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AUTO-OSCILLATIONS OF ELECTRON-HOLE DENSITY IN MOLECULAR SEMICONDUCTORS WITH IMPURITIES AT STATIONARY OPTICAL PUMPING

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Abstract The auto-oscillations of electron-hole density and temperature in organic semiconductors with traps for electrons and holes at stationary pumping are considered. It is shown that at some critical values of the pumping rate and the temperature of thermostat homogeneous density becomes unstable and the auto-oscillations arise. The region of existence of auto-oscillations against thermostat temperature, pumping rate, the dependencies of the characteristics of that region (average width and largest temperature) and frequency of the auto-oscillations are found.

INTRODUCTION

The formation of structures in nonequilibrium systems is subject of great interest [1-2]. It will be perspective to observe the self-organization process in electron-hole system of organic semiconductors[3].

In this article the auto-oscillations of the temperature and density of carriers in organic solids are studied. The observation of this phenomenon may be useful for production of sources of periodical oscillations and as a technique for the determination of various kinetic parameters of carriers.

THE MODEL OF THE SYSTEM

Let us consider a sample of the organic semiconductors with traps for electrons and holes in the form of a thin plate which is cooled by thermostat with the temperature Ti. Let the external irradiation create K electron-hole pairs per unit volume of the sample per second. If the condition $L \ll \varkappa / \upsilon$, where L is the plate thickness, $\varkappa$ the thermoconductivity coefficient, and υ the value that describes the energy exchange with thermostat (υ enters in the Newton boundary condition $\varkappa \partial T/\partial x = \upsilon(T-Ti)$), is fulfilled the thermal equilibrium within the crystal is reached far more quickly than the equilibrium between the crystal and the thermostat and the temperature is homogeneous within the crystal.

The free electrons and holes can be captured by impurity centers. As the result of the recombination of free electrons and holes with free or captured holes and electrons respectively the transition of the system to the highly excited state occurs followed by nonradiative relaxation with the energy transfer to the crystal lattice and therefore, by the heating of the crystal. The captured carriers can escape from traps due to the thermal activity or the external light irradiation. It is supposed that the crystal cools down when the carriers escape from traps and heats up when the reverse process occur. The heating of the crystal due to the external irradiation is taken into account.

In this case the dynamics of the system under consideration may be described by the following kinetic equations

$$\frac{d\,n_e}{d\,t} = K - \gamma n_e n_h - \gamma_{et_e} n_e n_e^- + \frac{n_{t_e}^+}{\tau_{t_e}} - \gamma_{et_h} n_e n_{t_h}^+ + \alpha^e K n_{t_e}^+ ;$$

$$\frac{d\,n_h}{d\,t} = K - \gamma n_e n_h - \gamma_{ht_h} n_h n_h^- + \frac{n_{t_h}^+}{\tau_t} - \gamma_{ht_e} n_h n_{t_e}^+ + \alpha^h K n_{t_h}^+ ;$$

$$\frac{d\,n_{t_e}^+}{d\,t} = \gamma_{et_e} n_e n_e^- - \frac{n_{t_e}^+}{\tau_{t_h}} - \gamma_{ht_e} n_h n_{t_e}^+ - \alpha^e K n_{t_e}^+ ;$$

$$\frac{d\, n^{+}_{t_h}}{d\, t} = \gamma_{ht_h} n_h n^{-}_h - \frac{n^{+}_{t_h}}{\tau_{t_h}} - \gamma_{et_h} n_e n^{+}_{t_h} - \alpha^{h}Kn^{+}_{t_h};$$

$$c_\rho \frac{d\, T}{d\, t} = \xi\, \vartheta_{eh} K + \vartheta_{eh}\gamma n_e n_h + (\vartheta_{eh} - \vartheta_{t_e})\gamma_{ht_e} n_h n^{+}_{t_e} +$$

$$\vartheta_{t_e}(\gamma_{et_e} n_e n^{-}_e - \frac{n^{+}_{t_e}}{\tau_{t_e}} - \alpha^{e}Kn^{+}_{t_e}) + (\vartheta_{eh} - \vartheta_{t_h})\gamma_{et_h} n_e n^{+}_{t_h} +$$

$$\vartheta_{t_h}(\gamma_{ht_h} n_h n^{-}_h - \frac{n^{+}_{t_h}}{\tau_{t_h}} - \alpha^{h}Kn^{+}_{t_h}) - \beta(T - Ti), \qquad (1)$$

