Discrete simulation of defect flows and fragmentation of 2D interfaces under contact interaction

D.D. Moiseenko[1,a], S.V. Panin[1,b], E.N. Iriskina[1,c], P.V. Maksimov[1,d], S.N. Kupriyanov[2,e] and I.G. Goryacheva[3,f]

[1] Institute of strength physics and materials science SB RAS, Tomsk, 634021, Russia

[2] Tomsk Polytechnic University, Tomsk, 634050, Russia

[3] Institute for Problems in Mechanics RAS, Moscow, Russia

[a] mdd@ispms.tsc.ru, [b] svp@ispms.tsc.ru, [c] eni@ispms.tsc.ru, [d] mpv@ispms.tsc.ru, [e] snk@ispms.tsc.ru, [f] goryache@ipmnet.ru

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Abstract. The paper is devoted to multiscale computer modelling of defect flows along interfaces in loaded solids. Interfaces are considered as 2D self-organized subsystems. Discrete approach of stochastic excitable cellular automata (SECA, [1,2]) was extended by adding of special algorithm of astable cellular automata (ACA) to simulate defect propagation and microcrack nucleation. SECA method provides 3D-modelling at mesoscale and it takes into account grain structure of the material; the ACA provides microscale simulations of 2D interface behaviour. Microcrack is considered as a specific "phase state" of local material volume. Defect flows are controled by specific "driving force" calculated from the values of material torsion, couple forces and hydrostatic pressures distributed at the interface. Numerical experiments of fragmentation and fracture in 2D interface show quasiperiodic cyclic character of microcrack nucleation and defect propagation. Computer simulation method based on excitable cellular automata allowed revealing undetected effects in the form of propagation of spiral waves in specimen under indentation. It is shown that rotational wave flows of defects are able to cause forming of quasiperiodical defect structures along the interface.

Introduction

The problem of computer simulation of plastic flow and fracture of multilayer composites in contact interaction seems to be very significant in view of presence of multiple interfaces. The latter should be considered as self-maintained 2D subsystems in a solid. Such kind of study can be undertaken only within the framework of multiscale models of defect flows at interfaces of loaded solid. Multiscale models have to take into account nonlinear wave character of local material excitations, which lead to pulsation of mass and energy in each local material volume. The model should necessarily include principles of local energy dissipation.

Numerical simulation based on cellular automata methods is generally carried out according to the algorithm described below:

1. generation of geometry of internal structure of specimen;
2. assignment of distribution of local material properties to each cell in the whole volume (for instance, dispersion of strength, elastic moduli, material degradation rate, dislocation density etc.);
3. assignment of links between active elements of cellular automaton;
4. definition of set of cell states and formulation of switching rules;
5. numerical simulation of evolution of perturbance pattern in cellular automaton as a result of excitations of various kinds.

Cellular automata one can divide into 3 basic types: bistable (BCA), excitable (ECA) and astable (ACA). Bistable cell can be found in one of two possible states. Excitable cell can run through serial states after single excitation (e.g. energy influx). Astable cells also run through serial states but this process can take place without any external influence. In order to take into account specific character of thermal and mechanical energy flows ECA was chosen as a simulation tool for study of deformed material behaviour at mesoscale. Active element of ECA is characterized by numerical parameters corresponding to the material (such as elastic moduli, mass density, the dislocation density, heat conductivity, specific heat capacity, the coefficient of thermal expansion and so on). Each cell is linked to its "neighbours" in 1-st coordination sphere. Heat and mechanical components of energy vary as a result of pair interaction with neighbour cells. Physical parameters associated with the cell also change.

1. SECA/ACA method overview

In the framework of SECA method area of a specimen simulated is divided into elementary volumes so automaton's active cells represent sites in the space where material of the specimen is located. Along with states each cell has the parameters corresponding to the medium volume simulated. The main concept of method is that deformation process is a result of energy transfer and transformation. Thermal and mechanical energy can change their values and they can transit to each other.

At each n-th time step of the algorithm active element interacts with neighbour cells. As a result of the interaction the element obtain energy from the neighbour cells. Value of mechanical energy of the element depends on the energy gradients between the cell and each neighbour. Total energy of medium elements is divided into components, which are allowed to changes of entropy, temperature and volume.

