UDC 537.37:537.226:541. 14

NONLINEAR RADIATION PROCESSES IN SOLIDS

Baktybekov K.S.

S.Seifullin Kazakh AgroTechnical University, Zhenis avenue, 62 Astana 010011 Republic of Kazakhstan, k.baktybekov@gharysh.kz

There are some features in the research of the mechanisms of radiation exposure to solids, that complicate the understanding and quantitative description of such processes. First, the system "substance + radiation exposure" is open. In an open system, deviations of thermodynamic parameters from their equilibrium values lead to processes of energy and matter transfer. Secondly, the processes that occur as a result of the interaction of materials with radiation exposure are nonlinear. Continuous exchange of matter and energy with the environment leads to the fact that the system realizes stable dynamic equilibrium states that are far from the state of thermodynamic equilibrium. This conditions characterized by the existence of a certain spatial or temporal ordering so-called dissipative structure.

Keywords*: chaos and structures, fractal, modeling of radiation defects, thermoluminescence.*

Introduction

Recently, the radiation treatment of materials has been increasingly used. In this case, the radiation energy of electromagnetic, X-ray or gamma rays, as well as beams of charged particles are used. The main importance, such work was acquired in connection with the use of nuclear power and the possible use of thermonuclear installations. Materials used in outer space often experience complex effects of micrometeorites, electromagnetic and corpuscular radiation. All these processes lead to a change in the structure of the material, and, consequently, to the acquisition of new properties, which are often undesirable when the material is used.

The result of the substance interaction and external action is the formation of new structures in the materials under research, leading to a change in their original properties. Nonlinear systems are affected by random small effects generated by nonequilibrium, instability, and manifested in the accumulation of fluctuations, bifurcations, phase and spontaneous transitions.

The smallest parameter's change, controlling the nonlinear system can lead to a giant response of the system to an external action and, as a rule, leads to the self-organization effect studied by synergetics [1, 2]. The self-organization shows that elements of a non-linear dynamical system start to be ordered in the system structure, which leads to the formation of regular (fractals) or irregular (multifractals) spatial structures [3-6]. Thus, it can be assumed a priori that new structures formed in materials as a result of interaction with external action have a structure with fractional cluster dimension, i.e. the fractal analysis methods fractal can be used for their description.

The processes occurring during the interaction of radiation with matter are the simplest cases in which strongly nonequilibrium condition of a solid are formed. When it is irradiation, the fast particle collides with the substance atom, chooses it out of the node into the interstitial space. In this case, the lattice site remains empty, and two defects are formed: a vacancy and an interstitial atom (Frenkel defects). If a particle is heavy, for example a neutron or an ion, and if the energy of the particle is large enough, then, having extracted one of the atoms from the node and losing some of the energy, it can continue to collide until its energy runs out. In turn, an atom knocked out of a node can also have enough energy to produce defects. As a result, a cascade is formed, in which there can be several hundred pairs of defects.

.

1. Processes in irradiated solids

Let us consider how the condition of the irradiated solid changes in time by recourses [7, 8]. The irradiation source continuously generates defects in a solid. At the same time, the processes in which the defects are destroyed are in the substance. First, it is the annihilation process, when two opposite defects occur and mutually destroy each other. Secondly, the defect can "die on drains" if it approaches the external surface or internal drains - defects of a different type. Consequently, in the irradiated material, as a result of external action, defects are continuously created, but as a result of processes occurring in the solid, they continuously disappear, as a result of the balance of these processes, a certain steady concentration of defects is maintained. We can see that in this case a typical weakly nonequilibrium system should be observed, which behaves like a closed equilibrium system, but does not evolve to a state of equilibrium, but to a stationary state with a certain constant concentration of defects in the volume. In this case defects should be distributed approximately uniformly in the volume, if we do not take into account the regions of the cascades that play the role of fluctuations in the concentration of defects. However, experiments have been carried out experimentally [9], where the figure of radiation damage is significantly different from that described, spatially organized structures are observed, which apparently corresponds to the regime of strongly nonequilibrium conditions. In literature recourse [10] the system explanation of defected divergence of theory and experiment on the base of representations of dynamic chaos, which are in recombination-stimulating processes.