where n_e , $n^{+}_{t_e}$ are respectively the density of free and captured electrons, n_h , $n^{+}_{t_h}$ are the densities of free and captured holes, T is the temperature of the crystal, γ is the probability of both free electron and hole to recombine, ϑ_{eh} is the energy that transfers to the lattice during the process, γ_{et_e},γ_{ht_h} are the probabilities of the capture of an electron and a hole respectively, γ_{et_h},γ_{ht_e} are the recombination probabilities of a free electron with a captured hole and a free hole with a captured electron, respectively, $1/\tau_{t_e} = \gamma_{et_e} N \exp(-\vartheta_{t_e}/T)$ is the probability of a captured electron to escape from a trap, $1/\tau_{t_h} = \gamma_{ht_h} N \exp(-\vartheta_{t_h}/T)$ is the same for the release of the captured holes, $N = 4\times10^{21}$ cm^{-3} is the number of molecules per unit volume of crystal, $\alpha^{e}K$, $\alpha^{h}K$ are the probabilities of both captured electron and hole to escape from a trap due to the external irradiation, respectively; ϑ_{t_e} , ϑ_{t_h} are the depths of the traps for electrons and holes respectively, $n^{-}_{t_e} = (n^{0}_{e} - n^{+}_{t_e})$, $n^{-}_{t_h} = (n^{0}_{h} - n^{+}_{t_h})$ are the densities of free traps for electrons and holes, n^{0}_{h} and n^{0}_{e} are the densities of traps for

electrons and holes, $c_\rho = \alpha T^3$ is the specific heat capacity of the crystal, $\xi\vartheta_{eh}K$ is the energy that transfers to the crystal lattice due to the external irradiation, $\beta = 2\nu/L$.

CALCULATIONS AND DISCUSSIONS

The equation $n_e + n_{t_e}^+ = n_h + n_{t_h}^+$ is satisfied due to the electroneutrality of the electron-hole plasma . Therefore the system (1) actually contains only four equations for variables n_e, $n_{t_e}^+$, $n_{t_h}^+$, T.

To study the dependence of the behavior of the system on the parameters one should find the stationary points of the system and investigate their stability. The numerical analysis shows that the system (1) has only one stationary point. The bistable and multistable states of that system are not found.

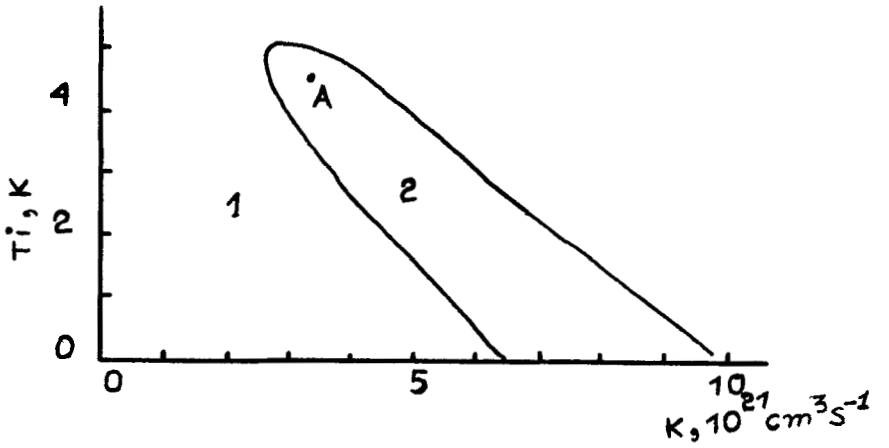

FIGURE 1 Region of auto-oscillations against the thermostat temperature Ti and pumping rate K. The densities of free and captured carriers and temperature for the stationary point A (Ti = 4.2 K, K = $3.8\times10^{21}cm^{-3}s^{-1}$) of the system are $n_e = 2.59\times10^{11}cm^{-3}$, $n_h = 5.40\times10^{9}cm^{-3}$, $n_{t_e}^+ = 1.42\times10^{16}cm^{-3}$, $n_{t_h}^+ = 1.42\times10^{16}cm^{-3}$, T = 6.55 K.

The results of the analysis of the stability of the stationary points are plotted in fig.1. All calculations were carried out at the following parameters:

$\gamma = \gamma_{ht_e} = \gamma_{et_h} = 10^{-6}$ cm^{3}s^{-1}, $\gamma_{et_e} = 10^{-9}$ cm^{3}s^{-1}, $\gamma_{ht_h} = 10^{-7}$cm^{3}s^{-1}, $\beta = 10^{10}$erg cm^{-3} K^{-1}s^{-1}, $\alpha = 114$ erg cm^{-3} K^{-4}, $\vartheta_{eh} = 3.6$ ev, $\vartheta_{t_e} = 9.7\times10^{-3}$ev, $\vartheta_{t_h} = 1.29\times10^{-2}$ev, $\alpha_e = \alpha_h = 0.003$, $n_e^0 = n_h^0 = 8\times10^{18}$ cm^{-3}, $\xi = 0.2$.

These parameters are characteristic for the crystal of anthracene.

Stationary points of the system are stable for the region 1 in fig.1. No auto-oscillations are expected in this case. If the parameters change from the region 1 to the region 2 the Hopf bifurcation occurs in the system, so the auto-oscillations should appear.