Energy transfer from active element to another one occurs step-by-step. At first stage the energy dE is transferred from element to another one, at second stage the energy obtained by one of the elements is divided.

1. a. at first time step as a result of interaction with neighbours the element can change its internal energy E_{ijk} on dE' by means of the work dA' spent by its neighbours.
   b. energy influx dE' can lead to change of the heat energy dQ_{ijk} and to the work production dA_{ijk} spent on change of element volume.
2. at second time step the volume change causes the work production dA'', which transit to neighbour elements.

The total internal energy of each elementary volume is known, so it is possible to obtain a distribution of normal components of stress tensor on the whole specimen with the help of Murnaghan equations [3].

In the framework of the proposed approach boundary active cells are divided into 3 types: «hard», «soft» and «intermediate». «Hard» boundary cells do not change own energy under interaction with internal automata of specimen. Interaction between such cells is not simulated. «Soft» boundary elements interact with all neighbours at 1st coordination sphere, both internal and boundary cells, and its energy is changed according to the expressions for energy flow. Finally, «intermediate» elements do not interact with neighbour boundary automata and change own energy as a result of influence of internal neighbour cells at first sphere.

Let the 3D cellular automaton simulates a specimen under mechanical loading, and face-centered cubic (FCC) arrangement of elements is used. Simulation of distribution of elastic energy in a solid under mechanical loading is realized by the following algorithm. The energy value of i-th element at n-th time step depends on its own energy value and the energy value of each k-th neighbour element at first coordination sphere of i-th element ($0 \le k \le K$-1, K is the number of elements at first sphere) at (n - 1)-th time step.

The input parameters of the model are the initial values of cell stresses { p_i^0 , $0 \le i \le I$ - 1} where I is the total number of cells. The initial elastic energy of i-th element is calculated as follows:

$$A_i^0 = \frac{(p_i^0)^2 \cdot V_{CA}}{2 \cdot Y_i^0}. \quad (1)$$

The energy of i-th cell at every n-th time step is calculated in the following way:

$$A_i^n = A_i^{n-1} + \sum_{k=0}^{K-1} \Delta A_{ik}^n + \Delta A_i^n \quad (2)$$

where ΔA_i^n is the external influx of energy to i-th element at n-th step:

$$\Delta A_i^n = \begin{cases} (A_b)_i^n, i \in I_b; \\ 0, \quad i \notin I_b \end{cases} \quad (3)$$

Here $(A_b)_i^n$ is the external influx of energy to boundary cell at n-th step, I_b is the set of indices of boundary elements of automaton. This value is calculated starting from the modulus of elasticity of internal element ($(Y_{in})_i^n$) neighbouring for given boundary element and the constant value of the strain ($(\varepsilon_b)_i$, a) or the stress ($(\sigma_b)_i$, b) of the boundary cell.

a. $$(A_b)_i^n = \frac{(\sigma_b)_i^2}{2 Y_{in}^n} V_{CA}; \quad (4)$$

b. $$(A_b)_i^n = \frac{(\varepsilon_b)_i^2}{2 (Y_{in})_i^n} V_{CA}. \quad (5)$$

The term ΔA_{ik}^n in Eq. 2 indicates the change of the elastic energy of i-th element as a result of interaction with k-th neighbour at n-th time step. It is calculated by the relation:

$$\Delta A_{ik}^n = \frac{(\sigma_{ik}^{n-1})^2 \varepsilon_{ik}^n V_{CA}}{2} \quad (6)$$

where σ_{ik}^{n-1} is the stress at boundary of i-th and k-th elements at (n - 1)-th time step, ε_{ik}^n is the strain of material contained in i-th element as a result of this stress, V_{CA} is the cell volume,

$$sig(x) = \begin{cases} \frac{x}{|x|}, x \neq 0, \\ 0, \quad x = 0 \end{cases}. \quad (7)$$

The stress σ_{ik}^{n-1} is calculated as the difference of the stresses of cell pair:

$$\sigma_{ik}^{n-1} = \sigma_k^{n-1} - \sigma_i^{n-1}. \quad (8)$$

To obtain the strain value the velocity of boundary v_{ik}^n is calculated according to Tornbull equation:

$$v_{ik}^n = m_{ik}^{n-1} \cdot \sigma_{ik}^{n-1}. \quad (9)$$

The strain ε_{ik}^n is expressed as follows:

$$\varepsilon_{ik}^n = \frac{v_{ik} \Delta t}{l_{CA}} = \frac{m_{ik}^{n-1} \sigma_{ik}^{n-1} \Delta t}{l_{CA}}. \quad (10)$$

