On one peculiarity of the model describing the interaction of the electron beam with the semiconductor surface

M A Stepovich, A N Amrastanov, E V Seregina, M N Filippov

1 Tsiolkovsky Kaluga State University, 26 Stepan Razin Street, Kaluga, 248023 Russia
2 Ivanovo State University, 39 Ermaka Street, Ivanovo, 153025 Russia
3 Bauman Moscow State Technical University (National Research University), Kaluga Branch, 2 Bazhenov Street, Kaluga, 248000 Russia
4 Kurnakov Institute of General and Inorganic Chemistry RAS, 31 Leninsky Prospect Street, Moscow, 119991 Russia

Abstract. The problem of heat distribution in semiconductor materials irradiated with sharply focused electron beams in the absence of heat exchange between the target and the external medium is considered by mathematical modeling methods. For a quantitative description of energy losses by probe electrons a model based on a separate description of the contributions of absorbed in the target and backscattered electrons and applicable to a wide class of solids and a range of primary electron energies is used. Using the features of this approach, the nonmonotonic dependence of the temperature of the maximum heating in the target on the energy of the primary electrons is explained. Some modeling results are illustrated for semiconductor materials of electronic engineering.

1. Introduction
Some methods for local analysis of semiconductors are based on the excitation of an informative signal by a beam of accelerated electrons (electron microscopy, spectroscopy of characteristic losses of electron energy, X-ray spectral microanalysis, etc.). However, when the electrons of low (1-8 keV) and medium (8-50 keV) energies decelerate in the semiconductor, only a small part of energy goes to the formation of informative signals, the most part of the energy goes to heating the sample [1, 2]. When the target is irradiated by a sharply focused electron beam, the heating of the sample can be significant, which can lead to an increase in the local temperature and, as a consequence, to a change in the characteristics of the semiconductor – this may lead to the necessity to take this into account on carrying out the quantitative measurements. Modeling the heating of semiconductor targets through an electron beam is the subject of this paper.

2. Simulation of electron beam energy losses
Many studies have been devoted to description of the distribution of energy losses in the interaction of an electron probe with a substance – see, for example, [3-7], while most models give only a qualitative agreement with the experimental results, and the application of each of them is usually limited by a comparatively narrow range of materials.
Among the available models, the most general approach to the description of energy losses by electron beams of medium energies was deduced in [6, 7], in which a model based on the possibility of a separate quantitative description of the contribution of the energy of the electrons absorbed in the target and backscattered electrons is described. This model can be successfully used to perform quantitative calculations for a wide class of materials in a wide range of primary-electron energies. According to this model, the energy loss density of the beam electrons looks like as:

$$\frac{P(M)}{P_0} = \frac{1}{\pi^2 a_i^2 z_{ms}} \left(1 - \eta + \frac{z_{ms}}{z_{ms}}\right) \left(\exp\left[-\frac{x^2 + y^2}{a_i^2} + \left(\frac{z - z_{ms}}{z_{ms}}\right)^2\right]\right) +$$

$$\frac{\eta a_i^2}{(1 - \eta) a_s^2} \exp\left[-\frac{x^2 + y^2}{a_s^2} + \left(\frac{z - z_{ss}}{z_{ss}}\right)^2\right]\right] +$$

(1)

Here the origin coincides with the point of incidence of the electron probe on the sample. $P_0 = IE_0/e$ – the primary beam power; $z_{ms}$ – the depth of maximum energy loss by primary electrons, that have experienced small-angle scattering and absorbed in the target, and $z_{ss}$ – the depth of the maximum energy loss by backscattered electrons [4-7], $a_i = Z_{ss}^2 z_{ms}$, $Z_1$ – ordinal number of an element in the periodic table; $\eta$ – backscattering coefficient of electrons, $\eta = 1.085ae\pi^{1/2}z_{ms}^{-1} \int_0^\infty \exp\left(-\left(z - z_{ss}\right)^2 z_{ms}^{-2}\right) dz_{ms}$, $a = 0.024Z^2A^{-1}$, $e$ – base of natural logarithms; $A$ – atomic weight of the element. Parameters $a_i$ and $a_s$ are determined from the relevant $a_i^2 = z_{ms}^2 + 0.72d_b^2$, $a_s^2 = 0.25z_{ss}^2 + 0.72d_b^2$, where $d_b$ – diameter of the probe [7].