2. The results of modeling radiation-thermal processes

For the structural transformations analysis, occurring in the systems with two types of interacting particles, a quantity called the conditional interaction potential (CIP) is introduced in literature resource [11, 12]. This parameter allows us to characterize the size of the resulting structures and to reveal their fractal nature.

To calculate the CIP it is necessary to have a figure of the particle distribution on the surface under study or to know the spatial coordinates of the interacting molecules at the required time. The digitized image is divided into the same cells, and the scale of the partition runs through all values, which is a multiple of the original surface. The value of the CIP is calculated for their pair of particles in each cell, according to formula

$$U = \frac{1}{2}\sum_{k}\sum_{i,j}\frac{q_i q_j}{r_{ij}} \tag{1}$$

where i, j – component index of pair, k – number of interaction radius, determined by partition number, q_i, q_j – conditional single «charges», used for difference between two kinds of participles in a system ($q_i = 1, q_j = -1$ или $q_i = -1, q_j = 1$ in dependence of initial conditions), r_{ij} – distance between interacting particle.

A characteristic feature of the dependence of the CIP on the partition scale is the presence of one or more maxima, which indicate the formation of aggregates of the same particles. The UWB change in time makes it possible to trace the evolution of the observed structure in a solid. As a rule, the UWB time dependence has a mini- mum in the negative region, which corresponds to a maximum of information entropy, which corresponds to a chaotic distribution of particles on the surface and in the volume of the crystal. If the system has synergistic effects, its entropy decreases to a certain value. In this case, the CIP particle in the system grows to a certain positive value and reaches saturation. The kinetic curves at the saturation stage have a quasi-oscillatory character, which corresponds to the dynamic processes of growth and destruction of the clusters formed. It should be noted that the maximum of information entropy falls on the minimum of the conditional interaction potential (Figure 1), which also confirms the chaotic distribution of defects at this time.

This information entropy according to Haken [13] is defined as the average value of the synergetic information *I*, acquired at birth or structure destruction with probability p_i:

$$I_i = -\ln p_i, \quad S = -\sum_i p_i \ln p_i, \quad \sum_i p_i = 1. \qquad (2)$$

This formula generally coincides with Shannon's entropy [14] -as a measure of the information necessary for determining the location of the system in a certain macrostate:

$$S = -\sum_i p_i \ln p_i, \qquad (3)$$

However, these expressions have a different physical meaning. The formulation (2) can be used to research the system dynamics in the process of its evolution, while the entropy (3) describes the statistical condition of the system at this moment.
In Table 1 are shown the calculated values of the characteristic dimensions of aggregates, random entropy, and the observed entropy in modeling of long-term irradiation on lattices of different sizes [12].

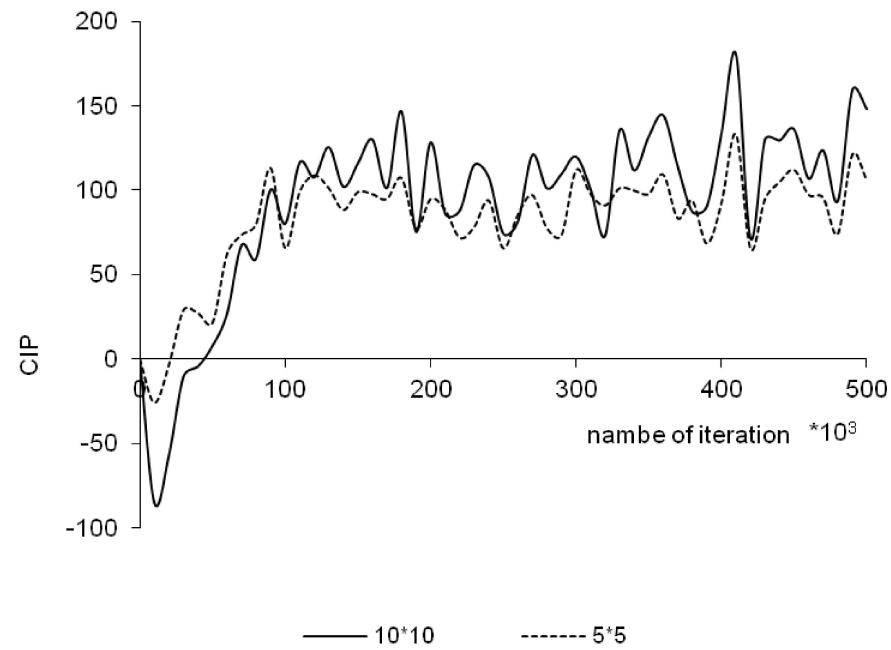
Table 1.The information entropy values, calculated for some characteristic aggregates sizes and in a volumetric sites of different sizes