Here m_{ik}^{n-1} is the mobility of boundary between material parts contained in i-th cell and its k-th neighbour at (n - 1)-th time step:

$$m_{ik}^{n-1} = (\sigma_{ik}^{n-1}) \exp\left(-\frac{Q}{k_B T_{ik}^{n-1}}\right) \quad (11)$$

where $(m_0)_{ik}^{n-1}$ is the maximal value of mobility (it depends on type of material containing in each of cells), k_B is the Boltzmann constant, Q_{ik}^{n-1} is the energy of the cell pair at (n - 1)-th time step, T_{ik}^{n-1} is the temperature at considered boundary:

$$T_{ik}^{n-1} = \frac{T_i^{n-1} + T_k^{n-1}}{2}. \quad (12)$$

Taking into account Eq. 6, 10 and 11, the term ΔA_{ik}^n in Eq. 2 is written as follows:

$$\Delta A_{ik}^n = \begin{cases} (m_0)_{ik}^{n-1} \exp\left(-\frac{Q_{ik}^{n-1}}{k_B T_{ik}^{n-1}}\right) \left(\sigma_i^{n-1} - \sigma_k^{n-1}\right)^2 V_{CA}, & \sigma_i^{n-1} \geq \sigma_k^{n-1} \\ 0, & \sigma_i^{n-1} < \sigma_k^{n-1} \end{cases} \quad (13)$$

The energy of i-th element is known, so it is possible to calculate the value of its stress σ_i^n:

$$\sigma_i^n = \sqrt{\frac{2A_i^n Y_i^n}{V_{CA}}} \quad (14)$$

where Y_i^n is the modulus of elasticity of i-th element at n-th time step.

Thus, at each time step the value of the «effective stress» σ_i is determined as the function of the mechanical energy A_i accumulated by i-th cell:

$$\sigma_i = \sqrt{\frac{2A_i Y}{V}}. \quad (15)$$

The value of the principal stress of i-th element $\tilde{\sigma}_i$ is calculated starting from the values of the effective stress of this element and its neighbours at 1st coordination sphere. For that the following operations are carried out:

1) The scalar values of the stresses acting on i-th cell from each of its neighbours are calculated (see Fig. 1):

$$\sigma_{ik} = \begin{cases} \sigma_k, & \delta(i,k) = 1 \\ 0, & \delta(i,k) = 0 \end{cases} \quad (16)$$

Here σ_k is the effective stress, $\delta(i, k)$ is the membership function of k-th element at 1st coordination sphere of i-th element of simulated cellular automaton. The value of this function equals 1 if the cell belongs to considered set, and it equals 0 if it does not belong to set.

2) The scalar value of the principal stress is calculated:

$$\tilde{\sigma}_i = \frac{1}{12} \sum_{k=1}^{12} \sigma_{ik}. \quad (17)$$

The value of the couple force vector of i-th cell $\vec{M}_i$ is calculated as follows:

1) The coordinates of the vectors directed from i-th cell centre centre to centres of each of its neighbours at 1st coordination sphere are calculated (see Fig. 1):

$$\vec{r}_{ik} = \vec{r}_k - \vec{r}_i, \quad (18)$$

where $\vec{r}_i$ is the radius-vector of i-th cell centre, $\vec{r}_k$ is the radius-vector of centre of k-th cell at 1st coordination sphere of i-th cell.

2) For each k-th element the indices l of the automata located at 1st coordination spheres of i-th and k-th element are determined.

3) The scalar values of the stresses are calculated (see Fig. 1).

(19)

4) The vector directed from each *k*-th automaton centre to centre of each *l*-th internal neighbour is determined (see Fig. 1):

$$\vec{r}_{kl} = \vec{r}_l - \vec{r}_k . \quad (20)$$

5) The couple force vector $\vec{f}_{lk}$ is calculated:

$$\vec{f}_{lk} = \frac{\vec{r}_{kl}}{|\vec{r}_{kl}|} \cdot S \cdot \sigma_{lk} \quad (21)$$

where *S* is the area of contact surface of neighbour elements.

