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Phenomenological model of athermal interaction of microwave radiation with the structures wide-gap semiconductor – oxide film

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Abstract. We propose a phenomenological model that explains the changes in the optical spectra of the structures wide gap semiconductor – oxide film, which takes place as a result of short-term microwave treatment. To explain the specific athermal microwave exposure, proposed was an integrated approach that is a combination of several processes that are described by various models. Interaction of processes caused by the resonant interaction of microwave radiation with the intrinsic oscillations of dislocations, which can lead to dislocation motion, has been considered. The length of dislocations, for which the condition of the resonant interaction is fulfilled, has been estimated. It has been shown that the combination of the considered processes can lead to appearance of additional centers of light absorption or scattering, which is manifested in the spectra of optical absorption and photoluminescence of the structures wide-gap semiconductor – oxide film.

Keywords: wide gap semiconductor, oxide film, athermal interaction, microwave radiation, dislocation.

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1. Introduction

Now, there is a sufficient number of experimental results showing the specific athermal effect of microwave radiation on materials. In particular, in the review [1] non-thermal action of microwave radiation on ceramic materials is considered.

So, in the papers [2-6] it has been shown that the short-term treatment of the structures oxide – semiconductor and crystalline semiconductors with microwave radiation of the frequency 2.45 GHz results in the increase of transmission in the optical range, appearance of additional bands in the photoluminescence spectra (PL) spectra of similar structures or redistribution of the intensity of PL bands [2-6]. And here, evaluation of the thermal short-term action of microwave radiation with the frequency 2.45 GHz, which was used in [2-6] in processing the structures oxide – semiconductor and crystalline semiconductors, has shown that the maximum heating of the sample during irradiation did not exceed 2 degrees.

However, there is still no model that would definitely explain the mechanism of non-thermal effects on the structures oxide film – semiconductor.

Considered in this work are the processes that explain the mechanism of athermal microwave effects on the structures wide-gap semiconductor – oxide film. Since the layers are localized near the interface wide-gap semiconductor – oxide film, there always are misfit stresses due to the mismatch of parameters characterizing the crystal lattices of oxide and substrate as well as thermal stresses arising during formation of oxide films. Dislocations will inevitably appear in these structures. Therefore, when considering the mechanisms of athermal microwave action on the structure, we will focus on the processes related with the possibility of dislocation motion under the influence of microwave radiation.

2. The process of mass transfer

In [1], the non-thermal effect of microwave field is explained by the phenomenon of mass transfer and related with it phase transitions in solids. According to the proposed model describing the diffusion-drift dynamics of vacancies flow under the influence of the electric component of the microwave field, the effects that lead to arising the directional mass transfer are caused by formation of the space charge near the structural inhomogeneities in the crystal bulk. Here, the forces similar in their nature to averaged ponderomotive forces act on the defects having charge.

As another reason for existence of non-vanishing after averaging over the period of the field of matter flows, the primary one-way permeability of the body surface for the flows of vacancies is considered. With substantial asymmetry of permeability, the influence of the field on mass transfer processes in a homogeneous crystal under conditions typical for microwave treatment of materials can be significant.

The averaged ponderomotive effect is equivalent (in the sense of generating the quasi-stationary flows of mass) to the action of stresses and leads to compression of the crystalline body along the vector of the electric field [1]. Mechanical stresses caused by exceed the radiation pressure of field by N^{-1} times, where N is the relative concentration of vacancies in the crystal [1]. It is related to the fact that the electric field acts only on the atoms neighboring to the vacant lattice point and therefore having uncompensated charge. On the other hand, these atoms are able to move during diffusion processes in the solid phase. In contrast to it, the effect of mechanical stress is applied to all the atoms of the crystal, the majority of which cannot be moved. Since the concentration of vacancies depends on the temperature, this effect can explain the decrease in the activation energy of mass transfer processes under microwave exposure observed in experiments [1].

