Available online at www.sciencedirect.com

ScienceDirect

Procedia Manufacturing 37 (2019) 30–37

Procedia MANUFACTURING

www.elsevier.com/locate/procedia

9th International Conference on Physical and Numerical Simulation of Materials Processing (ICPNS'2019)

Simulation of Self-sustained Relaxation of a Two-dimensional Metastable Medium by Means of a Traveling Wave

P.M. Bokov[a*], P.A. Selyshchev[b]

[a]*The South African Nuclear Energy Corporation SOC Ltd (Necsa), Building 1900, P.O. Box 582, Pretoria 0001, South Africa*
[b]*Department of Physics, University of Pretoria, Private bag X20, Hatfield 0028, South Africa*

Abstract

The traveling wave mode of self-sustained relaxation of a metastable medium, such as combustion and annealing of radiation-induced defects in solids, is studied. The mechanism of self-sustained relaxation and propagation of the traveling wave is a positive thermal-concentration feedback and heat transfer. The thermal-concentration feedback develops because the relaxation rate depends strongly on temperature, and the energy of the metastable state transforms into thermal energy in the process of relaxation. Hence, the relaxation leads to an increase in the medium temperature and, consequently, to further support of the relaxation. In this work, traveling waves are considered, and their features are investigated by computer simulation. The shape and speed of the traveling wave are investigated as a function of the medium properties, and the way of its initiation. We examined the shapes of wavefronts as they propagate on a plane, and observed two different regimes of traveling wave propagation. Sometimes the front of the traveling wave spreads as a whole and velocity of propagation is perpendicular to the wavefront. Sometimes small perturbations arise on the wavefront, and then grow by virtue of relaxation along the front, thus, the new area of the relaxed medium has the form of a narrow strip that propagates along the line of the front and maintains a constant width in the direction perpendicular to the front. We observe the appearance of one or more small perturbations, which arise in a symmetric way. The influence of boundaries on the traveling waves was also investigated.

Keywords: metastable medium; thermal-concentration feedback; self-sustained relaxation; travelling wave of relaxation.

* Corresponding author. Tel.: +27 (12) 305-5624;
E-mail address: pavel.bokov@necsa.co.za

10.1016/j.promfg.2019.12.008

1. Introduction

Autowave processes in condensed matter, including propagation on a surface, have been extensively studied [1]. These include autowaves in ferroelectric and semiconductor films, crystallization waves of supercooled liquid in a narrow layer, surface chemical reactions like burning, annealing of defects induced by ion irradiation, surface polymerization, etc. As a rule, these are switching waves in a bistable medium, which can be in either of two stationary states: metastable and stable. The mechanism of self-sustained relaxation and propagation of the traveling wave of relaxation is the positive thermal-concentration feedback and heat transfer. The thermal-concentration feedback develops because the relaxation rate depends strongly on temperature, and the energy of the metastable state transforms into thermal energy during the process of relaxation. The relaxation thus leads to an increase in the temperature of the medium and, consequently, further supports the relaxation. A positive feedback loop is therefore formed.

In this work two-dimensional traveling waves of self-sustained relaxation of a metastable medium, such as combustion [2] or the annealing of radiation-induced defects in solids [2-4], are considered. The properties of their propagation on a finite plane are investigated by means of computer simulation.

2. Mathematical model

Consider an active medium, which is formed by an ensemble of a given number of stationary (immobile) excitable elements. Each element can be in one of two states: either in the stable state, or in a metastable state with a certain increased energy. The metastable state of the medium is due to the presence of excited elements in a number greater than the equilibrium value corresponding to the given temperature. Any addition of energy exceeding the threshold level (activation energy) is capable of transferring the element from the metastable state to the equilibrium one. Thus, the relaxation of the medium from the metastable to the stable state has the Arrhenius dependence on temperature. At the same time, in the process of transitioning from the metastable to the stationary state, the energy of the element's excitation is converted into heat, which, due to the thermal conductivity, spreads through the medium and affects the neighbouring elements, and in turn causes their transition from the excited to the stable state. As a result, a wave of relaxation propagates in the medium. By analogy with the annealing of defects of a crystal structure, we may refer to the medium (or any part of it) in a metastable state as an unannealed medium (region), and the medium (region) in which the relaxation took place as an annealed region.

