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Research Article

Mathematical Model for Thermo-Electrical Instabilities in Semiconductors

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Abstract

Crystalline semiconductors under specific conditions, with an applied electric field, switch or oscillate between two conductive states, thus producing low frequency oscillations of electric current flowing through the sample and as a result of Joule heating oscillations of sample temperature. These phenomena are recognized to be thermo - electrical instabilities. Although current oscillations can be detected and registered experimentally, there is no device that can detect, register and allow us to study the sample temperature change in time. The purpose of this study is to learn about the relationship of electric current and sample temperature coupled with deep traps that play an important part in supporting the phenomenon. This can be done only by setting up a mathematical model that describes the phenomenon in detail. The equations that make up the model are continuity equations for free electron and deep traps carrier populations, as well as a heat conduction equation – a set of ordinary nonlinear inhomogeneous differential equations. The system is transformed into a so called “canonical form” as a result of linearization of the system at isolated equilibrium. It is achieved by expansion of the right hand sides of the equations into two variable Taylor series at isolated equilibrium involving linear non-singular transformation. The mathematical model for thermo-electrical instabilities in an n-type semiconductor with non-degenerate electron statistics has been studied as 3D dynamical system. The system of differential equations is broken down into component planar systems, each of them being tested for existence of limit cycles on a determined phase plane, followed by quantitative investigation of their local behavior at isolated equilibrium and at points on individual trajectories on phase plane dependant on single parameter T_0. Solutions of sets of initial value problems as time series of the variables: free electron concentration; sample temperature; deep trap population is presented. The investigation results show that oscillations of sample temperature follow those of current. Change in T_0 forces the system to adjust to new thermodynamical state by changing frequency and amplitude of the oscillations as well as dynamics of deep trap population.

Keywords

Dynamical System, Initial Value Problem, Time Series, Thermo-Electrical Instabilities, Semiconductor, Deep Traps

1. Introduction

Thermo electrical instabilities in semiconductors immersed in cryogenic media (low frequency oscillations of current and temperature of a sample as a result of Joule heating) have been a point of interest for researchers for many years and have been studied experimentally in a variety of semiconducting materials [1-3]. In [1] mathematical model based on 3 types of

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trap levels that account for both electron and hole capture for a thin cylindrical sample of crystalline $A^{II}B^{VI}$ compound with uniform distribution of temperature, electric field and electron-hole pair generation across the sample. System comprised of 5 differential equations taking into consideration kinetics of generation-recombination processes is investigated at steady state, taking all time dependences of the variables equal to 0 for simplified cases. Authors calculated threshold values for electric field and frequency of current and temperature oscillations comparing them with available experimental data.

Detailed, comprehensive and thorough research of the instabilities in chalcogenide and vanadium dioxide thin films have been conducted in [2], where thermo electrical instabilities are characterized in terms of negative differential conductivity observed in voltage current characteristics of solids. Heat flow in a semiconductor is compared with RC (resistor-capacitor) network, and effects of circuit design, presence of in homogeneities like metallic inclusions are analyzed. Steady state heat conduction equation together with coupled electrical and thermal processes in a sample are solved on grid in the finite difference approximation. [3] presents research of another model with differential equations for free electron concentration n, trap population n_t and sample temperature T for A^2B^6 compounds. Equations for n and T were solved numerically by means of Gear's method for stiff systems of ordinary differential equations. Time sequences of T(t) and phase trajectories on phase plane (n, T) were obtained as a result, for ambient temperature of T_0=283 K and different values of applied electric field.

Since it is impossible experimentally to detect oscillations of sample temperature, research of mathematical equations that describe the phenomenon is necessary. So far both simplified and more complex model investigations have been limited to study of either null-isoclines of systems of differential equations [1] or as in [3] only a partial investigation of suggested model. Construction of a simplified new model for more detailed study of the system of nonlinear ordinary differential equations in order to attempt to answer the questions how change of current and temperature are related to each other, and how deep traps involvement into instability progresses is presented in the paper. The quantitative analysis of periodic solutions can give insight into current-temperature relationship as well as behavior of deep traps in such a system.