The distributions of energy loss densities we calculated by (1) for kilovolt electrons in Si, GaAs, and CdTe normalized by the amount of energy released per target per unit time are illustrated in Fig. 1.
The possibilities of using this model for estimating the heat distribution in various semiconductor targets are the subject of this work. In this case, unlike [8], in the present work, the simulation was carried out for the case of the absence of heat transfer of the target with the external medium, which is usually realized in electron-probe technology.

3. **Modeling of heat distribution**

The time to establish a steady-state temperature regime of the analyzed microvolume is usually much shorter than the data set time during which the electron probe is positioned at a given point on the surface of the sample [6]. This makes it possible to look for a temperature distribution in the region of interaction of the probe electrons with the sample and in the adjacent regions of the sample on the basis of the solution of the stationary heat equation

\[
\left( \frac{\partial^2 \Delta T(x, y, z)}{\partial x^2} + \frac{\partial^2 \Delta T(x, y, z)}{\partial y^2} + \frac{\partial^2 \Delta T(x, y, z)}{\partial z^2} \right) = -\frac{P(x, y, z)}{k}. \tag{2}
\]

Here \( \Delta T(x, y, z) = T(x, y, z) - T_0 \), where \( T \) – sample temperature at point \( (x, y, z) \), \( T_0 \) – temperature after the establishment of a stationary regime under the influence of an electron beam, and \( P(x, y, z) \) – function describing energy losses by an electron probe in a target; \( \Delta T(x, y, z) \) must satisfy the following boundary conditions:

\[
\lim_{x \to \pm \infty} \Delta T = 0, \quad \lim_{y \to \pm \infty} \Delta T = 0, \quad \lim_{z \to \pm \infty} \Delta T = 0.
\]

Since in electron-probe technology the target irradiation by an electron beam is mainly carried out under conditions close to vacuum, the following boundary condition, meaning the absence of heat exchange with the external medium:

\[
\frac{\partial \Delta T}{\partial z} \bigg|_{z=0} = 0.
\]

Equation (2) can be solved in a standard way using the Green's function. The corresponding equation for the Green's function will have the form:

\[
\text{div grad } G = -\delta(x-x_0, y-y_0, z-z_0)
\]

with boundary conditions:

\[
\lim_{x \to \pm \infty} G = 0, \quad \lim_{y \to \pm \infty} G = 0, \quad \lim_{z \to \pm \infty} G = 0, \quad \lim_{z \to 0} k \frac{\partial G}{\partial z} \bigg|_{z=0} = 0.
\]

This equation as a Green's function of the Neumann problem in the upper half-space is solved by the method of mirror mappings and has a solution

\[
G = \frac{1}{4\pi} \left( \frac{1}{(x-x_0)^2 + (y-y_0)^2 + (z-z_0)^2} + \frac{1}{(x-x_0)^2 + (y-y_0)^2 + (z+z_0)^2} \right).
\]

Here \( (x_0, y_0, z_0) \) – point source coordinate. Heat distribution \( \Delta T(x, y, z) \) is defined as follows:

\[
\Delta T = \int_D G(x_0, y_0, z_0, x, y, z) \frac{P(x_0, y_0, z_0)}{k} \, dV_0, \tag{3}
\]

where \( D \) – heat distribution area \( (-\infty < x_0 < +\infty, \ -\infty < y_0 < +\infty, \ 0 \leq z_0 < +\infty) \), \( dV_0 = dx_0 dy_0 dz_0 \). Formula (3) was used to estimate the heating of semiconductor targets by an electron beam.
4. Results of calculations

The simulation results showed that the highest heating of all samples by medium energy electrons is observed at the lowest (from the considered range) energies, which is explained by the increasing of heating region with increasing primary electron beam energy. Therefore, the range of low electron energies of the probe is the most interesting for estimating target heating. At fixed beam energies, the smallest heating is observed for an easy target (Si), and the heaviest sample (CdTe) is heated most of all (see Fig. 2). This is due to the fact that as the ordinal number of the semiconductor increases, the interaction region of the electron probe with the target decreases.

![Figure 2](image)

*Figure 2.* Temperature distribution in Si (a), GaAs (b) and CdTe (c) by coordinate $z$. The calculations were carried out at $x = 0, y = 0$, for primary electron energies $E_0 = 2$ (curves 1), $4$ (2), $6$ (3) keV, at probe current $10^{-7}$ A.