We describe the autowave process with a system of reaction-diffusion equations in a two-dimensional rectangular region, i.e. $(x, y) \in \Omega = [a_x, b_x] \times [a_y, b_y]$:

$$\begin{aligned} &\frac{\partial n}{\partial t} = -\frac{n}{\tau(T)}, \\ &c_p \rho \frac{\partial T}{\partial t} = \kappa \left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} \right) + \theta \frac{n}{\tau(T)}, \end{aligned} \tag{1}$$

where t is time, n is the density (number per unit volume) of elements in the metastable state, T is the temperature, c_p is the specific heat capacity, ρ is the density, and κ is the thermal conductivity of the material, while θ is the energy released as a result of the transition of one element from the metastable to the stable state. τ is the characteristic defect lifetime under the assumption that depends on temperature according to Arrhenius Law:

$$\tau(T) = \tau_0 \exp\left(\frac{E_\mathrm{a}}{k_\mathrm{B} T} \right), \tag{2}$$

where E_a is the activation energy, k_B is the Boltzmann constant, and τ_0 is a constant depending on the properties of the material. The material is assumed to be thermally isolated from the environment, i.e. system (1)-(2) is subject to the homogeneous boundary conditions of the second kind all over the material perimeter, $\partial\Omega$:

$$\left.\frac{\partial T}{\partial x}\right|_{x=a_x}=\left.\frac{\partial T}{\partial x}\right|_{x=b_x}\left.\frac{\partial T}{\partial y}\right|_{y=a_y}=\left.\frac{\partial T}{\partial y}\right|_{y=b_y}=0. \tag{3}$$

At the initial moment in time, the density of elements in a sample is constant throughout the volume and equal to n_0. Also, at the initial moment in time the temperature of the material is equal to T_0 everywhere except for the area Ω^* of size Δx by Δy on the left boundary of the sample in which the temperature is increased by external heating to $T_1 = T_0 + \Delta T$, where ΔT is a given, as shown schematically in Fig. 1.

By introducing new dimensionless variables

$$v=\frac{n}{n_0},\ u=\frac{k_\mathrm{B}T}{E_\mathrm{a}},\ \beta=\frac{\rho c_p E_\mathrm{a}}{\theta n_0 k_\mathrm{B}},\ \tilde{t}=\frac{t}{\beta\tau_0},\ \tilde{x}=x\sqrt{\frac{\theta n_0 k_\mathrm{B}}{\kappa E_\mathrm{a}\tau_0}},\ \tilde{y}=y\sqrt{\frac{\theta n_0 k_\mathrm{B}}{\kappa E_\mathrm{a}\tau_0}} \tag{4}$$

problem (1)-(2) can be written in a dimensionless form [2]:

$$\begin{aligned}&\frac{\partial v}{\partial \tilde{t}}=-\beta v\mathrm{e}^{-1/u},\\&\frac{\partial u}{\partial \tilde{t}}=\frac{\partial^2 u}{\partial \tilde{x}^2}+\frac{\partial^2 u}{\partial \tilde{y}^2}+v\mathrm{e}^{-1/u}.\end{aligned} \tag{5}$$

In an infinite medium for zero initial temperature ($u_0 = k_\mathrm{B}T_0 / E_\mathrm{a} = 0$), and for $v_0 = 1$ (in accordance with (6)), the system of equations (5) may have a solution in the form of a traveling wave, and the solution of the problem depends on one parameter, β, with the physical meaning of the ratio of activation energy to energy stored in elements. A numerical solution of the problem (5) was obtained in [2] for a one-dimensional geometry. In the same work, it was shown that the behaviour of the solution depends significantly on the value of parameter β, and undergoes a qualitative change when β exceeds the threshold value, approximately equal to 6.5. When this threshold is exceeded, spatial-temporal oscillations of front shape (especially of the temperature front) and of wave velocity occur.