6) The required value of the couple force vector is determined:

$$\vec{M}_i = \sum_k \sum_l \left[\vec{r}_{ik}, \vec{f}_{lk} \right] \quad (22)$$

where $\left[\vec{r}_{ik}, \vec{f}_{lk} \right]$ is the vector product of the vectors obtained by Eq. 18 and 21.

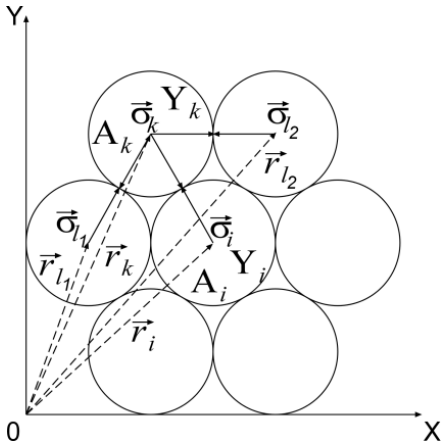


Fig. 1. 2D element of cellular automaton (*i*-th) and its first coordination sphere. Schematic picture of calculation of the principal stress and the couple force.

New method based on special algorithm of astable cellular automata is developed for simulation of processes in interfaces. This algorithm takes into consideration nonlocal wave character of evolution of inelastic deformation.

Active element of astable cellular automaton performs cyclic transfers through certain sequence of states. External influence on the element can accelerate or decelerate these transitions, but not stop them. In the simplest case ACA could be represented as a model of oscillator (see Fig. 2). Here levels of elastic energy can be formulated in terms of states of active element. Oscillation half-periods depend on non-local hidden variables of the system.

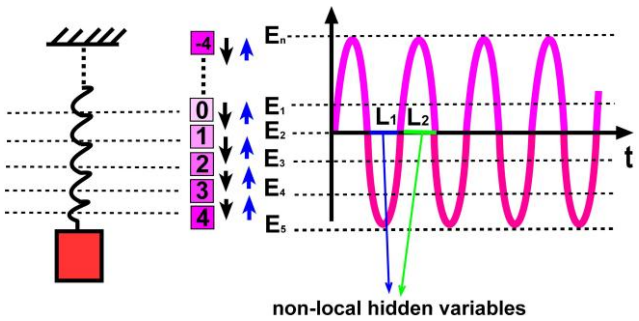
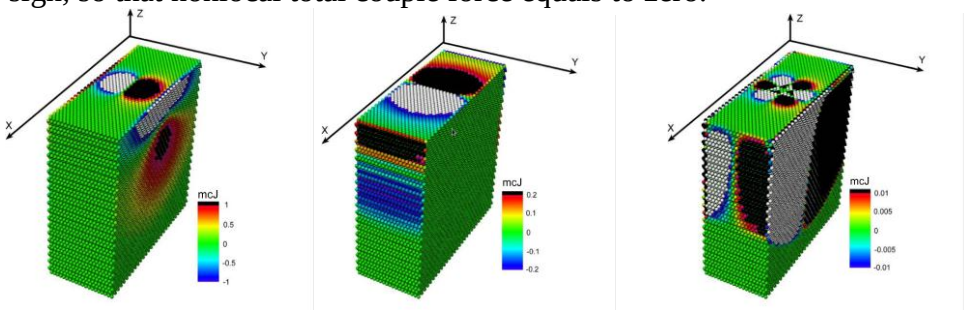


Fig. 2. The scheme of astable cellular automaton and wave character of its switching.

2. Numerical experiment of indentation of 3D specimen taking into account 2D interface

Specimen simulated was represented by cellular automaton in the form of system of active elements with the size of 0.5 μm in FCC packing. The specimen sizes were equal to 25× 10 ×25 μm. In the upper facet centre circle region with the diameter of 2.5 μm was located. In this region the velocity of growth of uniform hydrostatic stresses was assigned to 3.45 GPa/s. At every time step distribution of the values of the stress, the strain and the local couple force in the specimen was simulated. The time step was equal to 1 μs.

As one can see at Fig. 3 (a,b), distribution of the couple force components M_x and M_y show bending of specimen surface. At the same time, the numerical experiment results shows nontrivial pattern of distribution of the couple force components M_z in the form of symmetrical "leaf structure" near the indenter at free specimen surface (see Fig. 3, c). Note that the "leaves" alternate according to the couple force sign, so that nonlocal total couple force equals to zero.



a **b** **c**

Fig. 3. Distribution of the couple force components: a) M_x, b) M_y, c) M_z.