Figures 3, 4 and 5 show the calculated distributions $\Delta T(x, y, z)$ in Si, GaAs, and CdTe semiconductor materials and the dependence of the maximum temperature in the target on the energy of the primary electrons $\Delta T(E_0)$; the contribution of the energy scattered in the target by the absorbed and backscattered (reflected) electrons is separately shown.

The contribution of the absorbed in the target electrons to the total energy losses of the electron probe in the target and, correspondingly, to its heating, is determinant at a probe energy of less than 4...5 keV. For heavy semiconductors, the energy losses by these electrons become practically zero at an energy of about 8 keV. For light samples and samples with average ordinal numbers, the energy losses absorbed in the target and backscattered electrons become commensurate at an electron energy of the probe of about 8 keV. As for backscattered electrons, they are characterized by the presence of a maximum of about 5 keV, and then the curves decrease monotonically.

The presence of a rather sharp increase in the contribution of backscattered electrons to the total curve $\Delta T(E_0)$ leads to the formation of a "step" on the dependences of the maximum temperature on the energy of the primary electrons. We also note that the backscattered electrons have the least effect on the value of the maximum heating for light samples; this effect is observed most in heavy semiconductor targets.
Figure 3. The results of modeling the heating of a semiconductor target for parameters characteristic of single-crystal silicon: in the left figure, modeling the temperature distribution for electron energy 4 keV; in the right figure, the simulation of the distribution of the dependence of the maximum temperature on the energy of the primary electrons (curve 1) also the contribution to the curve 1 of the energy scattered by the electrons absorbed in the target (curve 2) and reflected (curve 3) is shown. Calculations were carries out at the probe current $10^{-7}$ A.

Figure 4. The results of modeling the heating of a semiconductor target for parameters characteristic of single-crystal gallium arsenide: in the left figure, modeling the temperature distribution for electron energy 4 keV; in the right figure, the simulation of the distribution of the dependence of the maximum temperature on the energy of the primary electrons (curve 1) also the contribution to the curve 1 of the energy scattered by the electrons absorbed in the target (curve 2) and reflected (curve 3) is shown. Calculations were carries out at the probe current $10^{-7}$ A.
Figure 5. The results of modeling the heating of a semiconductor target for parameters characteristic of single-crystal cadmium telluride: in the left figure, modeling the temperature distribution for electron energy 4 keV; in the right figure, the simulation of the distribution of the dependence of the maximum temperature on the energy of the primary electrons (curve 1) also the contribution to the curve 1 of the energy scattered by the electrons absorbed in the target (curve 2) and reflected (curve 3) is shown. Calculations were carries out at the probe current $10^{-7}$ A

5. Conclusions
The methods of mathematical modeling were used to study the heating of semiconductor targets using an electron beam of medium and low energies. The greatest heating of all samples by medium-energy electrons is observed at the lowest (from the considered range) energies. At fixed beam energies, the smallest heating is observed for light targets. The obtained heating estimates make it possible to select the optimal mode of action of the beam electrons on a semiconductor target when planning the experiment.

References
[1] Rau E I, Ditsman S A, Zaitsev S V, Lermontov N V, Lukyanov A E and Kupreenko S Yu 2013 *Bulletin of the Russian Academy of Sciences: Physics* 77 951
[2] Amrastanov A N, Kuzin A Yu, Mityuklyaev V B, Seregin E V, Stepovich M A, Todua P A and Filippov M N 2017 *Measurement Techniques* 60 534
[3] Donolato C 1981 *Phys. Stat. Sol. (a)* 65 649
[4] Kanaya K and Okayama S 1972 *J. Phys. D: Appl. Phys.* 5 43
[5] Oelgart Q and Werner U 1984 *Phys. Stat. Sol. (a)* 85 205
[6] Mikheev N N, Petrov V I and Stepovich M A 1991 *Bulletin of the Academy of Sciences of the USSR. Physical Series* 55 1
[7] Mikheev N N and Stepovich M A 1996 *Industrial Laboratory* 62 221
[8] Amrastanov A N, Ginzgeymer S A, Stepovich M A and Filippov M N 2016 *Bulletin of the Russian Academy of Sciences: Physics* 80 1290