For a sample of a finite size, the solution of the problem also depends on the initial and boundary conditions, and therefore on a larger number of dimensionless model parameters, including: the dimensionless width, $\tilde{L}_y$, and length, $\tilde{L}_x$, of the sample, the dimensionless magnitude, Δu, and the dimensionless width, $\Delta\tilde{y}$, and depth, $\Delta\tilde{x}$, of the initial heating area. In our study, as a rule, the heating magnitude, $\Delta u = k_\mathrm{B}\Delta T / E_\mathrm{a}$, and the heating depth, $\Delta\tilde{x}$, were fixed, while other parameters were varied one-by-one for four given values of β, namely for $\beta = 5.0$, $\beta = 6.8$, $\beta = 7.2$ and $\beta = 7.45$ taken from [2]. The adiabatic boundary conditions and initial conditions: $u_0 = 0$ and $v_0 = 1$, were assumed. The problem was solved by the finite difference method using a modified version of the algorithm from [5].

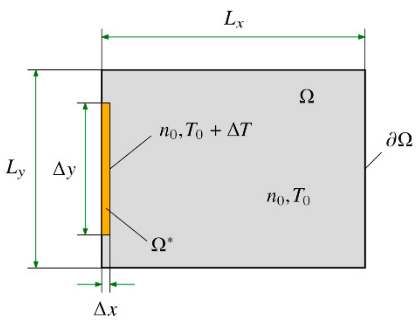

Fig. 1. Geometry of the problem and initial conditions.

3. Results and discussion

The propagation of the traveling waves under consideration has all the properties inherent to switching autowaves. When a one-dimensional wave is activated, it propagates at a constant speed and the waveform does not change. Wave propagation on the plane satisfies the principle of Huygens, and, therefore, wave diffraction takes place. There is, however, no wave interference since colliding waves destroy each other. The reflection of the autowave from obstacles and boundaries differs from the reflection of classical waves. In the case of a thermal-concentration wave, the “reflection” is merely a redistribution of heat fluxes. The speed of propagation of a smooth homogeneous wavefront depends on its curvature; a concave front propagates faster.

The activation of a self-sustained annealing wave has a threshold value of $\Delta\tilde{y}$ for a given $\Delta\tilde{x}$. For $\Delta\tilde{y}$ smaller than this threshold value, the self-sustained wave of relaxation does not develop: the relaxation wave quickly attenuates and heat redistributes over the sample. Depending on the parameters of the model, the shape of the relaxed zone may vary: "oval", "hat-shaped", "cascade", etc. shapes were observed. The transition from the relaxed to the non-relaxed area occurs abruptly, with a narrow transition zone. For $\Delta\tilde{y}$ above the threshold value, a self-sustained wave of relaxation forms, which runs over the entire volume of the sample, resulting in complete annealing of defects.

Depending on parameter β, two different regimes of traveling wave propagation are observed; this is in agreement with observations in [2]. Accordingly, for β smaller than the threshold value of approximately 6.5, the front of the traveling wave spreads as a whole and the velocity of propagation is perpendicular to the wavefront. For β above 6.5, small perturbations arise on the wavefront, and then grow by virtue of relaxation along the front. As a result, the new area of the relaxed medium has the form of a narrow drop-shaped strip that propagates along the line of the front and maintains an approximately constant width in the direction perpendicular to the front. The appearance of one or more small perturbations, which arise in a symmetric way, is then observed.

As example, the results of a simulation of a wave propagating in a rectangular region with dimensions: $\tilde{L}_x = 6000$ [arb. unit] and $\tilde{L}_y = 3000$ [arb. unit], are shown in Figs. 2—4. The wave is activated on the left boundary of the region by increasing at $\tilde{t} = 0$ the dimensionless temperature u from 0 to $\Delta u = 2/\beta$ [arb. unit] (where $\beta = 7.2$) in a narrow rectangular area of size $\Delta\tilde{x}\times\Delta\tilde{y} = 30\times1800$ [arb. unit] located symmetrically about the central axis.

