Mathematical modelling of heating of homogeneous metal targets with a focused electron beam

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Abstract. The problem of heat distribution in metal materials irradiated with sharply focused electron beams in the absence of heat exchange between the target and the external medium is considered with 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 is used. This method is applicable to a wide class of solids and a range of primary electron energies. Some modeling results are illustrated for different metal materials.

1. Introduction
Some methods for local analysis of solids are based on the excitation of an informative signal with 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 targets, 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]. Target heating can be especially important when using modern electron-probe technology, since the effective diameter of an electron beam interacting with a semiconductor target can be as high as 1-2 nm. When this happens, the density of the energy emitted by the electron beam in a target can range from 10 to 1000 W/cm³ [2], and the characteristic size (diameter) of the area of electron beam energy loss is no more than 1 or 1.5 micrometers. So, when the target is irradiated with a sharply focused electron beam, the heating of the sample can be significant, which can lead to an increase in the local temperature and this may lead to the necessity to take this into account on carrying out the quantitative measurements. In [3-5] we considered the influence of electron beam on semiconductor targets. Modeling the heating of metal targets with an electron beam is the subject of this paper.

2. Simulation of electron beam energy losses
For computation of energy losses of an electron beam in the condensed substance, we use 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 [6, 7]. 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 has the form:
\[ P(x, y, z) = \frac{1.085(1-\eta)P_0}{\pi^{\frac{3}{2}}a_i^2z_{ms}} \left( 1-\eta + \eta \frac{z_{ms}}{z_{ms}} \right) \exp \left( -\left( \frac{x^2 + y^2}{a_i^2} + \left( \frac{z - z_{ms}}{z_{ms}} \right)^2 \right) \right) + \frac{\eta a_i^2}{(1-\eta)a_i^2} \exp \left( -\left( \frac{x^2 + y^2}{a_i^2} + \left( \frac{z - z_{ms}}{z_{ms}} \right)^2 \right) \right). \]  

Here the origin coincides with the point of incidence of the electron beam on the sample; \( P_0 \) is the primary beam power; \( z_{ms} \) is the depth of maximum energy loss with primary electrons, that have experienced small-angle scattering and absorbed in the target, and \( z_{ms} \) is the depth of the maximum energy loss with backscattered electrons. \( z_{ms} = Z^{-\frac{1}{3}}z_{ms} \), \( Z \) is the effective target material number; \( \eta \) is the backscattering coefficient of electrons. Parameters \( a_i \) and \( a_s \) are determined from \( a_i^2 = z_{ms}^2 + 0.72d_b^2 \) and \( a_s^2 = 0.25z_{ms}^2 + 0.72d_b^2 \), respectively, where \( d_b \) is diameter of the probe.

For probe electrons with energy \( E_0 \) [keV] incident perpendicular to a target surface with density \( \rho_0 \) [g/cm\(^3\)], \( z_{ms} \) can be expressed in terms of total beam electron path \( R \) in a solid (see diffusion model [8]):

\[ z_{ms} = \frac{R}{2} \left[ 1 - \left( \frac{C\gamma}{1+\gamma} \right)^2 \right], \quad R[\mu m] = \frac{2.76 \cdot 10^{-2}AE_0^{\frac{5}{6}}}{\rho_0Z^{\frac{5}{6}}} \left( 1 + 0.978 \cdot 10^{-1}E_0 \right)^{\frac{5}{6}}, \]

Here \( A \) is the effective target material atomic weight, \( \gamma = 0.187Z \) and \( C \approx 1.1 \).

The distributions of energy loss densities calculated according to (1) for kilovolt electrons in Al (material with low effective target material atomic weight – light target), Cu (medium target), and Au (heavy target) normalized by the amount of energy released per target per unit time are illustrated in figure 1.

**Figure 1.** Distributions of the energy loss densities of beam of electrons in Al (a), Cu (b) and Au (c) normalized by the amount of power \( E_0 \) released in these targets and calculated for the electron beam energy \( E_0 = 2 \) (curves 1), 4 (2) and 6 (3) keV.
Note that in metal targets with medium and heavy effective targets material atomic weights the energy loss density of the beam electrons is significantly higher than in the corresponding semiconductor targets at the same energies [3-5].

