

FEATURES OF TRANSFER PHENOMENA IN POLYCRYSTALLINE FILM STRUCTURES

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Abstract:

The paper substantiates a physical approach to describing transport phenomena in polycrystalline semiconductor films. The case including the transfer of charge carriers across block boundaries (BB) is considered. The electrical conductivities of the barrier are found in the directions along the axes (perpendicular to the BB) and (parallel to the BB). It is shown that the greatest contribution to the change in the kinetic coefficients in the barrier regions is made by the potential dependence of the charge carrier concentration on the coordinate at $\varphi_A \gg kT$. The indicated parameters are for a polycrystalline film with arbitrary dispersion (with an arbitrary number of crystallites per unit length).

Keywords. Transport phenomena, polycrystalline semiconductor films, intergranular barriers, elementary unit of a crystal, dislocations, crystal, diffusion, minimum crystal, a block boundary, a boundaries of crystallites, electrical conductivity of the barrier, anisotropy of conductivity, electrical conductivity of a polycrystalline film, mean free path.

Introduction

In order to manufacture highly efficient film devices, including thermoresistive structures, in addition to possessing the art of a technologist, it is necessary to know the features of physical processes occurring in films under various external conditions and to identify their mechanisms. Knowledge of the regularities of current transfer in films of bismuth-antimony telluride can be a tool in identifying the nature of the tensorial effect.

To describe the transport phenomena in polycrystalline semiconductor films with intercrystalline barriers, we use the model elementary unit of a crystal [1] based on the following assumptions. It is assumed that under normal (equilibrium) conditions, all crystals consist of elementary units - miks ("minimal crystal"). Of particular interest is the problem of boundaries between them. The known experimental data suggest that the boundaries between the miks can also serve as sites for the development of dislocations. Apparently, it is not accidental that the maximum density of dislocations ($10^{11} \div 10^{12}$ per 1 cm^2) practically corresponds to the number of elementary units per 1 cm^2 of the crystal cross section with a linear mik size of $\sim 3 \times 10^{-6} \text{ cm}$. Some experimental data [2] give reason to believe that the really existing boundaries between miks are the paths along which matter (diffusion) and charges (electric current) are transported through the crystal.

The elementary unit of a crystalline solid body ("quantum of a crystal" or "minimal crystal" - "mic", symbol μk) is defined as follows. The minimum crystal - mic - is such a minimum amount of a crystalline solid that still retains the normal ("limiting") properties characteristic

of a massive sample of a given substance. A smaller crystal loses (substantially changes) these properties.

The linear dimensions of the mic are in the range $r_m = 10^{-5} \div 10^{-6}$ cm (for isotropic one- and diatomic crystals, the most reliable experimental data allow us to estimate $r_m = (3 \pm 1) \times 10^{-6}$ cm). Several mics connected to each other form a block. A block is a part of a crystal, consisting of several mics. The presence of boundaries separating mics means that "long-range order" in a crystal is possible only within a given mic, that is, it cannot exceed the linear dimensions of the elementary unit of the crystal. A polycrystal can, in principle, be considered as a strongly distorted crystalline macrostructure.

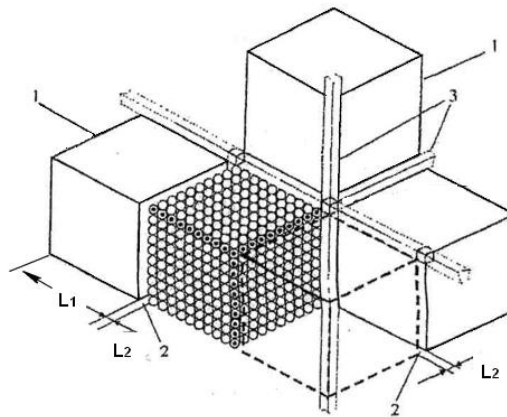


Figure 1. Fragment of the secondary structure of a cubic crystal [1]: 1 - elementary unit of the crystal - mic; L_1 is the width of a rectangular crystalline block; 2 - interblock layer of width L_2 .

A polycrystalline film of thickness d consists of identical rectangular crystalline blocks with a characteristic size L_1 , separated by interblock interlayers with a width L_2 . The electrical conductivity of the interblock layers is different from the electrical conductivity of each block (they are considered to be more resistive) and is assumed to be isotropic. Within the framework of the model, any region of the interlayer is characterized by the same value of electrical conductivity (the concentration of charge carriers), and the conductivity of the entire model grid depends only on the ratio of the electrical conductivities of blocks and interlayers and their geometric dimensions.

Let intergranular barriers exist at the block boundaries of a polycrystalline film with a nondegenerate electron gas, which ensure the depleting bending of the bands.

The electron concentration at any point of the film, including in the barrier regions, obeys Boltzmann statistics and is determined by the distance from the conduction band at a given location to the Fermi level. Let us designate the barrier height as φ_A , and the height of the barriers at the nodes (the contact point of three or more crystallites) at the boundaries of crystallites as φ_B .

The condition $\varphi_B > \varphi_A$ provides the lowest concentration of electrons in the nodes, i.e. nodes in the case of exhaustive bending of the bands in boundaries of crystallites are the most highly resistive regions in a polycrystalline film. Therefore, the nodes for electrons are practically

“locked” and at $\varphi_A \gg kT$, they make an exponentially small contribution to the conductivity. Current transfer in a polycrystalline film is carried out along the path crystallite - boundaries of crystallites - crystallite.

