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ANALYTICAL DESCRIPTION OF QUANTUM EFFECTS AT CURRENT FILAMENTATION IN CHALCOGENIDE GLASSES

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Abstract. Quantum effects occurring during current filamentation in a chalcogenide glass are considered. Under the conditions considered, the current filament appears as a set of concentric tubes with different temperatures. In every tube, the electron has a specific wave function and a specific energy level. The radii of the tubes appear to be proportional to natural numbers n. The dependence of maximal temperature on the electrical field is obtained. The Schroedinger equation is reduced to the first order differential equation. The type of energy of an electron at the tube is close to exciton energy dependence. The potential energy of an electron is described with the first order polynom of temperature. The temperature distribution in the filament is shown as an interference of the electron.

Keywords: chalcogenide glasses; current filament; quantization

1. **Introduction**

Formation of current filaments (current filamentation, or crowding) is a phenomenon that often occurs in chalcogenide glasses, which are considered to be the material of choice for the next-generation phase-change memory (PCM) devices [1,2]. This effect consists of a significantly higher current density in a certain coordinate region [3,4]. When the radius of the current filament decreases down to tens of nanometers, one can expect the appearance of quantum effects consisting in the fact that the diameter of the filament would take only certain, albeit close to each other, values. Taking into account that quantization of current and conductance were observed in, e.g., superconductors [5], carbon nanotubes [6], and metallic nanowires [7], this hypothesis is worth verification in application to chalcogenide glasses, too.

In this paper, the formation of a current filament is analyzed with allowance for quantum effects, and a simple analytical formula describing the quantization phenomena is presented. Additionally, a description of the filament is proposed as an object in which the energy of an electron has a form similar to the energy of an exciton in a solid or an electron in a hydrogen atom.

2. The model

In general, quantization can take place in all three coordinates. In the case of the current filament, however, only the radius will take certain values, since we assume that the length of the filament is L ~ 10^{-6} m, which is too large a value for the manifestation of quantum effects. Assuming in the first approximation that the electrons do not interact with each other, we suggest that it is possible to describe the quantum scale of the resulting filament with the formula:

$$\int_0^{r_c} \sqrt{2mkT(r)}\, dr = nh. \qquad (1)$$

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Here T is the temperature, k is Boltzmann's constant, m is the electron mass. Expression (1) is an integral of work in time, and when it becomes of the same order of magnitude as Planck's constant h, quantum effects should appear. Here, we integrate from zero to the radius of the filament r_c the momentum of an electron moving along the radial coordinate r in a medium with a certain temperature distribution. As a result, a value is obtained that has the same dimension as that of the angular momentum, yet is not exactly the momentum, as the angular momentum of an electron moving along the radius is equal to zero. The temperature in the stationary case is represented by the formula:

$$T(x) = T_0 + (T_m - T_0)exp\left(\frac{-ax^2}{4}\right). \tag{2}$$

Here

$$x = \frac{r}{r_0}, \qquad a = \frac{F^2}{F_S^2} exp\left(\frac{-1}{t_m}\right)\frac{1}{t_m^2} - 1; F_S{}^2 = \frac{2\lambda \Delta E}{\sigma_0 Lk},$$

where F is the electric field, F_0=10^6 V/m, λ is the heat sink coefficient, ΔE is the energy of activation of conductivity, T_m is a filament temperature of radius $x_c(n)$, T_0 is the room temperature, σ_0 is the initial conductivity, r_0 is a constant of the order of 1 μm, $t_m = \frac{kT_m}{\Delta E}$. In this consideration, the conductivity of the glass was taken in the form that summarizes its temperature and electric field dependences [3],[8],[9]:

$$\sigma = \sigma_0 \exp(-\frac{\Delta E}{\mathrm{kT}} + \frac{F}{F_0}).$$

Expression (2) describes the temperature in the filament as satisfactory; therefore, r_c can be taken as the radius of the filament, since outside the radius of the filament as the coordinate increases, the sample temperature is not described by a simple analytical formula. Taking into account that the action takes place on a small scale, formula (2) can be expanded in Taylor's series up to the second term and substituted in (1). As a result, we get an equation of the third degree:

$$p_m x - p_m \frac{T_m - T_0}{T_m}\frac{ax^3}{24} = n\frac{h}{r_0}, \tag{3}$$

where $p_m = \sqrt{2km_eT_m}$. Equation (3) is then reduced to the canonical form:

$$x^3 - \frac{24T_m}{a(T_m - T_0)}x + \frac{24nhT_m}{r_0 p_m a(T_m - T_0)} = x^3 + px + q = 0. \tag{4}$$

The roots of a given polynomial can be found using Cardano's formulas. Omitting the consideration of the choice of the legible roots, which will be presented in details elsewhere, we come straight to the expression for the current filament radius with a number n:

$$x_c(n) = \frac{3nh}{2r_0 p_m}; p_m = \sqrt{2kmT_m}. \tag{5}$$

The quantized radius was defined as Bohr radius or quantized resistance by using the Heisenberg principle. The current filament is formed gradually. First, a filament with a large radius is formed, then a filament of a smaller radius is formed inside the first filament, and in a few nanoseconds, a structure consisting of a number of concentric tubes is obtained.