The possibilities of using this model for estimating the heat distribution in various metal targets are the subject of this work: the simulation is carried out for the case of the absence of heat transfer of the target with the external medium (unlike [3-5]), 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:

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

(2)

Here \( \Delta T(x, y, z) = T(x, y, z) - T_0 \) is the value of target heating under the action of the electron beam, where \( T \) is the sample temperature at point \((x, y, z)\) after the establishment of a stationary regime under the influence of an electron beam, \( T_0 \) is the temperature before the influence of an electron beam, and \( P(x, y, z) \) is function describing energy losses with an electron beam in a target. \( \Delta T(x, y, z) \) must satisfy the following boundary conditions: \( \lim_{x \to -\infty} \Delta T = 0, \lim_{x \to +\infty} \Delta T = 0, \lim_{y \to -\infty} \Delta T = 0, \lim_{y \to +\infty} \Delta T = 0, \lim_{z \to -\infty} \Delta T = 0 \). 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: \( \frac{\partial \Delta T(x, y, z)}{\partial z} = 0 \).

Equation (2) were solved in a standard way using the Green's function [3-5].

4. Results of calculations

The simulation results showed that the highest heating of all samples is observed at the lowest (from the considered range) energies what is explained by the following: the size of the deceleration region of the electron beam is approximately inversely proportional to the fourth power of the initial electrons energy, therefore, as the initial electrons energy of the beam decreases, there is a significant increase in the bulk density of thermal energy generated in the sample [2]. 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 a light target (Al), and the heaviest sample (Au) is heated most of all – see figure 2 and figure 3.

The simulation results show that heating of heavy target (Au) at the used beam current is approximately an order of magnitude greater than heating of light target (Al). Moreover, for light targets, heating is essential for low electron energies of the beam, and for medium energies (from 10 keV and above) in many cases the heating of the light metal can be ignored, especially when using beam currents characteristic for scanning electron microscopes. For heavy metals with beam currents characteristic for X-ray microanalyzers, for low beam energies, heating can be quite significant: from ten degrees to several tens of degrees.
Figure 2. Temperature distribution in Al for coordinates x and z. The calculations were carried out at y = 0, for primary electron energies $E_0 = 2$ (a), 4 (b), 6 (c) and 8 (d) keV, at probe current $10^{-7}$ A.

Figure 4 shows the dependences of the of maximum temperature values of target heating under the action of the electron beam in the Al and Au targets on the energy of the primary electrons $E_0$; the contribution of the energy scattered in the target with the absorbed and backscattered (reflected) electrons is shown separately. The calculations are performed for x and y values equal to zero.

For light metals the contribution of electrons absorbed in the target 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 7-8 keV and the energy losses of these electrons become practically zero at an energy of about 10-11 keV. For heavy metals, the energy losses of 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 6-8 keV. As for backscattered electrons in these metals, they are characterized by the presence of a maximum of about 3-5 keV, and then the curves decrease monotonically.
Figure 3. Temperature distribution in Au by coordinates $x$ and $z$. The calculations were carried out at $y = 0$, for primary electron energies $E_0 = 2$ (a), 4 (b), 6 (c) and 8 (d) keV, at probe current $10^{-7}$ A.

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" (for medium metals) or local maximum (for heavy metals) 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 targets. The presence of such effect is explained with the difference of the densities of energy loss in these metals: for example, in figure 1 in these distributions there is a “step” for medium metals, and a local maximum for heavy metals. The presence of these features leads to a difference in the nature of the dependences $\Delta T(E_0)$ of the groups of metals under consideration.
Figure 4. The results of modeling the heating of the metal targets for parameters characteristic of Al (a) and Au (b): the simulation of the distribution of the dependences of the maximum temperature on the energy of the primary electrons (curves 1) also the contribution to the curves 1 of the energy scattered by the electrons absorbed in the target (curves 2) and reflected (curves 3) were shown. Calculations were carried out at the probe current $10^{-7}$ A.

5. Conclusions

The methods of mathematical modeling were used to study the heating of metal 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 metallic target when planning the experiment.

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