In addition, the conductance of the potential barrier in different directions is anisotropic. Using it, one can also find σ_δ^\perp and σ_δ^\parallel the electrical conductivity of the barrier in the directions along the axes (perpendicular to the block boundaries) and (parallel to the block boundaries). Taking into account the course of the barrier height along the axis x

$$\varphi(x) = \frac{e^2 N_d}{2\chi\chi_0} (\ell - x)^2 \quad (1),$$

which follows from the Poisson equation for the block boundaries barrier. In (1) N_d and $\chi\chi_0$ the doping level and the dielectric constant of the film material, ℓ is the width of the depleted region near the boundaries of crystallites. By simple integration in the case $\varphi_A \gg kT$, we find

$$\sigma_\delta^\perp \approx eN_d\mu_n \frac{2\varphi_A}{kT} \exp\left(-\frac{\varphi_A}{kT}\right) \quad (2)$$

$$\sigma_\delta^\parallel \approx eN_d\mu_n \sqrt{\frac{\pi kT}{\varphi_A}} \quad (3)$$

where, μ_n -is the electron mobility determined by the main scattering mechanism in the film material. Comparison of (2) and (3) shows a strong anisotropy of the potential barrier conductivity in mutually perpendicular directions.

The concentration of charge carriers in semiconductors with a narrow band gap, which include the compounds we are considering $A^{IV}B^{VI}$ and $A_2^VB_3^{VI}$, is usually high. Therefore, in real films of these semiconductors with crystallite sizes, at almost any reasonable surface states concentration and a very wide range of low temperatures, free carriers are not completely localized on the block boundaries.

We will consider the case that includes the transfer of charge carriers through the block boundaries. If $2\ell \gg \lambda_0$, the barrier regions are characterized by their own parameters, different from the bulk properties of the film material. The barrier region near the block boundaries includes the crystallite interface itself, which is a charged plane. Therefore, when concretizing the question of the parameters of barrier regions, it is necessary to know whether the existence of this charged plane, which must be overcome by charge carriers, affects the scattering mechanism and, accordingly, parameters sensitive to it (mobility, carrier concentration, etc.). The passage of charge carriers through the block boundaries with \vec{n} , the normal directed along the streamlines, i.e. perpendicular to the block boundaries does not contribute to the electrical conductivity, despite the fact that this process does not conserve exactly the momentum component that is acquired by the system from the electric field. In other words, when carriers pass through the charged block boundaries plane, changes in the electrical conductivity near this plane, in comparison with the homogeneous case, are associated only with the reflection of a part of the carriers from this plane, which do not contribute to the electrical conductivity.

Because of this, in the situation under consideration, the largest contribution to the change in the kinetic coefficients in the barrier regions is made by the potential dependence of the charge carrier concentration on the coordinate at $\varphi_A \gg kT$. (Usually the condition $2\ell \succ \lambda_0$ is provided at $\varphi_A \gg kT$).

Thus, at $2\ell \succ \lambda_0$, using (2) - (3), as well as the corresponding equivalent electrical circuits of crystallites, it is easy to calculate the kinetic coefficients of polycrystalline films. In particular, the electrical conductivity has the form

$$\sigma = eN_d\mu_n \frac{\varphi_A}{kT} \frac{L}{\ell} \exp\left(-\frac{\varphi_A}{kT}\right) \quad (4)$$

When $2\ell \prec \lambda_0$, which, apparently, in real films takes place more often than the opposite case, the kinetic coefficients near the barriers must be calculated taking into account the features of the passage of carriers through the barrier. Without specifying the nature of the potential barrier here, we will show one of the ways to calculate the parameters of a polycrystalline film in the case of $2\ell \prec \lambda_0$.

Let a potential barrier of size $2\ell \prec \lambda_0$ be created in a homogeneous semiconductor of length L_0 . When a semiconductor is placed in an electric field, the action of the barrier will be felt only by carriers located in the region of the barrier, i.e. the change in the parameters of the semiconductor will be only on the characteristic length 2ℓ , since the carriers that have not entered the barrier region and overcome it have a mean free path coinciding with the homogeneous case.

Let us denote by σ_δ the parameter of the region near the barrier at this length. Taking into account the additivity property of resistance in a series connection leads to the relation

$$\frac{1}{\sigma} L_0 = \frac{1}{\sigma_0} (L_0 - 2\ell) + \frac{1}{\sigma_\delta} 2\ell; \quad (5)$$

where σ_0 - is the parameter of a homogeneous semiconductor. Transforming (5), we find

$$\sigma = \sigma_0 \left[1 + \left(\frac{\sigma_0}{\sigma_\delta} - 1 \right) \frac{2\ell}{L_0} \right]^{-1} \quad (6)$$

Using this approach, one can find these parameters for a polycrystalline film with an arbitrary dispersity (with an arbitrary number of crystallites per unit length). It is easy to show that in the case of $L \succ 2\ell$, the electrical conductivity of the polycrystalline film coincides with expression (6), where L_0 must be replaced by L :

$$\sigma = \sigma_0 \left[1 + \left(\frac{\sigma_0}{\sigma_\delta} - 1 \right) \frac{2\ell}{L} \right]^{-1} \quad (7)$$

Expression (7) determines the electrical conductivity of a polycrystalline film at $2\ell \prec \lambda_0$ and any ratio between λ_0 and L .

If there is a tunnel-opaque barrier with a height $\varphi_A \gg kT$ at the boundary of the blocks, then near the boundary of the blocks, carriers with energies $E > \varphi_A$ contribute to the kinetic coefficients. In this case, for σ_δ in (7) one can write explicit expressions

$$\sigma_\delta = \sigma_0 \exp\left(-\frac{\varphi_A}{kT}\right);$$

Substituting them and taking into account $\varphi_A \gg kT$ gives

$$\sigma \approx \sigma_0 \frac{L}{2\ell} \exp\left(-\frac{\varphi_A}{kT}\right)$$

(8)

This expression differs from (4) in that it naturally reflects the absence of dependence of the electron concentration on the coordinate.

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