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DEVELOPMENT OF METHODS FOR STUDYING INTERGRANULAR SURFACE FEATURES IN SEMICONDUCTOR HETEROGENEOUS POLYCRYSTALS OF BISMUTH-ANTIMONY TELLURIDES WITH THE IMPOSITION OF ELECTRIC AND DEFORMATION FIELDS

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ABSTRACT

The article discusses the technique and tools for studying the role of the effective density of electronic surface states innanocrystalline semiconductor films when cyclic deformation is applied directly from the analysis of experimental data. The surface electron states play the role of recombination and trapping centers depending on the number of carriers, the electron capture section and hole, the concentration of surface states of their type and energy position . To determine the effective density of surface states, we found both a change in the Fermi level and a change in the density of the effective surface charge. The effective density of electronic surface states was determined from the measured variations in the active resistance and capacity of nanocrystalline films of bismuth-antimony tellurides upon the application of irreversible deformation, and its strain dependence was found. From data analysis, one can judge the irreversibility of heterogeneous structures during deformation, that is, the electronic structure of a nanocrystalline semiconductor film changes greatly when cyclic deformation is applied.

KEYWORDS: *Nanocrystalline Films, Grain Boundaries, Surface Electron States, Fermi Level, Interface Charge, Surface States, Effective Density Of Electron Surface States*

INTRODUCTION

Polycrystalline semiconductors are widely used in such technical devices as photoconverters, integrated circuits, varistors and others **[1,2]** . However, obtaining the necessary and, most importantly, stably repeatable properties of these materials is complicated by their structural features, the most important of which is the presence of grain boundaries. The electrical properties of polycrystalline semiconductors are largely determined by nonequilibrium electronic processes at grain boundaries. It is obvious that the improvement of the above devices should be based on a detailed understanding of these processes, on firmly established relationships connecting the measured electrophysical characteristics with the parameters that determine the electronic properties of grain boundaries. This stimulated numerous theoretical studies of

physical phenomena caused by grain boundaries, in particular, the barrier mechanism of electrical conductivity of polycrystalline semiconductors **[3–5].**

At present, the scale of the use of polycrystalline semiconductors, the grains of which have a size of the order of tens of nanometers, is increasing. This is due to the variety of their functional properties. A specific feature of nanocrystalline semiconductors is the presence of built-in interfaces in them - grain boundaries (GB), which have a decisive effect on the electrical properties of nanocrystals. At this stage, the physics of nanocrystalline film semiconductors is in its infancy. Therefore, the study of the response of these objects to superimposed physical fields will contribute to the creation of the physics of nanocrystalline semiconductors **[1, 3].**

The entire variety of grain boundaries in films of semiconductor mixtures is usually modeled by a single GB in an effective bicrystal. Its parameters are unknown. They are replaced by the averaged properties of the initial grains, which leads to the uncertainty of the results obtained. This is a serious shortcoming of the current situation in the field of semiconductor nanocrystalline films. The models used are one-dimensional. The electronic structure of grain boundaries is very sensitive to the capture of impurities by growing films. This contributes to the production of films with unique properties. The grain boundaries contain adsorbed atoms, vacancies, and other defects.

Materials

Nanocrystals have a highly developed intergranular surface. So, for example, in strain-sensitive films of bismuth-antimony tellurides, the average linear size of one granule is 50 nm ($5 \cdot 10^{-6}$ cm). For Bi_2Te_3-Sb_2Te_3 films, the geometric dimensions of which are 1x0.1x0.0003 cm^3, the total area of the intergranular surface reaches 60 cm^2.

Methods

Surface electronic states play the role of recombination and capture centers, depending on the number of carriers, the cross section for electron (Cp) and hole (Cp) capture, the concentration of surface states (Nss), their type, and energy position (Es).