In the course of spreading of the self-sustained annealing, the initial narrow rectangular area of high temperature expands forward and to the sides from the boundary and gets gradually rounded. The wavefront remains smooth and homogeneous. At $\tilde{t} = 9000$ [arb. unit] the temperature of the central part of the wavefront increases, and the area of relaxed material as well as the area of elevated temperature takes the form of a trapezoid (Fig. 2a). Then the area of elevated temperature extends forward rather than to the sides (along the wavefront line). The heated area takes the form of a segment, and two features, that lie symmetrically about the central axis of on the front line of the relaxed area, appear and the wavefront ceases to be smooth. The central part of the wavefront then rises again, and everything repeats (Fig. 2b—2d). In this case, the region of elevated temperature expands from the central burst to both sides along the wavefront, bending around it as a narrow band. After four such temperature bursts (from $\tilde{t} = 50000$ [arb. unit]), the relaxed area coincides with the heated one and has the form of a half-ellipse. At $\tilde{t} = 60000$ [arb. unit], two bursts of temperature, symmetric with respect to the central axis, appear and expand along the wavefront line as a narrow band (Fig. 3a—3b). The relaxed area increases by the width of the band. At $\tilde{t} = 65000$ [arb. unit], the wavefront reaches the lateral boundaries. Since the boundaries are adiabatic, the temperature near them increases, consequently the wave velocity near the boundaries increases, and the line of the front begins to level off (Fig. 4a). Later on ($\tilde{t} = 75000$ [arb. unit]), two narrow bands of elevated temperature propagate from the lateral boundaries along the wavefront (Fig. 4b). Further, both the relaxed and heated areas are expanded by the successive emergence and development of paired, symmetric temperature bursts. In this case, the line of the front becomes less curved. At $\tilde{t} = 99000$ [arb. unit], due to the joining in the centre of the two waves running along the front, three symmetrical temperature bursts appear. Further, the heated region expands by successive emergence and development of these three symmetric bursts, followed by five (Fig. 4c), then six and seven alternating bursts. The wavefront becomes generally flat, but the expansion of the heated region (up to the entire sample warming up) occurs as before by the emergence and development of 6 or 7 symmetric temperature bursts (Fig. 4d), and not by moving the front forward as a whole. Bursts arise, expand along the front and merge. Then new bursts arise and the process repeats until all metastable elements in the entire sample are relaxed.

