Assessment of the heating of conductive targets with an electron beam. Results of computational experiment

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Abstract. The problem of heat distribution in conducting (metal and semiconductor) materials irradiated by sharply focused low-energy electron beams in the absence of heat exchange between the target and the external medium was considered with the methods of mathematical modelling. The simulation is based on solving a multidimensional stationary heat equation using the Green's function. A model is based on a separate description of the contributions to the energy of absorbed and backscattered electrons dissipated in the target. It is applicable to a wide class of solids and the energy range of primary electrons. The results of calculations using the model under consideration of heating a target with an electron probe are given for various metallic and semiconductor materials. The obtained results can be used in the planning of experimental studies of conducting materials.

1. Introduction

Some methods for local analysis of condensed matter 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.). When a sample is irradiated with a focused electron beam (electron probe), considerable energy is released at the site of its fall onto the target, which can lead to an increasing of the local temperature [1, 2] and, as a consequence, the possible need to take this phenomenon into account when conducting quantitative studies. Consideration of the heating of a conductive target can be especially important when using modern electron-probe technology, since the effective diameter of the electron beam interacting with a semiconductor target can reach 1-2 nm. In this case, the density of energy released by an electron beam in a target can vary from 10 to 1000 W/cm³, and the characteristic size (diameter) of the microvolume of energy loss by electrons of the beam does not exceed 1 or 1.5 micrometers [2]. Thus, when a target is irradiated with an acutely focused electron beam, sample heating can be significant, this can lead to an increasing of the local temperature, which, in turn, can lead to the need to take this into account when conducting quantitative studies. Experimental determination of the heating temperature is greatly complicated by the small size of the region heat generation, that is why the results obtained have low accuracy and can only be considered as qualitative. Therefore, in practice, the calculated estimates of the amount of heating by an electron probe, based on the solution of the heat equation, are of particular value [3, 2].
2. Statement of the problem

Earlier [4-6], mathematical modeling was used to calculate the heating of semiconductor targets under an electron probe. In this paper, the objects of research are all conducting targets: both semiconductors and metals. In this case, as before, a model based on the possibility of a separate quantitative description of the energy contribution by the electrons absorbed in the target and backscattered electrons is used as a function of generating the heat source [7, 8]. This model can be successfully used to carry out quantitative calculations for a wide class of materials (practically from Al to Pt) in a wide range of energies of primary electrons (almost from units of kiloelectronvolts to 50 keV). The use of this model in carrying out calculations for heating targets with low-energy electrons and medium-energy electron beams for various conducting targets and comparing the results of calculations for metals and semiconductors is the main goal of this work.

3. About the mathematical model of the process

The temperature field in a conductive target irradiated by an electron beam can be calculated by solving the following three-dimensional stationary equation:

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

Here \( \Delta T(x, y, z) = T(x, y, z) - T_0 \) is the desired heating of the target when exposed to an electron probe, \( T \) is the temperature of the sample at a point \((x, y, z)\) after the stationary regime has been established under the influence of an electron beam, \( T_0 \) is the temperature of the sample before the electron beam, \( k \) is the thermal conductivity, and \( P(x, y, z) \) is the function describing the energy loss of the probe electrons in the target [7, 8]:

\[
P(M) = \frac{1.085(1-\eta)P_0}{\pi^2a_z^2z_{ms}} \left( 1 - \eta + \eta \frac{z_{ss}}{z_{ms}} \right) \exp \left[ - \left( \frac{x^2 + y^2}{a_1^2} + \left( \frac{z - z_{ms}}{z_{ms}} \right)^2 \right) \right] + \\
+ \frac{\eta a_z^2}{(1-\eta)a_z^2} \exp \left[ - \left( \frac{x^2 + y^2}{a_2^2} + \left( \frac{z - z_{ss}}{z_{ss}} \right)^2 \right) \right].
\]

Here the origin coincides with the point of incidence of the electron probe on the sample. \( P_0 = IE_0/\varepsilon_0 \) is the primary beam power, \( I \) and \( E_0 \) are current and energy of the electron beam, respectively, \( \varepsilon_0 \) is the electron charge; \( z_{ms} \) is the depth of maximum energy loss by primary electrons, that have experienced small-angle scattering and absorbed in the target, and \( z_{ss} \) is the depth of the maximum energy loss by backscattered electrons [4-7], \( z_{ss} = Z/\eta z_{ms} \), \( Z \) is ordinal number of an element in the periodic table; \( \eta \) is backscattering coefficient of electrons, \( \eta = 1.085ae^{\frac{1}{2}}z_{ms}^{-1} \int_{-\infty}^{\infty} \exp \left( - (z - z_{ss})^2 z_{ss}^{-2} \right) dz \), \( a = 0.024Z^2A^{-1} \), \( e \) – base of natural logarithms; \( A \) – atomic weight of the element. Note that for a massive target \( \eta = \int_{0}^{\infty} \eta(z)dz \approx 0.024eZ^{1.67}/A \). Parameters \( a_1 \) and \( a_2 \) are determined from the relevant \( a_1^2 = z_{ms}^2 + 0.72d_x^2 \), \( a_2^2 = 0.25z_{ss}^2 + 0.72d_y^2 \), where \( d_x \) is diameter of the probe.

