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# Modeling the Destruction of the *p-n* Junction by Electromagnetic Pulses

D. Sergeyev[1,2,*], K. Shunkeyev[2], N. Zhanturina[2], A.L. Solovjov[3]

[1] *T. Begeldinov Aktobe Avation Institute, 39, Moldagulova Ave., 030012 Aktobe, Kazakhstan*
[2] *K. Zhubanov Aktobe Regional University, 34, Moldagulova Ave., 030000 Aktobe, Kazakhstan*
[3] *B. Verkin Institute for Low Temperature Physics and Engineering of the National Academy of Sciences of Ukraine, 61103 Kharkiv, Ukraine*

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Within the framework of the density functional theory and methods of molecular dynamics, the process of destruction of a silicon *p-n* junction at the influence of an electromagnetic pulse (thermal effect) is considered. With an increase in the amplitude of the electromagnetic pulse, a nonlinearity of the mobility of quasiparticles arises and impact ionization processes occur, leading to the formation of various defects in the crystal lattice of the semiconductor. The evolution of the occurrence of point defects in a semiconductor by thermal deformation, as well as a further increase in their concentration, is shown. It is demonstrated that the primary passage of an electromagnetic pulse generates defects in a defect-free crystal. Further thermal impact of the pulse leads to an increase in the deviation of atoms, leading to the accumulation of defects and the destruction of the structure. With an increase in temperature, the *p-n* junction loses its rectifying properties and an instantaneous increase in the magnitude of the reverse current is observed due to the occurrence of an ionization current, which coincides in direction with the saturation current. It is revealed that thermal deformation significantly distorts the *p-n* junction profile. It was found that the destruction of the semiconductor structure occurs in the defect-free part of the crystal, and the defects stimulate destruction. In semiconductors doped with Li or Sr, the destruction time of the *p-n* junction increases due to the occupation of mobile Li or Sr ions by the formed silicon vacancies during the thermal action of the pulse. The results obtained can be useful in the development of semiconductor structures resistant to external influences of an electromagnetic pulse.

**Keywords:** Computer modeling, *p-n* junction, Electromagnetic pulse, Thermal effect, Molecular dynamics.

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## 1. INTRODUCTION

It is known that an electromagnetic pulse (EMP) is one of the damaging factors of a nuclear explosion (mainly high-altitude), which is an exotic phenomenon as a physical process [1]. The source of such EMP can be special electrical generators capable of generating powerful pulses with a short duration of the order of nanoseconds to tens of nanoseconds, and have a high energy density (see, for example, [2]). The emergence of such powerful EMP generators of "non-nuclear" origin has led to the creation of highly effective weapons that can be used for terrorist or criminal purposes to deliberately deliver electromagnetic strikes in order to disable the radio-electronic equipment (REE) of the alleged enemy by physically destroying its semiconductor components, or temporarily (suppression) of equipment malfunction in the form of a functional failure (Fig. 1) [3]. Note that lightning-induced EMP also poses a serious danger to modern electronic devices [4].

Under the influence of an external electromagnetic radiation, malfunctions of the REE are usually accompanied by irreversible physical processes in semiconductor devices associated with the destruction of the structure of the *p-n* junction, i.e. the most vulnerable electronic components are semiconductor devices.

To solve the problems of determining and ensuring the resistance of the electronic component base of the REE to the external effects of EMP, many models of physical processes in semiconductor structures under conditions of strong electromagnetic influence have been developed [5].

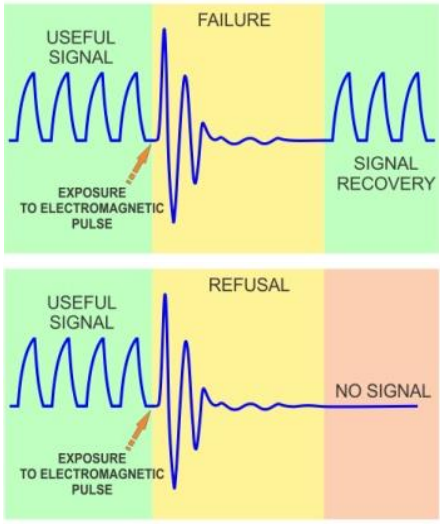



**Fig. 1** – Faults and failures in semiconductor devices under the influence of external electromagnetic pulse

The report of the US Air Force Laboratory analyzes various theoretical models describing the breakdowns of semiconductor devices (diodes and transistors), where the Wunsch-Bell (thermal) and Baruch-Budenstein (electrothermal) models [6] are indicated as

* serdau@mail.kz

the main models of the breakdown process, and the shortcomings of these models are also presented, associated with incorrect descriptions with a decrease in the duration of the acting EMP (in the region of nanosecond pulsed effects). However, until now, the basis for the development of models for describing the electromagnetic effect on semiconductor components are methods and algorithms designed to assess the EMP of a nuclear explosion in REE. The question of the identity of the impact of EMP of nuclear and non-nuclear origin on REE remains open. A full analysis of such physical processes requires further research in this direction.