The lattice size	Aggregates' Characteristic size	Observed system entropy	Chaotic distribution entropy
1000x1000	10x10	7.31 ± 0.10	9.21
	5x5	7.65 ± 0.12	10.59
500x500	10x10	7.09 ± 0.09	7.82
	4x4	7.48 ± 0.10	9.66
100x100	10x10	3.87 ± 0.05	4.60
	5x5	4.12 ± 0.00	5.99
100x100x100	10x10x10	6.83 ± 0.11	46.05
	4x4x4	8.58 ± 0.15	160.94

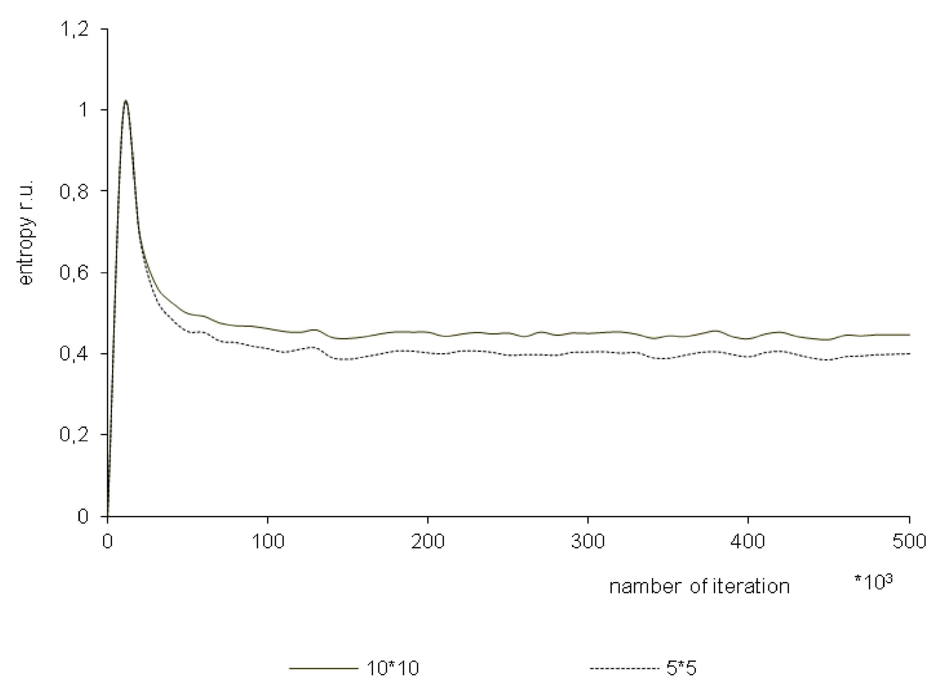
The defect structure destruction, formed by electron-hole centers accumulated in the crystal under the influence of radiation can be traced in the research of the process of thermoluminescence end thermally stimulated conductivity (TSC). The curves analysis of thermoluminescence (TL) arising in solids due to the recombination of charge carriers (electrons and holes) trapped by the lattice traps of a material is impossible without a detailed interpretation of the nature and mechanism of the dependence of thermoluminescence on crystal-chemical, physical-chemical and geological factors. It is known that the TL intensity depends on the number of recombining electron-hole centers in the crystal, the radiation dose rate and the duration of its exposure to the crystal. In connection with this, the TL process research was conducted of in order to elucidate the effect of the type of distribution of electron-hole centers in a crystal to the process.