The authors attempted to describe a behavior of an electron in every ring considering a thermal potential:

$$U(x) = C - \mathrm{kT}(x).$$

Here C is a constant with its value laying in the range from 1 to 4 eV; it describes total energy of an electron and cannot exceed the value of work function, otherwise, the electron will leave the filament and the material. The subtrahend in this equation is the kinetic energy of the electron.

The first order Schroedinger equation of this potential:

$$y' + y^2 + \frac{y}{x} - \frac{2mr_0^2}{\hbar^2}U(x) + \frac{2mr_0^2}{\hbar^2}E = 0, \tag{6}$$

$y(x) = (f'(x)), \psi(x) = Aexp(f(x)), \psi(x)$ is a Schroedinger function.

The thermal electron energy depends on the quantum filament radius. The dependence is similar to that of the exciton energy.

$$E_n = U\big(x(n)\big) - \frac{\hbar^2}{8mr_0^2x_n^2} \tag{7}$$

If $n \to \infty, E_n \to C - kT_0$. This result does not contradict physical meaning. E_n is the absolute value of energy for the electron in the conduction band.

The probability of the appearance of the filament with zero radius is zero because of $\psi^2(x)x = 0$ when n=0. Indeed, from the classical theory of the current filament [2], it follows that a filament with zero radius should be formed at an infinitely high electric field. The energy of an electron in a filament of zero radius is infinite and negative. This can be interpreted as if the electron is placed in an infinite field and at the same time is located in a quantum well. When $T_0 \to 0$, T_m decreases for a given n. On the contrary, the difference between the adjacent radii $x_c(n)$ increases. All this leads to a more pronounced manifestation of quantum effects.

In addition to the analytical solution, values of E_n were calculated numerically by solving the Schroedinger equation using Matlab software. The results are presented in Table 1. A good agreement between the analytically and numerically calculated values is observed. The subtrahend $\frac{\hbar^2}{8mr_0^2x_n^2} \ll C - kT$, which, in fact, means, that the quantization effects are rather weak. The most interesting is the first (more precisely, zero) energy level. As can be seen in Table 1, this energy very much differs in value from the subsequent values lying in the interval kT_m. The change of the sign of the potential energy did not affect the position of the energy level E_0. The wave functions were calculated and the behavior of an electron seems similar to the interference of light. For the electron, the probabilities to be found exist in a certain area of the sample appear to be periodical with different magnitudes (Fig. 1). The ring-like (or, rather, tube-like) areas with different temperatures are separated from each other. The temperature distribution is continuous in the case of large areas where quantum effects disappear. Thus, we assume that this energy near zero coordinates corresponds to the colder region of the glass and that the filament has the shape of empty tubes with similar temperature distributions with a cold area existing at the center of the current filament.

Table 1. Calculated values of electron energy

n, quantum number	E_n, eV (numerical)	E_n, eV (analytical)
0	1.6092	-
1	1.9482	1.9512
2	1.9594	1.9591
3	1.9670	1.9665
4	1.9717	1.9711

Also, the formula for calculation of the temperature T_m in each ring was derived:

$$\frac{9n^2\hbar^2}{r_0^2} = F'(t_m),\ F'(t_m) = \frac{2m\Delta E t_m^4}{\left(\beta exp\left(\frac{-1}{t_m}\right) - t_m^2\right)(t_m - t_0)} \tag{8}$$

Here $\beta = F^2/F_s^2$, $t_m = \frac{kT_m}{\Delta E}$ is the maximum temperature of heating for each ring, $t_0 = \frac{kT_0}{\Delta E}$. The value of t_m cannot possibly be smaller than t_0 and $n \to \infty$ if $t_m \to t_0$. It means that filaments do not form at low currents. The width of every filament is of the order of 10 nm.