Many modern models are focused on solving a homogeneous heat equation, where the values of the amplitude and duration of the acting pulse are set and the damage to electronic components is estimated, taking into account the elementary external heating of the structure. In [7, 8], simplified models are considered based on the solution of the heat equation, taking into account the localization of thermal power as the main factor of the influencing EMP, i.e. implying the main influence on the destruction of the semiconductor conditional (given by the value of the amplitude of the EMP) thermal processes. In [6], by numerical simulation of processes in electronic components, taking into account their design and technological parameters and parameters of the acting EMP, the electrical characteristics of the functional disruption of the operation of electronic equipment and thermal damage to their constituent electronic components were determined.

Further development of the description of the physical processes under consideration is connected with the phenomenological model (physico-topological model), which takes into account some parameters of the semiconductor, such as the band gap, intrinsic impurity concentration, mobility and lifetime of free charge carriers, etc. [9]. However, even such more advanced models do not allow one to reliably predict the level of resistance of semiconductor structures to EMP.

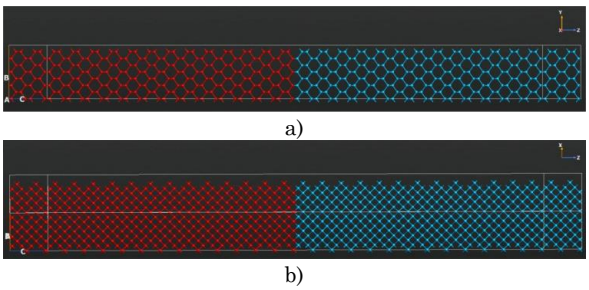
In our opinion, taking into account only the effect of thermal heating of the semiconductor element design is not sufficient, and in order to "illuminate dark corners" in this complex physical process, one should resort to atomistic modeling, i.e. take into account to assess the parameters of the influence of various defects in the crystal lattice of a semiconductor, stimulated by high-energy EMP. The fundamental factor of such destruction is the occurrence of various defects in the crystal lattice of the semiconductor under the influence of EMP, which will "transfer" the solid body into highly nonequilibrium states of the condensed phase, and a detailed study of such phenomena is necessary for the further development of technology for creating EMP-resistant semiconductor materials.

At present, there are many experimental techniques (for example, femtosecond interference microscopy) for studying pulsed phenomena in various time ranges. However, these methods provide only indirect information about the extreme state of matter. This led to the widespread use of various physical and mathematical modeling methods for studying the state of matter [10]. One of the proven tools in this direction is the atomistic methods of the density functional theory and molecular dynamics. The application of atomistic methods to the study of the interaction of high-energy EMP with matter makes it possible to study the mechanisms of thermal deformation and destruction, as well as to model all stages of the interaction of EMP with a condensed phase. The contribution of produced and intrinsic defects to the kinetics of destruction of a substance remains an important aspect [11]. Therefore, the purpose of this work is to study the process of destruction of semiconductor structures by methods of atomistic modeling [12, 13].

## 2. SIMULATION MODEL AND METHODS

Atomistic modeling is carried out in the following sequence: creation of a computer model of a semiconductor device (optimization of the geometry of a semiconductor, creation of a passivated layer, creation of the geometry of a diode (p-n junction), evaluation of the structure taking into account the formed defects), calculation of the main parameters (substantiation and choice of a calculation method, choice of exchange correlation functional, choice of pseudopotential and base grid, setting calculation parameters), processing of obtained numerical data, analysis of obtained results.