The effect of the action of the averaged ponderomotive force is greatly enhanced in the case of an inhomogeneous structure of material as well as in materials, in which there are mobile defects (*e.g.*, vacancies) possessing substantially higher electric susceptibility as compared with the average unit of the crystal lattice. A necessary condition for ponderomotive effects is the presence of macroscopic structural inhomogeneities in material, such as free surfaces or boundaries between the crystalline grains. Estimations show that the averaged ponderomotive effect can significantly affect the diffusion processes in polycrystalline materials [1].

According to [7], even a small rearrangement of atoms near dislocation can cause the displacement of the dislocation line by the interatomic distance, so the decrease in activation energy of mass transfer processes under microwave exposure should lead to a separation of dislocations from stoppers.

3. The resonant interaction of microwave radiation with a dislocation

In [8], we considered the model of the resonant interaction of microwave radiation with a dislocation.

According to [7], the equation for the displacement $u(y, t)$ of the dislocation loop with the length l, rigidly attached to the ends and oscillating (similar to the elastic string) under the action of periodic external influence, can be written as

$$m_l \ddot{u} + B\dot{u} - \gamma \frac{\partial^2 u}{\partial y^2} = \sigma b \qquad (1),$$

where m_l is the effective mass of dislocation per unit of length, γ – effective line tension of the dislocation, $\sigma = \sigma_0 e^{i\omega t}$ – oscillatory shear stress caused by external influence, b – absolute value of the Burgers vector. The boundary conditions are as follows $u(0, t) = u(l, t) = 0$. The parameter B in the expression (1) corresponds to the attenuation constant. The term $\gamma \frac{\partial^2 u}{\partial y^2}$ describes the restoring force per unit of length. The γ value is estimated from the expression

$$\sim ½\, Gb^2 , \qquad (2)$$

where G is the shear modulus.

The value m_l is determined as

$$m_l. \approx \rho b^2 , \qquad (3),$$

where ρ is the density of material.

According to [7], for the dislocation loop the dependence of $u(y, t)$ can be described by the expression

$$u(y, t) = A\, \sigma_0\, (ly - y^2)\, e^{i\omega t} \qquad (4)$$

where $A = \sigma / 2\gamma$.

After substituting Eq. (4) to Eq. (1) and integrating from $y = 0$ to $y = l$ we obtain

$$-\omega^2 m_l \frac{Al^3}{6} + i\omega B \frac{Al^3}{6} + 2\gamma A l = b \qquad (5)$$

or

$$A = \frac{b}{2\gamma}\left[1 + i\omega\tau - \frac{\omega^2}{\omega_0^2}\right]^{-1} \qquad (6)$$

where

$$\omega_0^2 = \frac{12\gamma}{m_l l^2} \qquad (7)$$

and

$$\tau = \frac{Bl^2}{12\gamma} . \qquad (8)$$

When attenuation is weak, the value

$$\nu_0 = \omega_0/2\pi \tag{9}$$

plays the role of the resonant frequency, at which $|A|$ reaches its maximum value limited only by the attenuation constant.

If substitute the expressions (2) and (3) to (7) for the frequency ω_0, we will obtain:

$$\omega_0^2 = \frac{12 \cdot \frac{1}{2} \mathrm{Gb}^2}{\rho \mathrm{b}^2 l^2} = \frac{6G}{\rho\ l^2} \ . \tag{10}$$

From (7), we can estimate the size of dislocations, for which the microwave frequency ν = 2.45 GHz used in our experiments will be resonant. For the case $\nu = \nu_0$ we obtain

$$l^2 = \frac{3}{2} \frac{G}{\pi^2 \rho\ \nu_0^2} \ . \tag{11}$$

Substituting the values of G and ρ for silicon carbide and oxide films of SiO_2, TiO_2, Gd_2O_3, Er_2O_3 into Eq. (11), we conclude that the frequency $\nu = 2.45\times10^9\ \mathrm{s}^{-1}$ is resonant for the dislocations with the length $l \approx 10^{-4}$ cm.

Thus, the resonant interaction of the microwave radiation with the frequency $\nu = 2.45\times10^9\ \mathrm{s}^{-1}$ can lead to detachment of the dislocations with $l \approx 10^{-4}$ cm and their movement both in the silicon carbide substrate and the oxide layer. The movement of dislocations, in turn, will lead to change in the distribution of internal stresses in the structure, and, hence, the subsequent change in the number and configuration of dislocations.