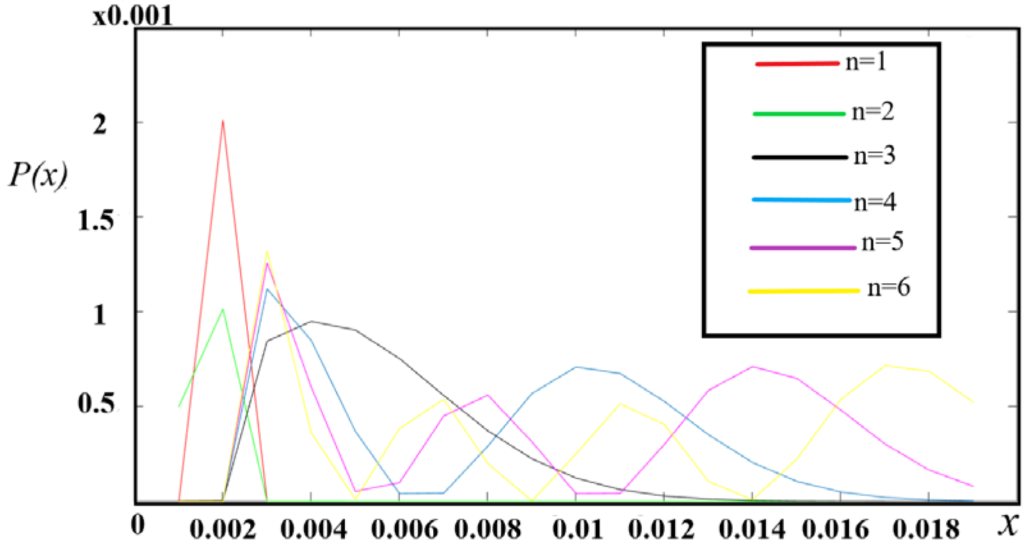

Fig. 1. The wave functions of the electron at the potential $U(x) = C - \mathrm{kT}(x)$, $T_0 = 300K, T_m = 1000K, F = 4 \cdot 10^6\, V/m$

Figure 2 shows the relation between the maximum temperature and the electric field. In the case presented in Fig. 2, the quantum number *n* (in this case, *n* = 2 and $\frac{9n^2h^2}{r_0^2} = 5.49 \cdot 10^{-5}$, which is shown as a solid blue horizontal line) intersects the graph of the function *F*. The maximum temperature t_m is searched at the points of the intersection of the two lines. The most probable t_m is the maximal root of equation (8).

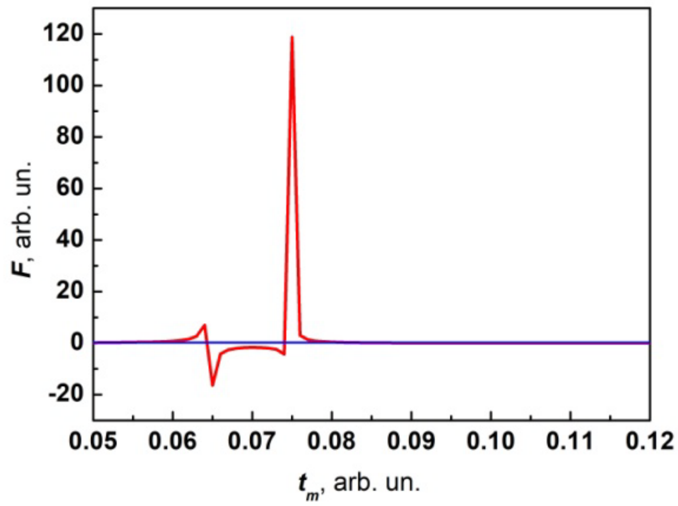

Fig. 2. The relation between the maximum temperature and the electric field. In the case considered, *n* = 2 and $\frac{9n^2h^2}{r_0^2} = 5.49 \cdot 10^{-5}$ (shown as a horizontal line)

3. Conclusion

In this work, an attempt was made to develop a quantum approach to the formation of a current filament in a cylindrical sample of chalcogenide glass with a conductivity that exponentially depends on the inverse temperature taken with a negative sign. It is shown that quantum effects can manifest themselves in current filaments on scales of tens of nanometers at high fields and a glass sample thickness of the order of a micrometer. The radius of the filament has been refined; the formed filament has a certain radius and a certain maximum temperature in the center. A law has been established according to which the maximum temperature depends on the electric field**.** Every filament represents a set of concentric tubes, each up to ten nanometers wide, with a specific temperature that drops sharply from maximum to room temperature. An exception is the central region of the filament; the authors believe that a cold "spot" is formed in the very center of such a filament. The second-degree differential equation describing the probability of an electron to be in a certain quantum of the filament has been replaced by an equation of the first degree, which simplified the approach.

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