2. Model Details

To set up a system of equations that describe the dynamics of electrons at conduction zone E_c n and on deep traps n_t, which play an important part in thermo-electrical instabilities in semiconductors, the generation-recombination model by Schoell [4] was employed. The author [4] considered the two trap level model for analysis of instabilities of the current density and electric field that were classified in his book as first order phase transitions. Choice of the model is preferred because the right hand side expressions are polynomials with respect to position independent variables n and n_t that gives a clear understanding of the mechanism which drives the instability. Equations for the electron concentration at E_c and on deep traps, taking into account thermal emission rates, are considered for an n-type homogenous semiconductor with non-degenerate electron statistics. Along with the equation for change in sample temperature, well known as heat conduction equation, it completes the dynamical system (1):

$$\begin{aligned} \frac{d\boldsymbol{n}}{dt} &= n^2(-T_1^S - X_1^*) + (N_D - n - n_t)X_{th} - \\ &-n(n_t(X_1 - X_1^*) + T_1^S(N_t - N_D) - N_D X_1^*); \\ \frac{d\boldsymbol{n_t}}{dt} &= -\left(X_{op} + X_{th}n_t + T^*(N_D - n - n_t) - X_1\right); \\ \frac{d\boldsymbol{T}}{dt} &= \left(\frac{k}{c\rho}\frac{d^2T}{dx^2} - \frac{T - T_0}{t_c} + \frac{ne\mu E^2}{c\rho}\right). \end{aligned} \tag{1}$$

The variables and constants in the system are: n=n/N_D, n_t=n_t/N_D, T=T/T_0, t_c, T_0– free electron concentration, electron concentration on traps, sample temperature, thermal relaxation time of a sample and temperature of the cooling media; N_d, E, c, ρ, k, μ – are effective donor concentration, applied electric field (constant), heat capacity of a sample, its density and heat conduction, and electron mobility. Temperature dependence of the physical parameters like heat capacity, heat conduction, thermal relaxation time, electron mobility, electron concentration in a temperature interval of T_0=(77-197) K is taken into consideration based on accessible data, both experimental as well as theoretical research from [5-11]. Physical constants taken for spatially homogeneous n-Si sample of size (0.8 x 0.5 x 0.5) cm with partially compensated donors $N_A < N_D$, where acceptors are assumed to be the ground state (E_1 =0.302 eV), and shallow donors to be the first excited state (E_2=0.011 eV) of the deep traps [4, 9, 12]. Figure 1 represents the two level model in detail.

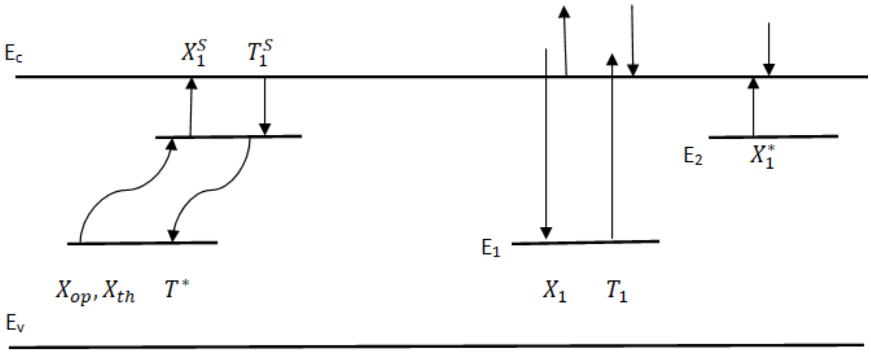


Figure 1. *Two level generation-recombination model for first order phase transitions in semiconductors by Schoell [4].*

As a result of combination of the thermal X_{th}, optical X_{op} excitements and impact ionization X_1 of the ground state E$_1$ in the presence of an applied constant electric field, electrons are transferred onto the first excited state E$_2$. From E$_2$ electrons are emitted onto the conductive zone with the rates X_1^S for thermal and X_1^* for field aided emission, or back to the ground state E$_1$. Temperature independent optical excitement X_{op} populates the ground states with a new supply of electrons to continuously support oscillations of current and temperature. T_1^S, T^* - recombination at the excited and ground states; two electron Auger recombination at the ground state T_1 is combined with T^* in the equations. Direct transitions between conduction E$_c$ and valence band E$_v$ are ignored [4].

Expressions for the generation rates X_1^S, X_{th}, X_1^* and X_1 are given by:

$$X_1^S = X_1^{S0}\exp(-\tfrac{E_2}{T});\ X_1^* = X_1^{*0}\exp(-\tfrac{E_2}{e\lambda E})$$

$$X_{th} = \mathrm{e}_0\exp(-\tfrac{E_1}{T});\ X_1 = X_1^0\exp(-\tfrac{E_1}{e\lambda E})$$

Where X_1^{S0}; e$_0$; X_1^{*0}; X_1^0; T_1^S; T^*– are constants [4]; λ - electron mean free path; E – applied constant electric field; e - electron charge. Optical excitement rate X_{op} calculated from [7].

Equation for electron dynamics n in the conduction zone E$_c$ accounts for field impact ionization and recombination, as well as thermal generation of electrons from E$_2$, field impact ionization and recombination at E$_1$ and E$_2$. Dynamics of the deep trap population n$_t$ accounts for optical, thermal, field impact ionization of electrons from E$_1$; recombination through E$_2$.

