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# Mathematical modelling of energy conversion of pulsed electron beam in BaF<sub>2</sub> crystal

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Abstract. This paper presents the results of mathematical modeling of spatiotemporal distribution of energy in a  $BaF_2$  crystal in an area of dissipation of energy of an pulsed electron beam. Fluence is varied from 0.188 to 0.626 J/cm<sup>2</sup>. Electron beam pulse duration was 24 ns, and the maximum electron energy of 280 KeV. Based on the obtained of energy distributions temperature change of the material during irradiation were calculated.

#### 1. Introduction

Through a combination of unique electrical and optical properties of  $BaF_2$  is a promising material for a wide range of constructional applications. Using pulsed electron beams allows generating short-lived defect concentration sufficient for detection and research of the mechanisms of defect formation in solids. However, the impact on ionic crystals pulsed electron beams (PEB) has some specific features compared with low-intensive sources of radiation.

In an area of energy dissipation of pulsed electron beam is formed strong electric field and the temperature rises along with the generation of non-equilibrium electron-hole pairs, which affects the efficiency of formation and decay of an electron-hole excitation and also on the postradiation processes. Effect of temperature increase in an area of energy dissipation is not enough studied, making it difficult to correct account of this factor in the analysis of research results.

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#### 2. Calculation of distribution of the injected electrons in BaF<sub>2</sub> crystal

Feature of interaction of accelerated electrons with matter manifests itself in a change driving directions, which is conditioned mainly by the elastic scattering on the nuclei of atoms, while the change in the energy of the electrons occurs mainly is due to inelastic scattering by electrons. Therefore, changing the magnitude and direction of the velocity vector of the electron can be considered independently [1].

Ionization energy losses of electron per unit path length determined by Bethe-Bloch formula [2, 3], accurate enough in energy range of electrons  $10^4 \le E \le 10^7 \text{eV}$ .

$$\left(-\frac{dE}{dz}\right)_{I} = \frac{2\pi e^{4} N_{A}}{m_{0}c^{2}\beta^{2}} \frac{Z}{A} \rho \cdot \left\{\ln\frac{\tau^{2}(\tau+2)}{2(\bar{I}/m_{0}c^{2})} + 1 - \beta^{2} + \frac{1}{(\tau+1)^{2}} \left[\frac{\tau^{2}}{8} - (2\tau+1)\ln 2\right] - \delta\right\}$$
(1)

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Where Z, A – atomic number and mass of a element;  $N_A$  – Avogadro's number; e,  $m_0$  – charge and electron rest mass; c – speed of light in vacuum;  $\beta = \upsilon/c$ ;  $\beta^2 = 1 - (\tau+1)^{-2}$ , where  $\upsilon$  – electron velocity;  $\tau = E/(m_0c^2)$  – kinetic energy of electrons in units  $m_0c^2$  ( $m_0c^2 = 0.511$  MeV);  $\overline{I}$  – average ionization potential of the atom;  $\delta$  – correction for the effect of density.

The average ionization potential  $\overline{I}$  (in eV) is defined by the Sternheimer formula [4]:

$$\bar{\mathbf{I}} = \mathbf{Z} \cdot (9,76 + 58,8 \cdot \mathbf{Z}^{-1.19})$$

(2)

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For substances with a complex chemical composition, the braking ability can be determined with good accuracy by summing a braking ability of the constituent elements, thus calculation is performed with the replacement  $Z \rightarrow Z_{ave}$ ,  $A \rightarrow A_{ave}$ ,  $\overline{I} \rightarrow I_{ave}$ . For BaF<sub>2</sub> crystal obtained  $Z_{ave} = 24.67$ ,  $A_{ave} = 58.44$ ,  $I_{ave} = 397.34$  eV.

To calculate the distribution of injected electrons in the sample and the absorbed energy density applied a variation "enlarged" collisions of Monte Carlo method using the angular distribution of Moliere-Bethe [3]. In the calculations the thickness of sample was chosen equal to the maximum extrapolated path of electrons  $R_o$ . In normalized coordinates  $\tau = z/R_o$ , for BaF<sub>2</sub> crystal was calculated a universal curve of distribution injected electrons, which depends only on the properties of this material (figure 1).

## 3. Calculation of energy release in BaF<sub>2</sub> under the influence of PEB

In the calculations used spectrum of PEB [3], which was determined experimentally by attenuation in thin foils, as described in [5]. Modelling of distribution of energy release produced considering the action of the retarding field of injected space charge [3].