The geometry of the electron-hole junction is shown in Figure 2. The model of the *p-n* junction is 52 layers of silicon (2106 atoms), one half (26 layers) of which is doped with electrons (marked in blue in the figure), the other half is doped with holes (marked in the figure in red). The concentration of electrons and holes, depending on the type of semiconductor, varies from $10^{13}$ cm$^{-3}$ to $2 \times 10^{19}$ cm$^{-3}$.



a)

b)

**Fig. 2** – The geometry of the *p-n* junction

The optimization of the geometric parameters of semiconductor structures will be carried out within the framework of the electron density functional theory with the generalized gradient approximation (GGA). The setting of the semi-empirical Slater-Koster method was carried out as follows: k-point was chosen (7, 7, 100), Bassani. Si was chosen as the basis [14].

The process of destruction of the *p-n* junction structure was studied by the method of molecular dynamics [15]. According to this method, systems consisting of N interacting atoms are described by the system of Newton's equations:

$$m_i \frac{d^2\mathbf{r}_i(t)}{dt^2} = \mathbf{F}_i\left[\mathbf{r}_1, \ ..., \ \mathbf{r}_N\right], \quad (1)$$

or taking into account $\frac{d\mathbf{r}_i(t)}{dt} = \mathbf{v}_i(t)$:

$$m_i \frac{d\mathbf{v}_i(t)}{dt} = \mathbf{F}_i\left[\mathbf{r}_1, \ ..., \ \mathbf{r}_N\right], \quad (2)$$

where $m_i$, $\mathbf{r}_i$ and $\mathbf{v}_i$ – mass, coordinate and the velocity of $i$-th particle ($i = 1, \ ..., \ N$), $\mathbf{F}_i$ – force, acting on $i$-th particle. By solving the system of equations 1, 2, it is possible to determine the particle trajectories. Tersoff_Si_2005 [16], StillingerWeber_Si_1985 [17], ReaxFF_HOSiAlLi_2012 [18] were chosen as potentials.

Computer simulation of the current-voltage characteristics (CVC) of the p-n junction was carried out using the Slater-Koster method in combination with the Non-Equilibrium Green's Functions (NEGF) method [19, 20]. When calculating the CVC, the bias voltage varied from – 1 V to 1 V, energy – from – 2 eV to 2 eV, k-point was chosen 21 × 21. To calculate the CVC, the transmission spectrum (function) of the p-n junction under consideration is first determined:

$$T(\varepsilon) = \mathrm{tr}\left[\Gamma^L G \Gamma^R G^\dagger\right] = \mathrm{tr}\left[\Gamma^R G \Gamma^L G^\dagger\right], \quad (3)$$

where $\Gamma^{L(R)}(\varepsilon)$ is broadening matrix (broadening function) of the left (right) electrode, $G(\varepsilon)$, $G^\dagger(\varepsilon)$ are retarded and advanced green's functions, $\varepsilon$ is energy. Further, using the transmission function, the CVC of the p-n junction is determined based on the landauer equation:

$$I = \frac{2e}{h}\int_{-\infty}^{+\infty} T(\varepsilon)\left[f\left(\frac{\varepsilon-\mu_R}{k_B T_R}\right) - f\left(\frac{\varepsilon-\mu_L}{k_B T_L}\right)\right] d\varepsilon, \quad (4)$$

where $e$ is the electron charge, $h$ is the Planck constant, $f(\varepsilon)$ is the Fermi energy distribution function of quasiparticles, $k_B$ is the Boltzmann constant, $T_L$, $T_R$ are the current temperatures and $\mu_R$, $\mu_L$ are the electrochemical potentials of the right and left electrodes. The numerical data obtained were processed using the Origin program.

## 3. RESULTS AND DISCUSSION

As can be seen, the destruction of the p-n structure occurs due to thermal deformation (Fig. 3). At the initial stage of destruction, we observe the temperature displacement of atoms from the crystal lattice site to the interstices, i.e. the primary passage of EMP generates defects in a defect-free crystal. With an increase in the electron temperature, the deviations of atoms increase, accumulations of defects are observed, which then lead to destruction. At the moment of destruction, a sharp increase in the kinetic energy of the quasiparticles is observed.