4. Parametric resonance

As it is well known [9, 10], in the case of parametric resonance, periodic modulation of some parameter of the system can result in oscillations of the growing nature, the equilibrium state of the system becomes unstable, and leaving this state has the character of oscillations with a progressively increasing amplitude. In the case of dislocation, the length of dislocation can be the modulated parameter because the atoms that are stoppers for dislocation, in turn, themselves are a source of vibrations. The most intense oscillations are excited in the case when the frequency of parameter modulation is twice exceeded the intrinsic frequency of the system. More accurate calculations [9, 10] show that the swinging the oscillations takes place in the whole frequency range $\Delta\omega$ around the frequency $2\omega_0$. If to introduce the notation $\omega = 2\omega_0 + \Delta\omega$, where $\Delta\omega$ is small detuning, it is possible to show that in the absence of friction the parametric resonance arises within the frequency range

$$-\frac{h\omega_0}{2} < \Delta\omega < \frac{h\omega_0}{2} \, . \tag{12}$$

In the presence of attenuation the $\Delta\omega$ value is determined as

$$|\Delta\omega| < \sqrt{\left(\frac{h\omega_0}{2}\right)^2 - 4\varsigma^2} \ , \tag{13}$$

where ζ is the attenuation parameter.

Therefore, due to the parametric resonance, detach of dislocations not only with the length l determined by the expression (11), but also dislocations with the length $l_1 \sim 2l \sim 2\times10^{-4}$ cm from stoppers may occur.

Moreover, oscillations of dislocations with the frequency about 10^9 Hz can be considered as hypersonic oscillations. At the same time, the propagation of hypersound in the crystal can lead to phenomena similar to the effect of “radiation shaking”: the appearance of hypersonic waves affects the spatial remote defects, causing their diffusion or restructuring. Also, the interaction of waves of elastic stresses with the existing point defects can lead to activationless migration of interstitial atoms, to influence on the probability of nonradiative processes in the luminescence centers, *etc*. [11].

5. The process of redistribution centers of emission and absorption

Since the binding energy between the impurity atom and dislocation is a function of the position of the defect relatively to dislocation [7], the motion of the dislocation caused by microwave exposure (the processes leading to the motion of dislocations as a result of microwave exposure are discussed in Sections 1-3) should lead to a redistribution of the irradiation centers and absorption in the structures.

Due to the presence of free or unsaturated bonds in the dislocation core [12] when the distance between dislocations and impurity atom is changed, as a result of the movement of dislocations, the conditions may arise when electron tunneling is possible, in particular, from the impurity to a dislocation, which can lead to a change in the charge state of the impurity. Similarly to the impurity atoms, vacancies and interstitials are also attracted to the dislocations, and the intrinsic point defects can be fully absorbed by the edge dislocations [7].

In addition, according to [7] in the athermal processes the motion of dislocations can result in the appearance of non-equilibrium point defects.

In the result of interaction of the dislocations with impurities and lattice defects in the band gap of the crystal, the related energy levels appear. Therefore, the band structure near the dislocation is extremely complicated [12]. In general, the dislocation creates isolated centers that can act as centers of both radiative and nonradiative electron-hole recombination [12]. According to [13], the energy released in nonradiative recombination of electron-hole pair in SiC is sufficient for that atom to overcome barrier impeding its displacement to another position. That is, there is a local rearrangement of the lattice of the hexagonal polytype in the cubic one, and cubic polytype layer is formed [13].

6. Conclusion

Thus, being based on the considering processes of interaction of microwaves radiation with dislocations, which result in changes in the number and configuration of dislocations, one can conclude that the microwave exposure should lead to a redistribution of recombination centers in the structures semiconductor – oxide layer. It, in turn, causes appearance of additional bands in the photoluminescence spectra or to redistribution of intensities inherent to separate bands in the photoluminescence spectrum, as well as to changes in the spectra of optical transmission.

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