The dynamics of sample temperature T in time depends on applied constant electric field, heat dissipation through cooling of the sample at T$_0$, and change in the concentration of free electrons in E$_c$ and their mobility. Variation of T over the length x of the sample was set as boundary value problem with boundary conditions of type 3 [12]. Obtained solutions T(x) for different values of T$_0$ are substituted into the equation for followed investigation of nonlinear autonomous system (1).

3. Methods

System (1) was studied as a set of three planar systems: (n, T), (n, n$_t$), (n$_t$, T). Each of the planar systems was tested for the presence of a limit cycle based on Bendixon's criteria at fixed values of generation rates X_1^S, X_{th}, X_1^* and X_1; optical excitement X_{op}, as well as parameter T$_0$ for determined range of values of appropriate variables, which form a "square" on the phase plane, before being cast into so called "canonical form" by means of linear nonsingular transformation [13]. The right hand side nonlinear expressions of the system (1) for an appropriate planar system are expanded into two variable Taylor series at an isolated equilibrium. The first order derivatives of the expansions were used to form a Jacobian matrix; firstly for determining that the equilibrium is isolated, as well as for obtaining quadratic characteristic equations with respect to characteristic number λ. For the case when λ is a complex conjugate (for periodical trajectories on the phase plane), transformation (3) was employed to express a planar system in form (2) when equilibrium is at origin. The transformation (3) provides real functions of real variables to produce values of real and not complex domain. Linear parts of the system (2) are then set as a Cauchy problem with sets of initial conditions:

$$\begin{cases}\frac{\mathrm{du}}{\mathrm{dt}} = \alpha\mathrm{u} - \beta\mathrm{v} + \varphi(\mathrm{u},\mathrm{v}) \\ \frac{\mathrm{dy}}{\mathrm{dt}} = \beta\mathrm{u} + \alpha\mathrm{v} + \psi(\mathrm{u},\mathrm{v})\end{cases} \qquad (2)$$

$$\mathrm{t} = 0;\ \mathrm{u} = \mathrm{u}_0;\ \mathrm{v} = \mathrm{v}_0$$

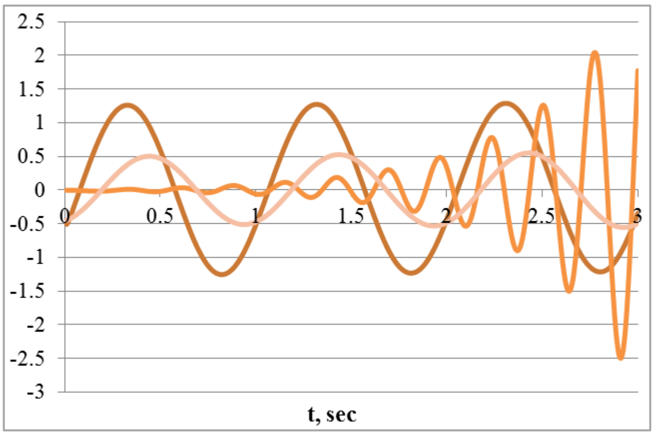
$$u = (\alpha - a)x + cy;\ v = \beta x; \qquad (3)$$

$$u_0 = (\alpha - a)x_0 - y_0;\ v_0 = \beta x_0.$$

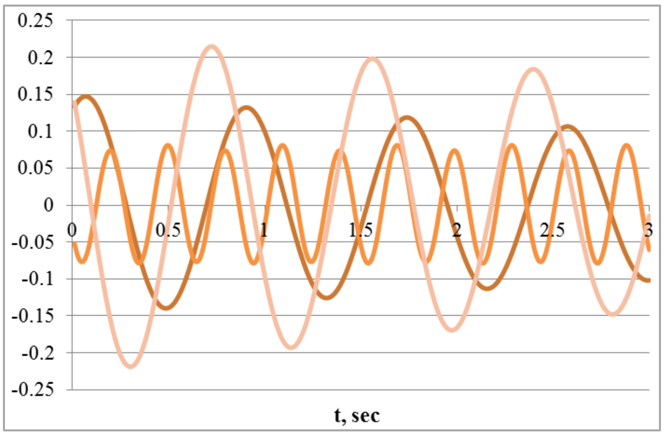
Here x, y – variables and x_0, y_0 - initial values of an appropriate planar system accordingly; a, c – elements of Jacobian at an isolated equilibrium; $\lambda_{1,2} = \alpha \pm \beta i$ - roots of characteristic equation; $\varphi(u,v)$, $\psi(u,v)$ – nonlinear parts (second and higher order terms) of two variable Taylor series expansions. The initial value problem (2) was solved with variation of constants method for inhomogeneous linear systems. Real parts of the solutions were separated and plotted against time.