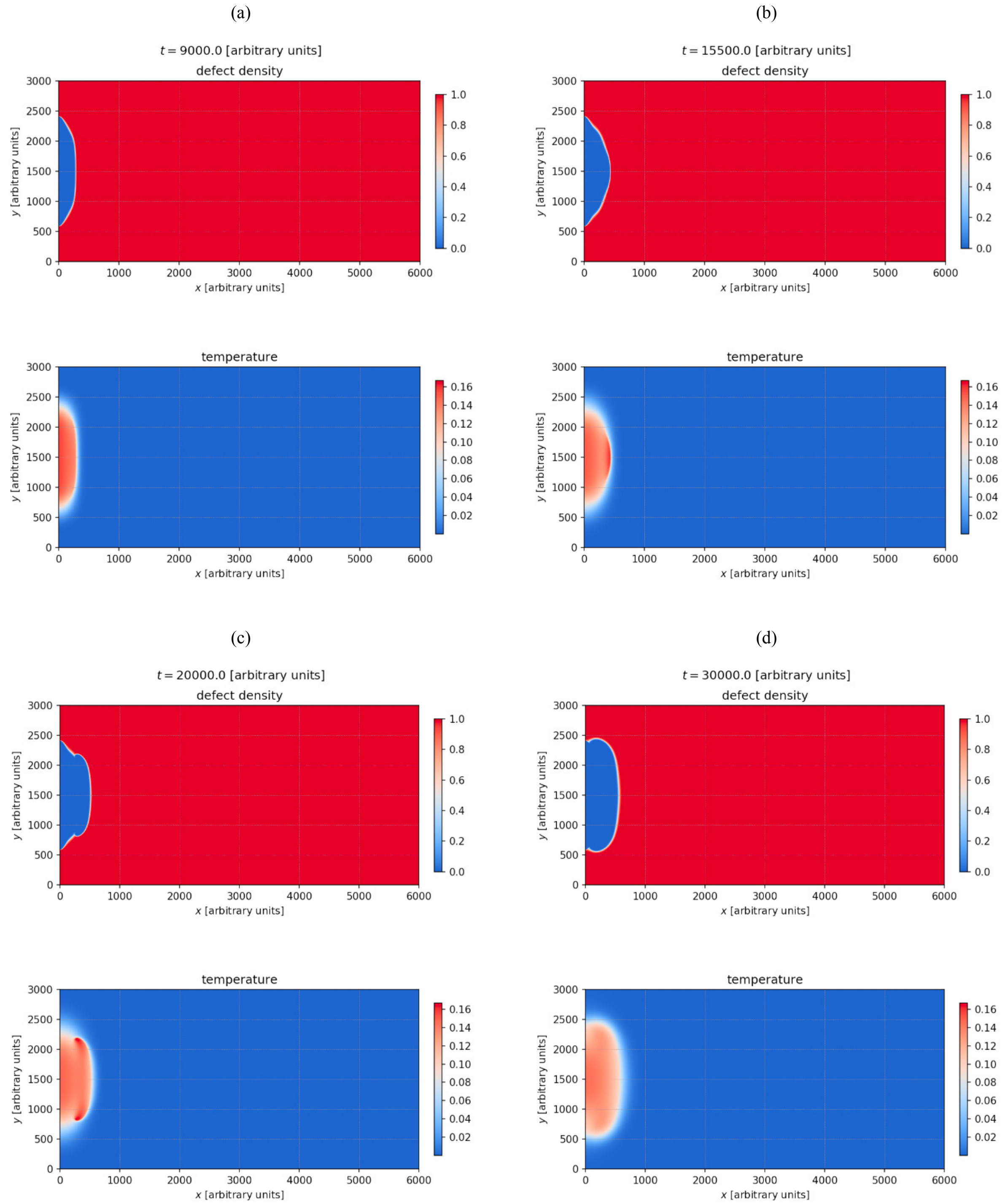

Fig. 2. Propagation of the self-sustained wave of relaxation in the beginning of the process.