For detailed research of the processes to occur the graphs of dependencies of all the components of the couple force vs. time depth were plotted. Diagrams of torque value dependence versus time and depth are plotted in order to investigate deformation processes in depth of specimen under the "leaves". The analysis of these graphs allows revealing spiral waves of inelastic deformation propagating from the "leaves" deep into the specimen (Fig. 4).

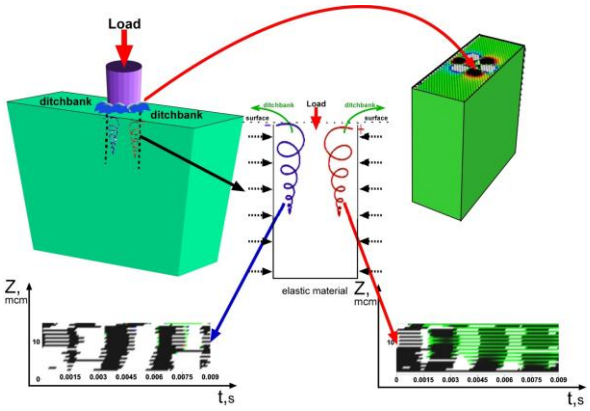


Fig. 4. The scheme of generation of spiral waves under the indenter.

Nonlinear processes such as spiral wave propagation are necessarily accompanied by dissipation of energy. Approaches of linear continuum mechanics and equilibrium thermodynamics do not allow answering the question about which part of elastic energy is spent on production of entropy. The answer can be given in the framework of multiscale approaches only [4, 5].

New original principles of dissipative processes in deformable solid were also proposed in papers of G.C. Sih [6] (see Fig. 5, a). This theory is based on concepts of pulsation of mass and energy. These concepts allow escaping principles of momentary interaction and momentary equilibrium. That is the common point of proposed cellular automata approaches and the theory of G.C. Sih (see Fig. 5, b).

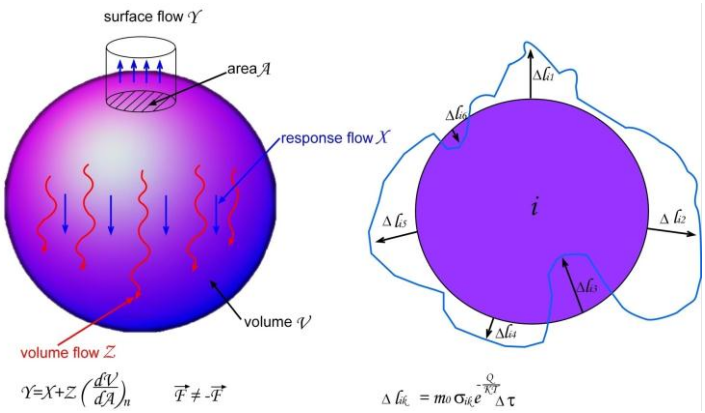


Fig. 5. The scheme of dissipative processes: a) volume and surface flows (G.C. Sih, [6]), b) SECA.

Thus, the new method of anharmonic astable cellular automata (AACA) was developed for simulation of processes of material fragmentation along the "coating-substrate" interface. Due to above-mentioned features of ACA, it is possible to simulate processes of fatigue fracture of material. With the help of AACA it is possible simulating, for example, propagation of fatigue crack in material (see Fig. 6). In this case the probability of cell switching to the state "damaged" can be chosen as the value, which is reciprocal to the ultimate stress in crack point.

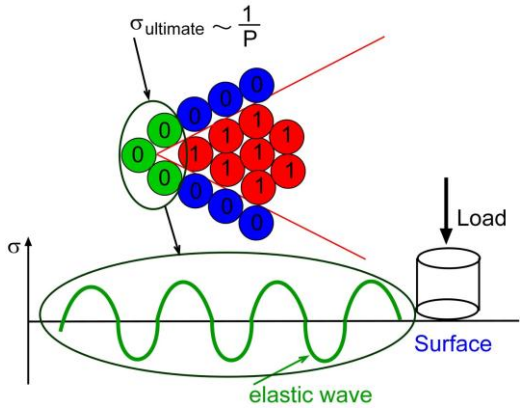


Fig. 6. Use of AACA for simulation of growth of fatigue crack.