The dependencies of the width of the auto-oscillation region with regard to the pumping rate ΔK and largest thermostat temperature Ti_{max} in the auto-oscillation region against depths of the traps are found (fig.2,3).

For the crystal with large band gap the Ti_{max} increases.

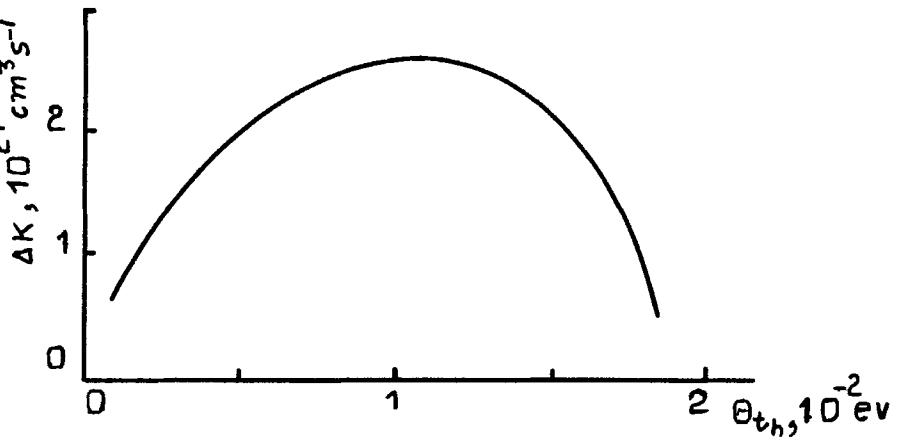

FIGURE 2 Dependence of the average width of the auto-oscillation region against the pumping rate ΔK on the depths of the traps. $\vartheta_{t_e} = 0.75\times\vartheta_{t_h}$.

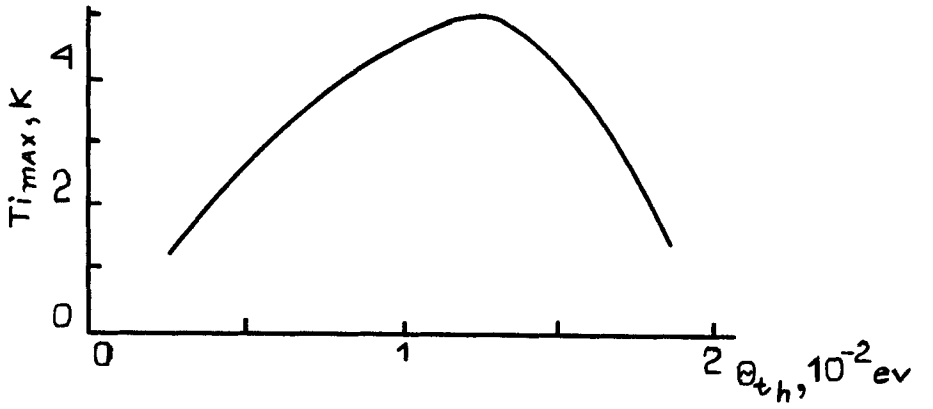

FIGURE 3 Dependence of the largest thermostat temperature Ti_{max} in auto-oscillation region on the depths of the traps. $\vartheta_{t_e} = 0.75 \times \vartheta_{t_h}$.

The dependence of the frequency of arising auto-oscillations in case of parameters nearby the boundary of the auto-oscillation region on the traps are shown in fig.4.

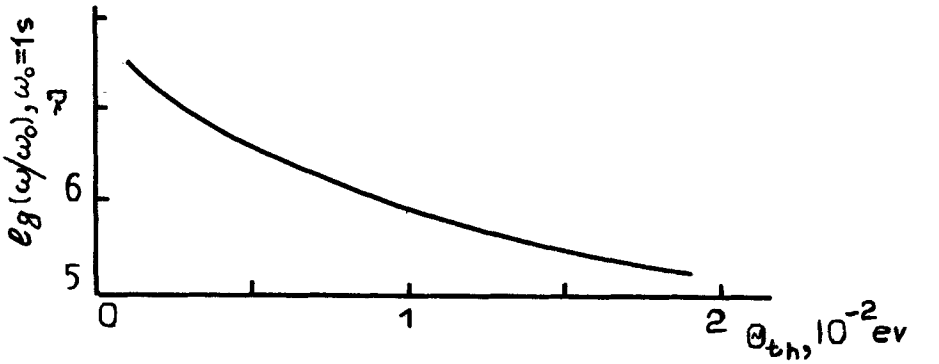

FIGURE 4 Dependence of the frequency of the auto-oscillations nearby the auto-oscillations region on the depths of the traps. $\vartheta_{t_e} = 0.75 \times \vartheta_{t_h}$.

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