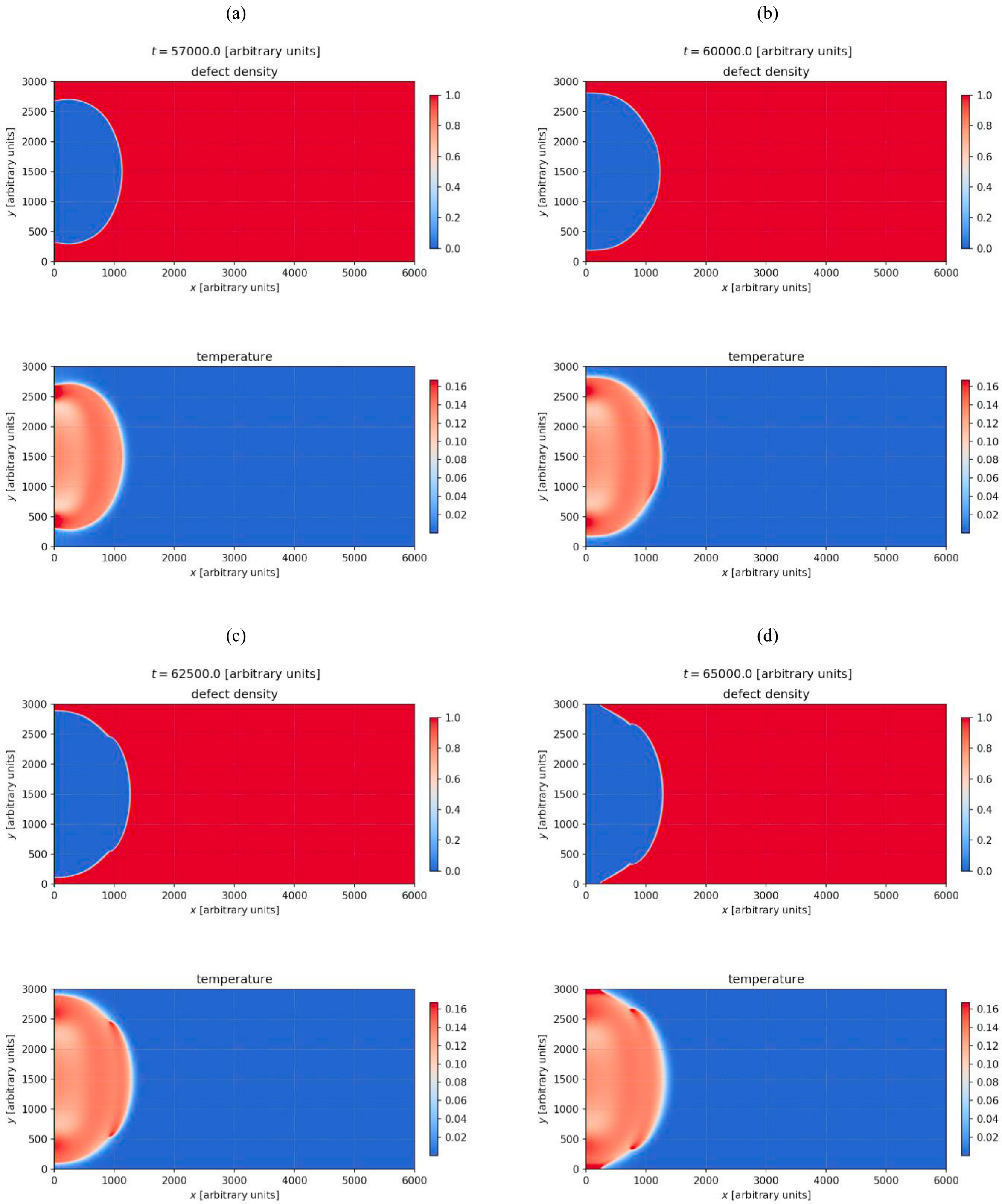

Fig. 3. Propagation of the self-sustained wave of relaxation before the wave front reaches the lateral boundaries.