When TL end TSC modeling, the experimental data of the activation energy and the heating rate from the work [7] for the NaCl crystal were used as the process parameters. The capture centers associated with radiation defects are mainly annealed to room temperature, and are F, F - aggregate and V-centers. The simplest mechanism of the recombination process realized in the model used is the migration of free charge carriers of the same sign to the captured charge carriers of the opposite sign. The TL curves correctness was verified by the Voigt's formulas (4), Broinlich formula (5), and Lushchik formula (6), which used in methods for determining the depth of the traps [15].

.



a)



b)

Fig.1. CIP dependence (a) and the specific value of information entropy (b) the structure of radiation defects from the duration irradiation of a two-dimensional NaCl crystal with a lattice of 1000x1000 at a dose rate of 0.1% for two characteristic sizes of aggregates.

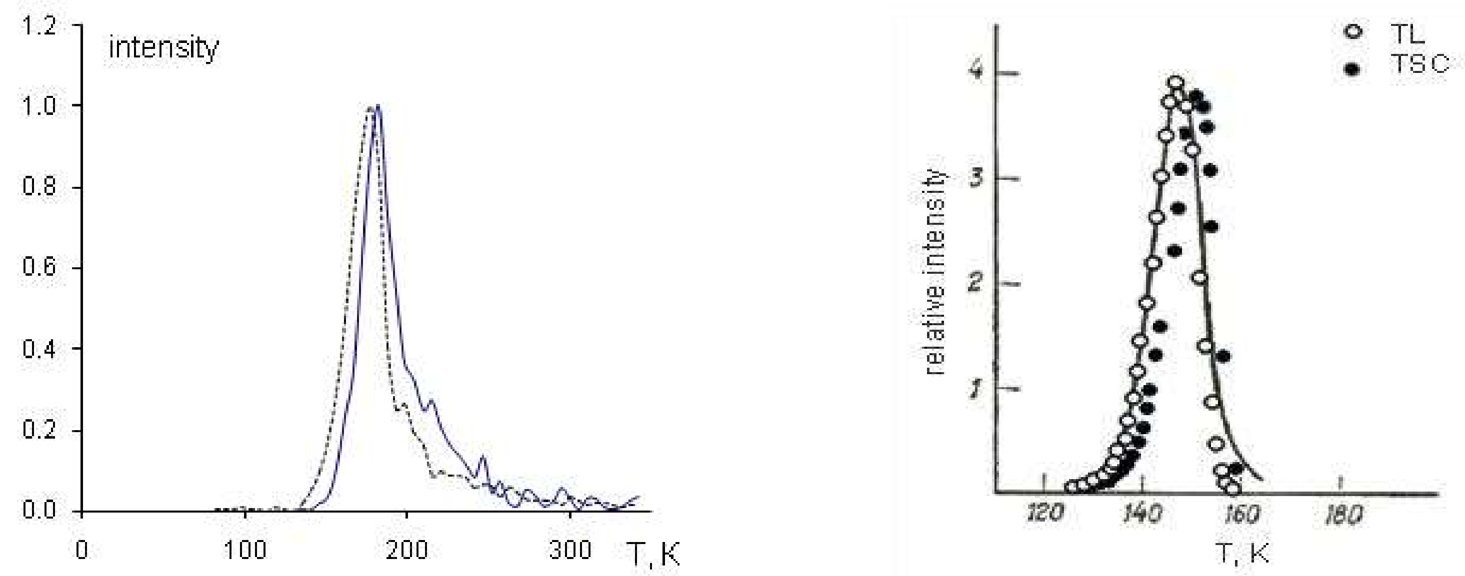
There are shown the TL and TSC processes of modeling results in a NaCl-type lattice and the experimental data of the authors [7] in fig 2. The activation energies of the *E* centers calculated using the parameters obtained in modeling the TL process satisfy semi-empirical relationships:

$$18T_m \le E/k \le 25T_m\,, \tag{4}$$

$$E = \frac{kT_{m1}\cdot T_{m2}}{T_{m1}-T_{m2}}\ln\left(Q_1T_{m2}^2/Q_2T_{m1}^2\right), \tag{5}$$

$$E = kT_m^2/\left(T_2^* - T_m\right), \tag{6}$$

where Q – the rate of crystal heating; T_m is the maximum temperature of thermoluminescence; T_2^* - temperature at half the maximum intensity of glow from the high-temperature side; k is the Boltzman's constant; indices *1* and *2* denote the parameters for two TSL curves.



a) b)

Fig.2. Curves TL и TSC: a) NaCl, computer modeling, *E/k* = 3868 K; …….. TL _____ TSC;
b) NaCl:Ag, experimental data [7], *E/k* = 3868 K

Conclusion

Thus, it can be argued that the mathematical model with the initial multifractal defect distribution adequately reflects the real system and can be used to the research the thermoluminescence phenomenon.

REFERENCES

1 Nikolis G., Prigogin I. *Self-organization in non-equilibrium systems.* Moscow, World, 1979, 512 p.

2 Glensdorf P., Prigogin I. *Thermodynamic theory of structure, stability and fluctuations*. Moscow, World, 1973, 280 p.

3 Zaslavsky G.M., Sagdeev R.Z., Usikov D.A., Chernikov A.A. *Weak chaos and quasi-regular structures.* Moscow: Science, 1991, 240 p.

4 Kronover R.M. *Fractals and chaos in dynamic systems. Fundamentals of the theory*. Moscow, Postmarket, 2000, 353 p.

5 Mandelbrot B. *The fractal geometry of nature*. San Francisco, Freeman, 1982, 459 p.

6 Bozhokin S.V., Parshin D.A. *Fractals and multifractal*s. Izhevsk, SRC "RHD", 2001, 128 p.

7 Lushchik Ch.B., Vitol I.K., Elango M.A. Decay of electronic excitations into radiation defects in ionic crystals. Uspehi Phisicheskih Nauk, 1977, Vol. 122, Issue 2, pp. 223 – 251. [in Russian]

8 Lisitsyn, V.M. Formation and Evolution of Primary Defectiveness in Ionic Crystals. *Proceeding of the Tomsk Polytechnic University,* 2000, Vol. 303, Issue 2, pp. 7 – 23. [in Russian]

9 Khmelevskaya V.S., Malynkin V.G. Dissipative structures in metallic materials after irradiation and other types of strong impact. Materials Science, 1998, Vol. 2, pp. 25 – 32. [in Russian].

10 Avilov A.B., Arapov B.A., Oxygenendler B.L. On the role of dynamic chaos in recombination-stimulated atomic processes. *Letters in ZhTPh*. 2000, Vol. 26, No. 2, pp. 23 – 27. [in Russian]

11 Baktybekov K., Vasil'eva I. The simulation of interaction of dielectric materials with soft space radiation. *Proceedings of the 9th Intern. Symposium on Materials in a Space Environment*. Nordwijk, 2003, pp. 719 – 721.

12 Baktybekov K.S., Vasilieva IF, Vertyagina E.N. Modeling of the aggregation of radiation defects in solids. *Bulletin of KarGU. Natural sciences*. 2003, Vol. 31, pp. 165 – 172.

13 Hacken G. *Information and self-organization*. Moscow, World, 1991, 240 p.

14 Shannon C.E. A mathematical theory of communication. *Bell Systems Tech. J.* 1948, Vol. 27, pp.379 – 423.

15 Broinlich P. Thermoluminescence and thermally stimulated current - methods for determining trapping parameters. *In the collection: "Physics of Minerals"*. Ed. A.S. Marfunin. Moscow: World, 1971, pp.134 – 155. [in Russian]

Article accepted for publication 14.05.2018