Formula (3), together with the calculated distribution universal injected electrons (Fig. 1), allows the calculation of the density distribution of the space charge  $\rho(z_i, t_m)$  in absolute coordinates for PEB of arbitrary shape with a different beam current density at any moment of excitation.

$$\rho(z,t) = \sum_{i=1}^{k} \rho_i(z) = \frac{e(1-\gamma_0)}{\int_{0}^{1} \phi(\tau) d\tau} \cdot \sum_{i=1}^{k} \frac{N_{0i}}{R_{0i}} \phi(\tau)$$
(3)

Where  $\gamma_0$  - the proportion reflected electrons;  $N_0$  - number of electrons in monoenergetic pulse; e - electron charge;  $\rho(z)$  - function of the distribution of the space charge in absolute units;  $\phi(\tau)$  - function of the distribution of the injected electrons,  $R_0$  - distance extrapolated path of the electrons.





Figure 1. Normalized distribution of injected electrons in  $BaF_2$  at different energies of incident electrons  $E_o$ 

**Figure 2.** Dynamics the forming of profile energy release in  $BaF_2$ . Fluence of PEB is 0.188 J/cm<sup>2</sup>.

The dynamics of the formation of the energy profile for  $BaF_2$  shown in figure 2. In contrast to the monoenergetic beam (figure 1), profile excitation of the sample at the beginning of irradiation pulse is shifted from the irradiated surface and after reaching maximum of a extrapolated path, determined by the electrons with maximum energy (t  $\approx 10$  ns), returns to the irradiated surface.

Accounting a spectral-time parameters of pulsed electron beam leads to complex spatiotemporal energy release function W(z,t) in the sample. The time dependence of energy release to the surface layers of the sample has a a complicated form with multiple peaks. With increasing z coordinate layer - distribution W(z, t) acquires a dome shape. It should be noted that with increasing distance from the irradiated surface of the material decreases time of irradiation of a layer.



Figure 3. Calculated time dependences of energy release at different distances from the irradiated surface  $BaF_2$ . Fluence of PEB is 0.188 J/cm<sup>2</sup>

**Figure 4.** Dependence of influence of a injected space charge field and the vacuum gap on the initial fluence  $W_{0.}$  a - fluence PEB on the irradiated surface (d- with vacuum gap); b - absorbed energy (f- with vacuum gap); c- energy stored in the electric field of the injected charge (e- with vacuum gap)

Results in figure 4 shows that at short-circuited geometry of irradiation, the ionization energy losses of electrons is much higher loss due to the inhibitory effect of the electric field of the injected charge. Reducing the absorbed energy relative to the incident energy on the surface caused mainly by reflected electrons. In the case of geometries with a vacuum gap before the irradiated surface due to deceleration of the electrons in the electric field of the space charge decreases the energy density incident on the surface (dashed curves in figure 4), which leads to a further decrease in the proportion of the absorbed energy.

# 4. Calculation of a temperature change in field dissipation of energy of PEB in BaF<sub>2</sub> crystal

Calculation of heating the material in the field of energy dissipation PEB, was based on the resulting spatiotemporal energy release in the material  $W_i(z, t)$ , discussed in more detail in [6].

Figure 5 shows the results of calculating distribution of heat ( $\Delta$ T) in BaF<sub>2</sub> crystal at the initial temperature of the material (T<sub>M</sub>) 293 K. Irradiation is accompanied by an increase in temperature caused by thermalization of nonequilibrium electrons and holes. Profile of the temperature distribution is determined by the spatial distribution of the absorbed energy.

Figure 6 shows the calculated dependence  $\Delta T$  at the maximum of the energy release from the  $T_M$  for BaF<sub>2</sub> crystal at the end time irradiation of PEB. In the area of dependencies  $\Delta T(T_M)$  where  $T_M < 80$  K, the determining factor of high heat is the low heat capacity of the material. With increasing  $T_M$  above 80 K, values of  $\Delta T(T_M)$  are becoming almost constant. In this area the heating caused mainly by the high energy release.





**Figure 5.** Calculated a formation dynamics of a the profile of temperature distribution (T) in  $BaF_2$ . Fluence of PEB is 0.188 J/cm<sup>2</sup>. The initial temperature of the material is 293 K

**Figure 6.** Calculated dependence  $\Delta T$  at the maximum of the energy release from the  $T_M$  for BaF<sub>2</sub> crystal at the end time irradiation of PEB Fluence of PEB is indicated for each curve

# 5. Conclusion

At research of temperature dependences of the spectra of pulsed cathodoluminescence, values of decay component, as well as the temperature dependence of the yield of products of irradiation, an important factor is the temperature of the material in which the measurements are carried out. Consequently, as shown in this paper, the presence of spatiotemporal inhomogeneity of temperature of the crystal, as well as a significant heating of the material during irradiation PEB, even at low fluence, will make a significant distortion in the measurement results. This effect of inhomogeneous change of a temperature must be taken into account in the research of the temperature dependence of the yield of products of irradiation and kinetic processes postradiational.

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