It is reasonable to assume that at weak fields created by EMP, the mobility of carriers in a semiconductor is almost independent of the field. However, if the EMP field is significantly large, the quasiparticle mobility becomes nonlinear and, in some cases, the drift velocity is saturated. Under such conditions, impact ionization processes occur. When exposed to a powerful EMP, scattering often occurs through the emission of optical phonons, i.e. when a strong EMP interacts with matter, carriers acquire field energy and lose it due to the predominance of phonon emission over absorption. This leads to the appearance of a state in which the electron temperature is several orders of magnitude higher than the temperature of the crystal lattice. Such extreme overheating of a substance is accompanied by compression and tension, thereby causing the birth of both point and linear structural defects. We believe that under the influence of a pulsed energy input into a substance over a short period of time, depending on the pulse amplitude, the crystal structure can be restored, then we are talking about temporary failures of an electronic device (Fig. 1), on the other hand, it depends on the types and "sizes" born defects, as well as from intrinsic defects of the semiconductor. Such defects determine the electrical transport properties of a semiconductor device. Thermal deformation strongly affects the potential profile of the p-n junction; in the pre-fracture state of the junction, we observe its strong distortion (Fig. 4).

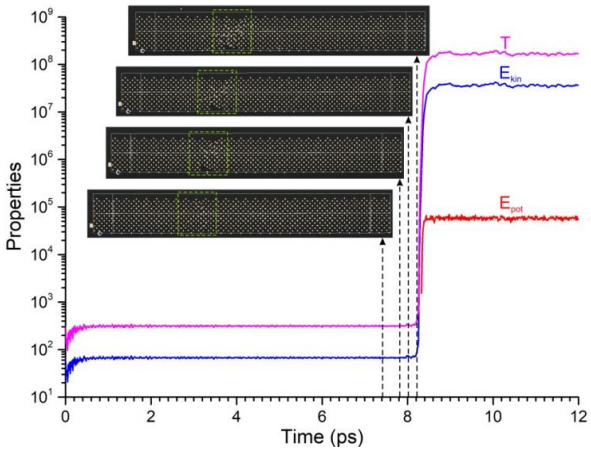



**Fig. 3** – Destruction of *p-n* junction (change in temperature, kinetic and potential energy over time)

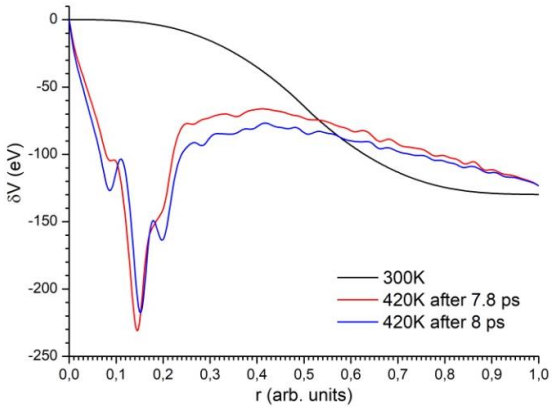



**Fig. 4** – Potential profile of *p-n* junction at different temperatures of quasiparticles (300 K and 420 K)

The EMP energy can be estimated using the expression:

$$\varepsilon_s = \int_0^\infty s(t)s^*(t)dt\,, \tag{5}$$

where $s(t)$ a function describing a signal, $s^*(t)$ complex conjugate function. For real signals, expression (5) is transformed

$$\varepsilon_s = \int_0^\infty s^2(t)dt\,. \tag{6}$$

From expression (6) it is obvious that the signal energy is directly proportional to the square of the amplitude. Then it can be assumed that the EMP energy with certain amplitude is sufficient to detach the atom from its original position, and for the irreversible displacement of the atom, it is sufficient to overcome only half of the interatomic bonds (1.18 Å). Note that the current temperature of the semiconductor has a noticeable effect on the value of the threshold energy of displacement of atoms. From the evaluation of the EMP energy, it is obvious that the thermal heating of a semiconductor element under the influence of a low level of EMP cannot lead to its complete failure, it only temporarily "knocks down" the operating mode. In this case, it is reasonable to assume that failures in semiconductor devices and electronic equipment based on them mainly occur under the influence of a powerful external EMP, which significantly exceeds the operating electrical loads.