4. Results

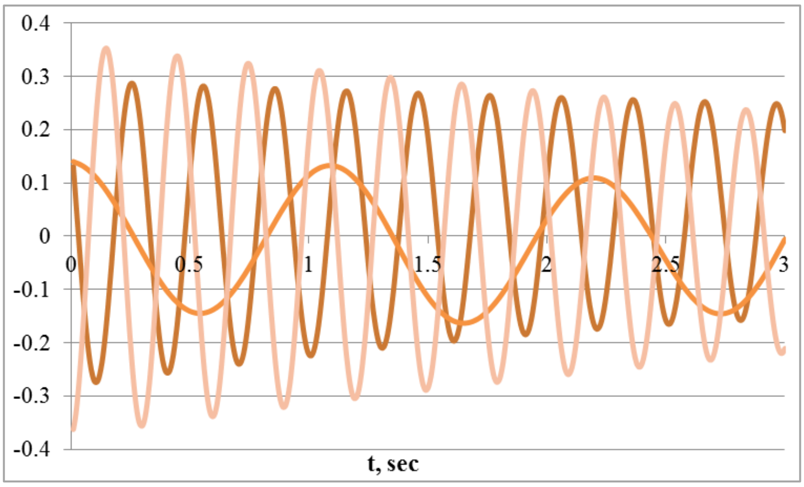
Figure 2 presents time sequences of obtained real parts of the solutions of (2) for the planar systems dependant on the single parameter T_0. Variations of n, n_t and T in time are overlaid in the graphs. At $T_0 = 77$ K, amplitudes of n and n_t are large, while that of T is small, relative to n and n_t. As T_0 grows the amplitude of all variables T, n and n_t decrease. With growing T_0, the amplitude of T become larger relative to those of n and n_t. At higher T_0, the amplitude of n_t is limited to smaller deviations in time. A decrease in the frequency of n_t with a growing T_0 is also observed.



(a)



(b)



(c)

Figure 2. *Time sequences for n-brown; n_t–orange; T-pink at different values of temperature of cooling media T_0: (a) – 77 K; (b) – 137 K; (c) – 197 K.*

5. Discussion

At a low value of T_0, small amplitude of T shows rapid cooling of the sample Figure 2a; large amplitudes of n_t and n indicate lower carrier population at conduction band E_c, so the transfer of electrons onto E_c from traps is happening in larger volumes. With growing T_0 Figure 2b, c, electron transfer from traps is no longer possible at the same volume, because of the constant recombination rates and limited number of allowed states per unit volume at E_c. The lowering of the frequency of n_t also points to that. As a result, an adjustment through an increase of frequency is taking place for both n and T, since the sample's cooling is taking a longer time; oscillations of T fall behind the changes of current in time.

Comparing the findings of the research with those of [3] would be appropriate here. Study of the system in [3] included as part of the research, time sequences of T(t) in transition from regular to chaotic oscillations, as well as accompanying phase trajectories of planar system (n, T). No further investigation of interrelationships of the variables n, n_t, T were conducted and yet time sequences of n, n_t can give information about the involvement of deep traps, interrelationship with other variables of the system through their own behavior in time. In Figure 2 time sequences of each of the variables were overlaid to show not only how these variables change in time, but also how their frequencies, amplitudes, and phase differences relate and evolve with respect to each other and a growing T_0.

The next step in the research of the dynamical system (1) is conducting analysis of the phase trajectories of the planar systems depending on the parameter T_0 which will give a clearer view of the interrelationship of the variables n, n_t and T.

6. Conclusions

The fact that alternating current passing through solids creates heat due to Joule heating has been known for a long time and has found far reaching applications in the modern world. Yet the relationship between current and temperature remained unknown, since it is impossible to detect variations of temperature in time, experimentally. Theoretical research of this relationship in solids, based on information accessible to the author, has never been conducted in full. Findings of this research give interesting insight into the delicately balanced system where change in one variable causes strong effects on the others, depending on parameter T_0. Change in the temperature of the cooling media forces the system to adjust to a new thermo dynamical state by changing the frequency and amplitude of oscillations, thus giving an idea of the level of density states occupation at the conduction zone; oscillations of sample temperature always follow those of current, and this delay is present throughout the interval of change of T_0.

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Author Contributions

Mukaddas Arzikulova is the sole author. The author read and approved the final manuscript.

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Data Availability Statement

The data is available from the corresponding author upon reasonable request.

Conflicts of Interest

The author declares no conflicts of interest.

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