 < a \le 0.3$) have been studied as well as on bond parameter γ, length of the chain and spatial structure of the model. In order to investigate these parameters numerical solution of the system of equations was found using computer and applying the following boundary conditions:

$$y_0 = 0;$$
$$y_{N+1} = 0; \qquad (2)$$

To determine a degree of vibration synchronism we calculated the mean phase difference for oscillator vibrations in a chain. Phase difference for a couple of the neighbouring oscillators was calculated by the formula:

$$\Lambda\Phi = \sin^2\left(\frac{y_j/x_j - y_{j+1}/x_{j+1}}{2}\right)$$

(3)

and it means that synchronization of vibrations is considered in a space but not a synchronization of the time realization taken separately. It was found that with an increase of the bond parameter between oscillators the mean phase difference of vibrations in the chain is reduced tending to zero (fig. 2).

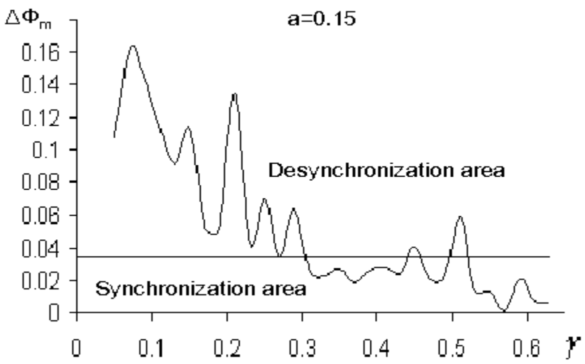

Fig. 2. Dependence of the mean phase difference of vibrations for a chan of Ressler oscillators on the bond parameter between the oscillators.

For estimation of the influence of a degree of chaotic state on the possibility of synchronization in one-dimensional system of the oscillators one can see that with an increase of parameter a and, hence, a degree of chaotic state in vibrations of each of the oscillators synchronic character of vibrations is reduced. It is absolutely absent in a strong chaotic state (a=0.3) (fig. 3).

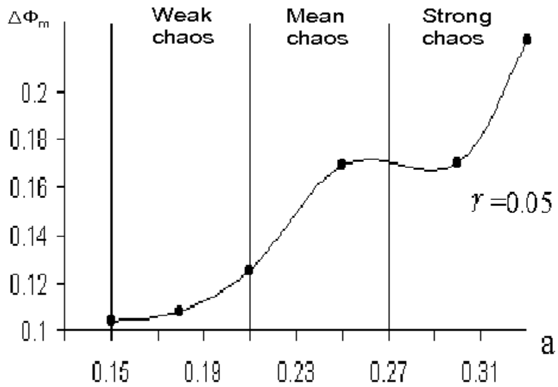

Fig. 3. Dependence of the mean phase difference for vibrations in the chain of Ressler oscillators on parameter a (the case of strongly bound oscillators).

Strong chaos just corresponds to the real system of the atoms vibrating in the sites of crystal lattice. But any real crystal lattice is a spatial-distributed system. Therefore, it seems reasonable to proceed from consideration of one-dimensional chain of Ressler oscillators to spatially-distributed system.

3. SPATIALLY-DISTRIBUTED MODEL

Two-dimensional model used in the work is a couple of two chains each containing 50 Ressler oscillators, which are crossed in a single point, i.e. they have one common site being an oscillator -Ref. 3 (fig. 4).

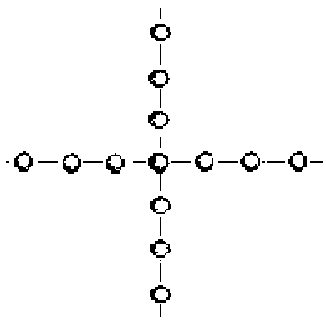

Fig. 4. Spatially-distributed model chain of the bound Ressler oscillators.

A system of equations along the axes x and y has the following form:

For x: $$\dot{x}_j = -\omega_j y_j - z + \gamma(x_{j-1} - 2x_j + x_{j+1})$$

$$\dot{y}_j = \omega_j x_j + a\, y_j$$

$$\dot{z}_j = b + z_j\,(x_j - c)$$

(4)

For y:

$$\dot{x}_j = -\omega_j y_j - z_j$$

$$\dot{y}_j = \omega_j x_j + a\, y_j + \gamma\,(y_{j-1} - 2y_j + y_{j+1})$$

$$\dot{z}_j = b + z_j\,(x_j - c)$$

(5)

Equations for the common oscillator for both chains can be written as:

$$\dot{x}_j = -\omega_j y_j - z + \gamma\,(x_{j-1} - 2x_j + x_{j+1})$$

$$\dot{y}_j = \omega_j x_j + a\, y_j + \gamma\,(y_{j-1} - 2y_j + y_{j+1})$$

$$\dot{z}_j = b + z_j\,(x_j - c) \qquad (6)$$

As a result of the study of this two-dimensional system the following results were obtained (see fig. 5).