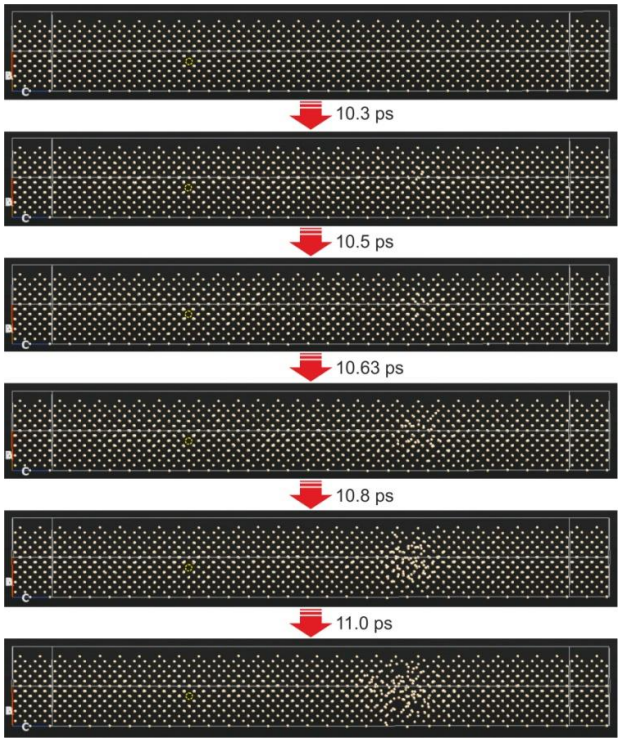



**Fig. 5** – The evolution of the destruction of p-n junction with vacancy defects

Real *p-n*-junction contains a relatively high concentration of growth and technological defects and is in a non-equilibrium disordered state. With the accumulation of defects in the excited region of the crystal, the root-mean-square deviations of atoms increase, almost as at the melting temperature. Under such conditions, overheating of the defective semiconductor structure occurs. Figure 5 shows the evolution of the destruction of an electron-hole junction with vacancy defects at a temperature of ~ 395 K (in the figure, the locations of vacancy defects are marked with a yellow dotted line). Usually, the melting process begins at the intersections of defects; however, as can be seen from Fig. 5, the destruction of the structure occurs in the defect-free part of the crystal.

The CVC of the *p-n* junction in the pre-destructive state are shown in Figure 6. As can be seen, with increasing temperature, the diode loses its rectifying properties. There is a sharp increase in reverse current. An increase in the reverse current is explained with the appearance of an ionization current that coincides in direction with the saturation current of the p-n junction. The ionization current leads to a redistribution of potentials in an electronic device, and also stimulates overheating of the p-n junction, which can lead to thermal breakdown.

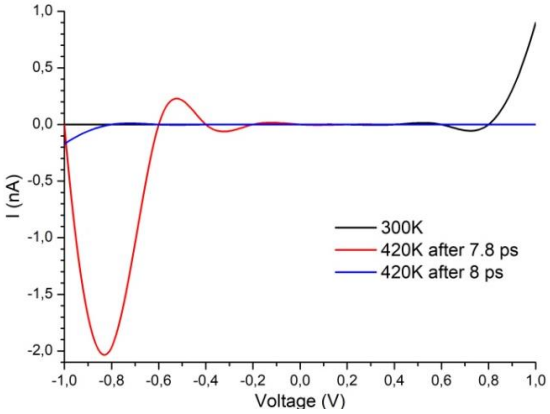



**Fig. 6** – CVC of *p-n* junction at different temperatures of quasiparticles (300 K and 420 K)

The destruction temperature slightly increases in silicon *p-n* junctions doped with lithium Li. We believe that this is due to the high mobility of Li ions under the action of an electric field and the occupation of the formed silicon vacancies, temporarily reanimating the site of destruction. Figures 7 and 8 show the diffusion properties of Li and Sr in Si.