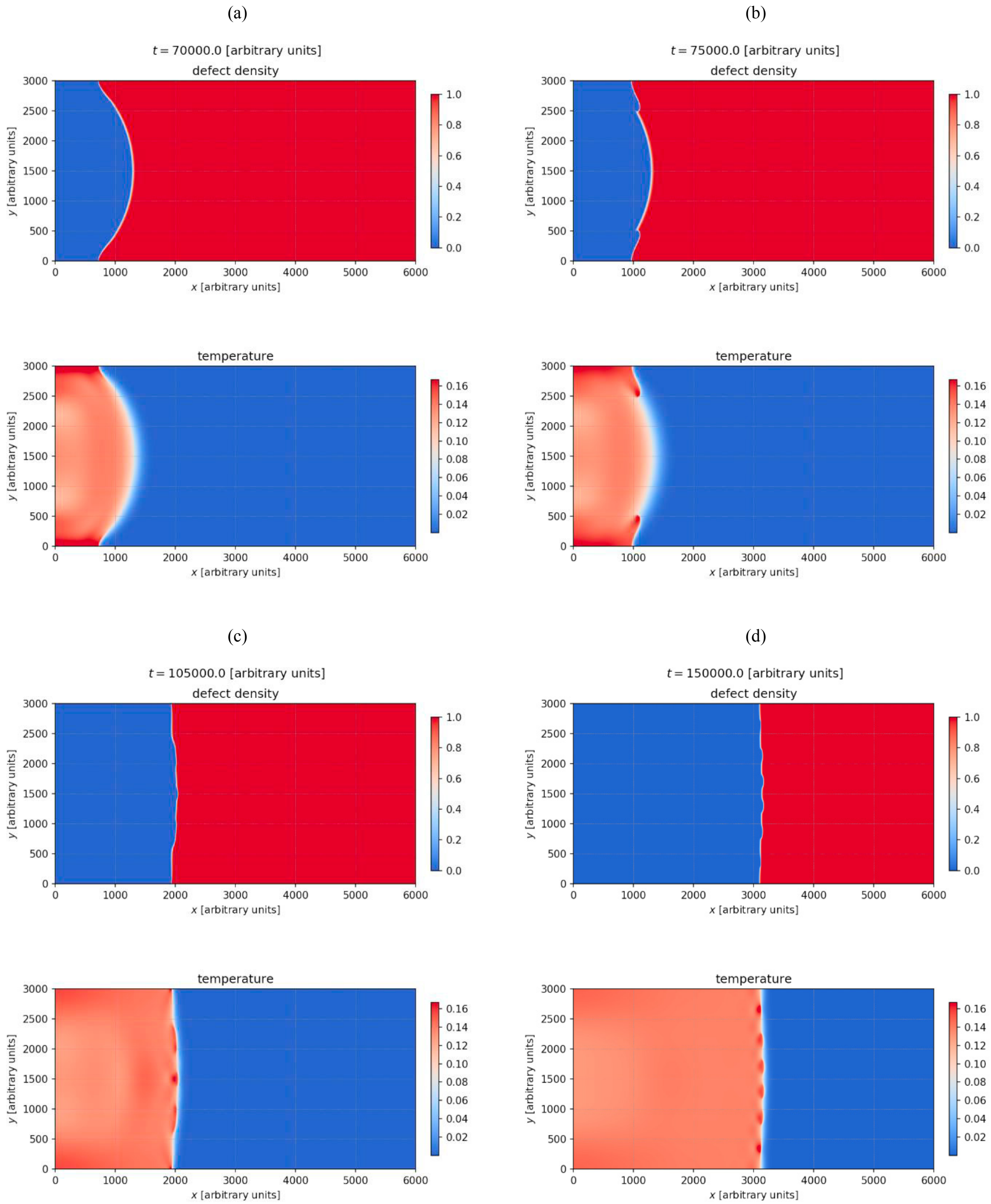

Fig. 4. Propagation of the self-sustained wave of relaxation after the wavefront reaches the lateral boundaries.

A wave activated in the centre of the region has similar properties. Soon after activation, the heated region expands and takes the form of a circle, regardless of whether the original shape of the activation pulse was quasi-circular or square. At this time, it coincides with the annealed area. Then, local areas of elevated temperature appear symmetrically and expand along the line of the front (circumferentially) in both directions and eventually merge, thereby increasing both the heated and annealed areas. Then everything repeats, but the number of bursts increases.

Since the appearance of temperature spikes has a threshold nature, it can be assumed that they are the result of instability, which develops due to thermal-concentration feedback, as well as in the one-dimensional case.

4. Conclusions

Initialization of the self-sustained relaxation waves has a threshold value with respect to the initiation energy, which is defined by the dimensions of the heated area and the magnitude of the heating. Below this threshold value, the self-sustained wave of relaxation does not develop, while above it, a self-sustained relaxation wave forms and then runs over the entire volume of the sample, resulting in complete relaxation of all excitable elements in the sample.

If the initial heating is performed uniformly along the entire width of the sample then, due to the symmetry of the problem, the solution remains one-dimensional (the dependence of solution on the lateral coordinate disappears). At the same time, it qualitatively repeats the results published in the literature for the one-dimensional case. Accordingly, when the non-dimensional parameter β, which is the ratio of activation energy to energy stored in elements, is below a threshold value of approximately 6.5, the annealing front propagates at a constant speed. For β above this value, oscillations of both the wave speed and of the temperature profile are observed.

If the initial heating is done over a part of the external boundary, the solution of the problem is two-dimensional, and its behaviour depends again on parameter β. Thus, for $\beta = 5.0$, the relaxation front has a smooth regular shape and the relaxation propagates in a direction perpendicular to the front. For β above the threshold value the propagating wave exhibits a more complex behavior: bursts of temperature appear and expand along the wavefront line as a narrow drop-shaped band, thereby increasing the relaxed area by the width of the band.

Thermally insulated boundaries lead to the straightening of the wavefront: in the vicinity of the boundary, the velocity of its propagation increases, resulting in the alignment of the front reduction of its total curvature.

Acknowledgements

This research was financially supported in part by the National Research Foundation (NRF) of South Africa (Grant 96281 of the first author). Any opinion, finding and conclusion or recommendation expressed in this material is that of the author(s) and the NRF does not accept any liability in this regard.

References

[1] Autowave Processes in Systems with Diffusion (ed. M. T. Grekhova), Institute of Applied Physics, USSR Academy of Sciences, Gorki (1981), pp. 6, 77, 117.

[2] R. O. Weber, G. N. Mercer, H. S. Sidhu, and B. F. Gray. Combustion waves for gases (Le = 1) and solids (Le → ∞), Proceedings of the Royal Society of London A: Mathematical, Physical and Engineering Sciences, 453 (1997) 1105-1118.

[3] P. M. Bokov and P. A. Selyshchev. Propagating self-sustained annealing of radiation-induced interstitial complexes. IOP Conference Series: Materials Science and Engineering, 110(1):012055 (2016).

[4] P. A. Selyshchev and P. M. Bokov. Kinetics of Annealing: Basic Relationships and Nonlinear Effects. In J. F. R. Archilla, F. Palmero, M. C. Lemos, B. Sánchez-Rey, and J. Casado-Pascual, editors, Nonlinear Systems, Vol. 2: Nonlinear Phenomena in Biology, Optics and Condensed Matter, pages 283–314. Springer International Publishing, Cham (2018) 283-314.

[5] C. Rossant. IPython interactive computing and visualization cookbook. Packt Publishing Ltd (2014).