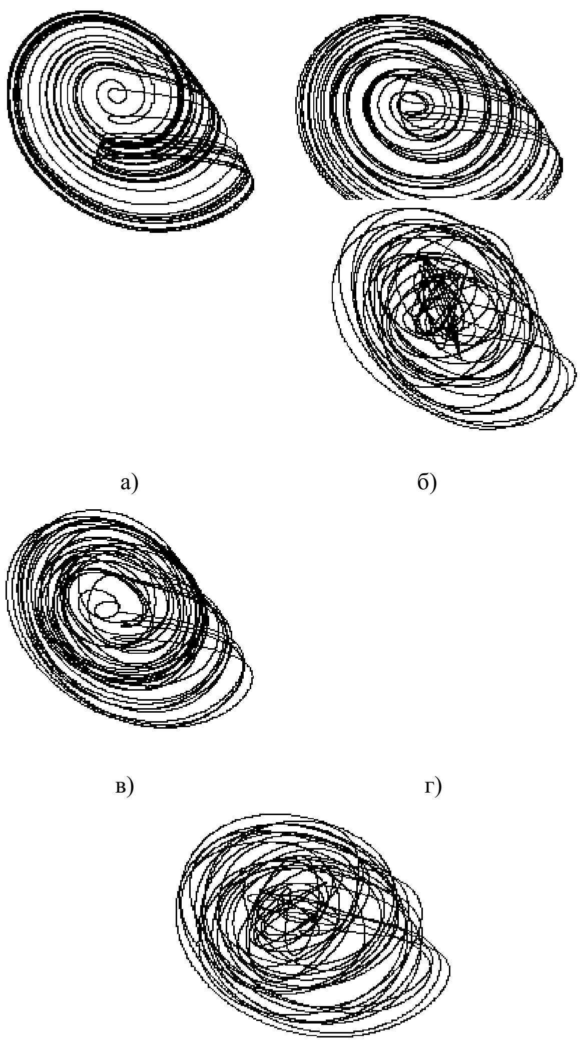

Fig. 5. The change of mechanical trajectory of 25-th oscillator in dependence of the bond parameters: a) $\gamma_x = 0$, $\gamma_y = 0$; b) $\gamma_x = 0$, $\gamma_y = 0.8$; c) $\gamma_x = 0.1$, $\gamma_y = 0.8$; d) $\gamma_x = 0.5$, $\gamma_y = 0.8$; e) $\gamma_x = 0.8$, $\gamma_y = 0.8$.

The figure represents mechanical trajectory of the oscillator situated at the intersection of two chains in a dependence of the bond parameters. As it can be seen the increase of the bond parameters along one of the axes significantly distorts the mode of Ressler attractor. However, in spite of more complicated visible structure of attractor for strongly bound chains (γ_x = 0.8, γ_y = 0.8) the degree of their synchronization only slightly differs from that one for completely unbound chains (γ_x = 0, γ_y = 0).

In the process of the real melting of a solid in the range of premelting there are no quite long chains of the bound atomic sites. It is explained by different factors and, first of all, by the keen increase of the number of vacancies in a solid in premelting state. Thus, two-dimensional model must be checked-up for the dependence of the degree of synchronous state of vibrations on the length of a chain (Fig. 6).

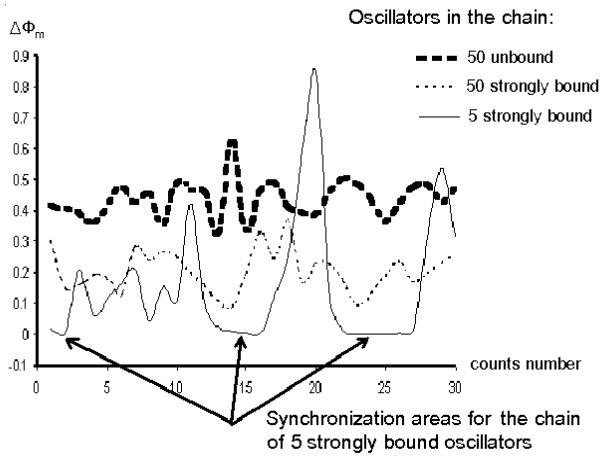

Fig. 6. Dependence of degree of synchronization for two-dimensional chains of Ressler oscillators on the bond degree between the oscillators and the number of oscillators in the chain.

Fig. 6 demonstrates that with a decrease of the chain length for a strong bond between the neighbouring oscillators (the case which is realized in premelting state) there appear stable areas of strong synchronization. Numerical calculations show that the degree of synchronous state of vibrations in these areas is by 3-4 orders of magnitude higher than that one in the case of 50 strongly bound oscillators. Thus, in spite of the fact that two-dimensional model of 5 oscillators is considered solely for the case of a strong chaos, the order of synchronization can attain the same values as in one-dimensional model with a weak chaos for rather long periods of time.

4. CONCLUSIONS

Thus, according to the model of synchronization a cluster represents dynamically and energetically active pattern forming the new phase state of a substance called mesophase. Existence of a cluster as an active structure element is due to the interaction of collective degrees of freedom for the limited number of the bound spatially distributed vibrating atoms. Interaction in such system results in a stationary generation of energy unlike of local generation as in the case of nonexcited systems. Generation of the energy has statistical self-sustained character thus resulting in extension of transition processes in time and fluctuation character of the process as a whole. Therefore, macroscopic approach based on the methods of non-linear dynamics allows to interpret the mechanism of appearing correlations in the excitation area.

5. REFERENCES

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