\( \Delta T(x, y, z) \) must satisfy the following boundary conditions:

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

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

The solution of the heat equation under consideration was obtained using the Green’s function [3-5, 9]. Heat distribution $\Delta T(x, y, z)$ is defined as follows:

$$\Delta T = \int_{D} G(x_0, y_0, z_0; x, y, z) \frac{P(x_0, y_0, z_0)}{k} \, dV_0.$$  

Here $G$ is a Green’s function, $(x_0, y_0, z_0)$ is the point source coordinate, $D$ is heat distribution area ($-\infty < x_0 < +\infty$, $-\infty < y_0 < +\infty$, $0 \leq z_0 < +\infty$), $dV_0 = dx_0\,dy_0\,dz_0$.

For our problem

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

4. Results of mathematical modelling

The results of the computational experiment for the parameters of targets characteristic of a wide range of semiconductor materials used in practice are described in sufficient detail in [4-6, 9]. And some results of calculations of heating a copper target for a wide range of electron energies are presented in figure 1. Note that a copper target is a target with parameters typical for medium metal targets. These results allow us to estimate the change in heating temperature as a function of the electron energy of the probe. We note that qualitatively similar dependences were obtained by us for semiconductor materials, and the results of these calculations allow us to compare heating values for both metal and semiconductor samples, to evaluate the general patterns and characteristics of heating of metal and semiconductor targets. Hereinafter, the x and y axes of the Cartesian rectangular coordinate system are on the flat surface of the target, and the z axis is directed deep into the target and $z=0$ on the target surface.

Figure 2 shows the calculated heating of the targets in depth for an electron energy of 10 keV, which can be considered boundary for low (units of kiloelektronvolts) and medium (tens of kiloelectronvolts, up to about 50 keV) electron energies. The calculations were carried out for a probe current of $10^{-7}$ A, which in a certain sense can be considered boundary for various electron probe devices: smaller currents, incl. smaller by several orders of magnitude, are characteristic for scanning electron microscopes, and high currents – for X-ray microanalyzers.

The most interesting results are in computational experiment for low electron energies. This can be explained by the fact that the size of the electron deceleration region of the beam is approximately inversely proportional to the fourth power of the initial electron energy and therefore there is a significant increase in the bulk density of thermal energy generated in the sample [2]. A comparison of the results of calculations for conducting samples with average parameters: a copper target and a target of gallium arsenide is shown in figure 3 and figure 4.
Figure 1. The results of modeling the heating of a metallic target for parameters characteristic for Cu for probe current $10^{-7}$ A and electron energies 2 (a), 6 (b), 10 (c), 15 (d), 20 (e), 25 keV (f).

Figure 2. Calculated temperature distribution in a copper target (a) and in a gallium arsenide target (b) for a beam energy of 10 keV and a probe current of $10^{-7}$ A.

At the same other conditions, denser targets heat up more strongly (effective sequence numbers of target materials $Z_{Cu} = 29$ and $Z_{GaAs} = 32$, effective relative atomic masses of target materials $A_{Cu} = 64$ and $A_{GaAs} = 72$).
Figure 3. The simulation results of temperature distributions in Cu. The calculations were performed for the electron energy of the beam 2 (a) and 4 (b) keV at current probe $10^{-7}$ A.

Figure 4. The simulation results of the temperature distribution in GaAs. The calculations were performed for the electron energy of the beam 2 (a) and 4 (b) keV with probe current $10^{-7}$ A.

To illustrate the results of modelling the temperature distribution over depth in figure 5 shows plots of $\Delta T(z)$ dependencies in a copper target for $x$ and $y$ values equal to zero. These dependences allow estimating the maximum values of target heating. The calculations were performed for energies 2 (curve 1), 6 (2), 10 (3), 15 (4), 20 (5) and 25 keV (6) with probe current $10^{-7}$ A. It follows from these data that the main heating of the target is observed in the near-surface region is about 0.5 microns. This result is also characteristic for light targets (for example Al, $Z_{\text{Al}} = 13$ and $A_{\text{Al}} = 27$) at low electron energies, however, at medium energies from about 20 keV, substantial heating is also observed at 2...3 $\mu$m. And for heavy targets (for example Au, $Z_{\text{Au}} = 79$ and $A_{\text{Au}} = 197$), the main heating at the considered electron energies for a significant number of tasks can be taken into account to a depth of 0.1...0.15 $\mu$m.
Figure 5. The results of modelling the temperature distribution over $z$ in Cu at $x$ and $y$ equal to zero. Calculations were performed for energy 2 (curve 1), 6 (2), 10 (3), 15 (4), 20 (5) and 25 keV (6) with probe current $A^{-7}$ A.

Note that under the same conditions, the heating of metal targets is substantially less than the heating of targets made from semiconductor materials – see figure 6.

Figure 6. 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.

For metal targets, as well as for semiconductor targets, a non-monotonic dependence $\Delta T(E_0)$ was found. We note in particular that for semiconductors, this dependence had a local maximum for practically the entire class of materials: light, medium and heavy – see figure 7. For metals, the local
maximum was characteristic only for heavy targets – see figure 8. The explanation for this is the high thermal conductivity of metal targets, which "smoothed out" the effect of the back scattered electrons on the dependencies $\Delta T(E_0)$.

**Figure 7.** The results of modeling the heating of a semiconductor targets for parameters characteristic of single-crystal Si (a), GaAs (b), CdTe (c): the simulation of the distributions of the dependences of the maximum temperature on the energy of the primary electrons (curve 1) also the contribution to the curves 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 8.** The results of modeling the heating of a metal target for parameters characteristic for Au: 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 conducting (metal and semiconductor) materials using an electron beam of medium and low energies. The greatest heating of all samples by the 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 the conducting targets when planning the experiment.
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