Spiral waves discovered as a result of 3D simulation of plastic deformation evolution lead to generation of complex oscillating excitations in 2D interfaces. So the spiral wave parameters were used as the initial values for AACA 2D simulation.

The results of simulation of propagation of defect flows along 2D interface between coating and surface are shown at Fig. 7, 8. Here P is the probability of crack growth, L is the period of crack life, D is the latence period of repeated crack opening.

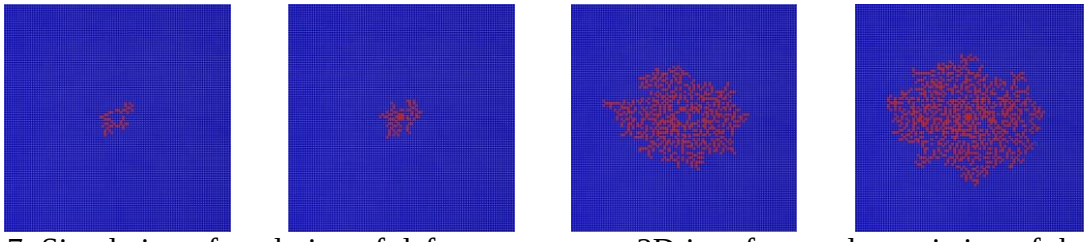


Fig. 7. Simulation of evolution of defect structure at 2D interface under variation of the hidden variables: P = 0,1; L = 25; D = 5.

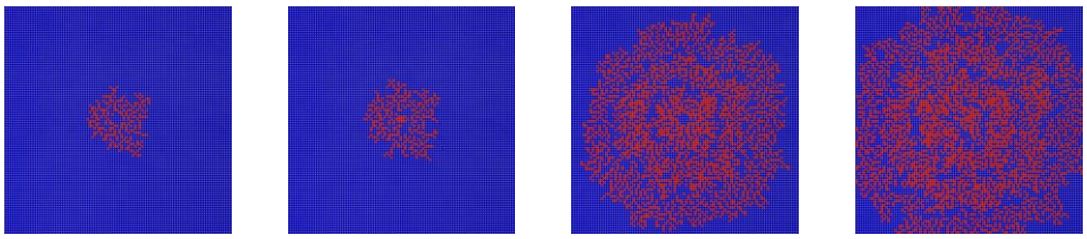


Fig. 8. Simulation of evolution of defect structure at 2D interface under variation of the hidden variables: P=0,2; L=25; D=5.

The results represented at Fig. 7 – 8 show that under change of the value of the parameter *P*, which is associated with the ultimate stress, character of evolution of fracture pattern changes essentially. For instance, at Fig. 7 one can see quasi-homogeneous alligatoring (crack network). At the same time, the results presented at Fig. 8 show quasiperiodic character of fracture. These patterns allow making a conclusion about undulatory propagation of defects.

Along with ultimate stresses characterizing local interaction only, astable cellular automaton takes into account influence of behaviour of the whole system on local active element. For example, latent period of crack opening can depend on non-local hidden variables of the system (sound velocity, thermal energy produced during vibration, rate of chemical reaction or phase transitions under various temperature values etc.). Thus, due to astable character of cellular automaton and taking into account its anharmonicity it is possible to describe such non-local characteristics in an explicit form.

Summary

Analysis of numerical experiments of specimen indentation allowed making a conclusion that spiral waves generate on the surface and propagate deep into the specimen. Existence of spiral waves of inelastic deformation was predicted theoretically by professor Egorushkin and academician Panin [4, 5]. However, direct numerical experiments for real structures at mesoscale, which could confirm this theory, were not carried out. SECA method takes into account explicitly local couple forces realizing the scheme “shear + rotation”. Therefore this method allows obtaining a result, which is in a good agreement with forecast of this theory.

The computer simulation method based on anharmonic astable cellular automata allowed investigating the effect of spiral structures on the interface and predicting a possibility of generation of concentric waves of mass excess. This process is accompanied by forming of defect structure.

Combination of 3D and 2D models allows providing multiscale simulation of defect structure generation along the interface. Under propagation through the interface the spiral wave initiates wave character of structure-phase transformations in the interface area.

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