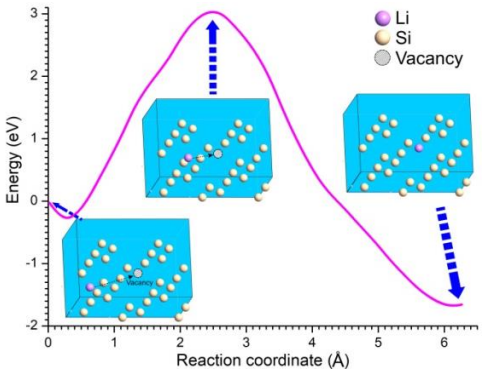



**Fig. 7** – Diffusion of the Li atom in the crystal lattice of Si

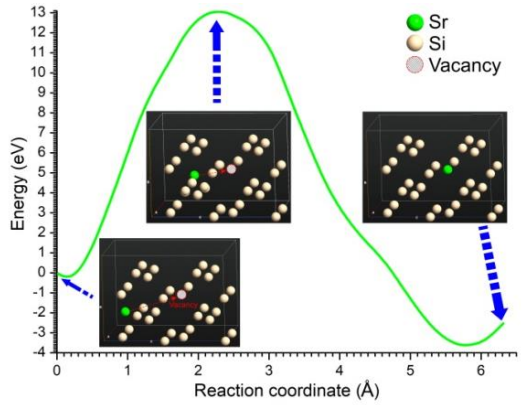



**Fig. 8** – Diffusion of the Sr atom in the crystal lattice of Si

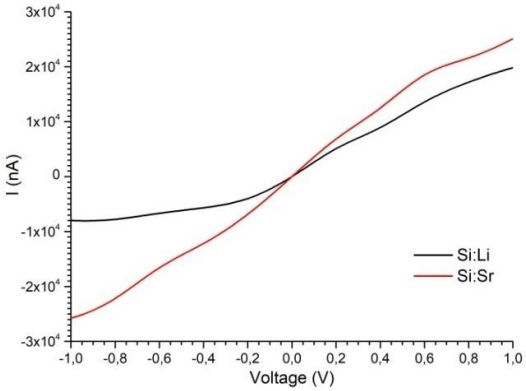



**Fig. 8** – CVC of a silicon electron-hole junction doped with Li and Sr

To overcome the barrier and occupy the place of Si vacancies, the Li ion requires ~ 3 eV of energy, and the Sr ion ~ 13 eV. However, an increase in the concentration of Li and Sr in Si leads to a deterioration in the rectifying properties of the *p-n* junction. Figure 9 shows the CVC of *p-n* junctions with 7 % Li and Sr content.

## 4. CONCLUSIONS

Thus, in this work, on the basis of atomistic modeling, the process of destruction of a silicon p-n junction is considered. The dynamics of the occurrence of defects in a semiconductor by thermal deformation is shown. The CVC of the diode before the destruction of the semiconductor structure are given. It has been established that the destruction of a defective semiconductor structure occurs in the defect-free part of the crystal. An increase in the destruction time of *p-n* junctions doped with Li or Sr due to the occupation of silicon vacancies by Li or Sr ions is shown. The obtained scientific results expand the understanding of the physical processes occurring in semiconductor structures under the influence of EMP, and can be useful in developing methods for testing semiconductor structures for resistance to external EMP influences, guidelines aimed at improving the reliability and stability of semiconductor components of REE.

## ACKNOWLEDGEMENTS

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# Моделювання руйнування *p-n*-переходу електромагнітними імпульсами

Д. Сергєєв[1,2], К. Шункєєв[2], Н. Жантуріна[2], А.Л. Соловйов[3]

[1] *Актюбінський авіаційний інститут імені Т. Бегельдінова, пр. Молдагулова, 39, 030012 Актобе, Казахстан*
[2] *Актюбінський регіональний університет імені К. Жубанова, пр. Молдагулова, 34, 030000, Актобе, Казахстан*
[3] *Фізико-технічний інститут низьких температур ім. Б. Веркіна НАН України, 61103 Харків, Україна*

У рамках теорії існування густини та методів молекулярної динаміки у статті розглядається процес руйнування кремнієвого p-n-переходу під дією електромагнітного імпульсу (термічний ефект). Зі збільшенням амплітуди електромагнітного імпульсу виникає нелінійність рухливості квазічастинок і відбуваються процеси ударної іонізації, що приводять до утворення різноманітних дефектів у кристалічній решітці напівпровідника. Показано еволюцію виникнення точкових дефектів у напівпровіднику шляхом термічної деформації, а також подальше збільшення їх концентрації. Показано, що первинне проходження електромагнітного імпульсу породжує дефекти в бездефектному кристалі. Подальший термічний вплив імпульсу приводить до збільшення відхилення атомів та накопичення дефектів і руйнування структури. З підвищенням температури *p-n*-перехід втрачає свої випрямляючі властивості і спостерігається миттєве збільшення величини зворотного струму за рахунок виникнення струму іонізації, який збігається за напрямком зі струмом насичення. Виявлено, що термічна деформація суттєво спотворює профіль *p-n*-переходу. Встановлено, що руйнування напівпровідникової структури відбувається в бездефектній частині кристала. У напівпровідниках, легованих Li або Sr, час руйнування *p-n*-переходу збільшується за рахунок заселення рухливими іонами Li або Sr утвореними вакансіями кремнію під час теплової дії імпульсу. Отримані результати можуть бути корисними при розробці напівпровідникових структур, стійких до зовнішнього впливу електромагнітного імпульсу.

**Ключові слова:** Комп'ютерне моделювання, *p-n*-перехід, Електромагнітний імпульс, Тепловий ефект, Молекулярна динаміка.