Under these conditions, it becomes topical to develop methods and tools for studying the role of the effective density of electronic surface states of nanocrystalline films directly from the analysis of experimental data. Here, too, the entire set of electrically active grain boundaries (GBs) in a nanocrystalline film is modeled by one effective GB. **[6-7].**

For a neutral transition, two parameters remain free: the interface charge Qi and the applied voltage U. Under the conditions U=0, the interface charge is determined by the spatially homogeneous Fermi level F. It can be calculated by integrating the density of statesN_{ss} (E_i) on the interface:

$$Q_i = q \cdot \int dS \int \{ dE \cdot N_{ss}(E) \cdot f(E) \} \qquad (1)$$

where $f(E) = \dfrac{1}{1 + \exp\left\{\dfrac{E - F}{kT}\right\}}$, $F_i(U = 0) = F_o$ - Fermi level

It is assumed that before charges are captured by traps, the interface is electrically neutral; otherwise, the constant charge must be subtracted from the right side. If we take the differential with respect to the Fermi level F, then from formula (1), where S is the effective surface area, we get:

$dQ/dF = q \cdot S \cdot N_{ss}$ (2)

The change in surface charge with respect to the Fermi level gives the concentration of surface states N_{ss}.

$\frac{dQ_{ss}}{dF}$ is obtained from the expression $\frac{\Delta Q_{ss}}{\Delta F}$ at $\Delta F \rightarrow 0$.

Thus, to determine the effective surface states density, it is necessary to find both the change in the Fermi level Δ F and the change ΔQ_{ss} in the effective surface charge density.

The Fermi level F as well as Q can change when external fields are applied - temperature or deformation, or when impurity atoms are introduced. In [4], the situation was studied when F and Q changed due to a change in the temperature of the polycrystalline CdTe film.

The change in Q_{ss} is associated with a change in the effective capacitance $C(\varepsilon_i)$. The surface charge is equal to Q=CU. Under the influence of external forces

$$\Delta Q_s = C \cdot \Delta U + U \cdot \Delta C \quad (3)$$

The total charge changes Q_s also contains an induced charge due to different values of the electric voltage U_{11} in the absence ($U_{11}(0)$) and the imposition ($U_{11}(\varepsilon_i)$) of deformation ε_i.

Means

$$\Delta Q_{ss} = U \cdot \Delta C \quad (4)$$

The dependence of the resistance of nanocrystalline films can be represented as:

$$R = A \exp\left(-\frac{F}{kT}\right) \quad (5)$$

Here A is a geometric factor.

As nanocrystalline films are deformed, both A and F change. The Fermi level in metals does not change. Another thing is heterogeneous semiconductor films. For them, the change in specific conductivity during deformation is more important than the change in the geometric factor A. I.e. in nanocrystalline semiconductors, the change in the Fermi level is more significant than the change in A. Therefore, when strain εi is applied, formula (5) has the form

$R(\varepsilon_i) = A_0 (1 + \gamma_I \cdot \varepsilon_i) \cdot \exp (- [F (\varepsilon_i) - \delta_i \cdot \varepsilon_i] / kT)$ (6)

Here: $\delta_I \cdot \varepsilon_i$ is the effective change in the energy position of the band gap, and $\gamma_i \cdot \varepsilon_i$ is the change in the geometric factor.[7].

Formula (6) can be written as

$R(\varepsilon_i) = A_0 \cdot \exp (- [F (\varepsilon_i) - b_i \cdot \varepsilon_i] / kT)$ (7)

where$b_i=\delta_i + \gamma_i$

Such a record will allow one to find the change in the Fermi level F with deformation. We used a high level of automation in the process of measuring the resistance of the film before and during the application of cyclic deformation. As a result, we have:

$kT\cdot Ln[R(\varepsilon_i)/R((\varepsilon_{i-1})]=b_i\cdot(\varepsilon_i-\varepsilon_{i-1}) - \Delta F_i$; здесь$\Delta F_i = F(\varepsilon_i)–F(\varepsilon_{i-1})$ (8)

and, i = 1,2,3,…, *N*, where within one cycle $N = 10^3$.

In this way,

$-\Delta F(\varepsilon_i) + b_i(\varepsilon_i-\varepsilon_{i-1})=kT\cdot Ln[R(\varepsilon_i)/R((\varepsilon_{i-1})]$ [8-11].

Results

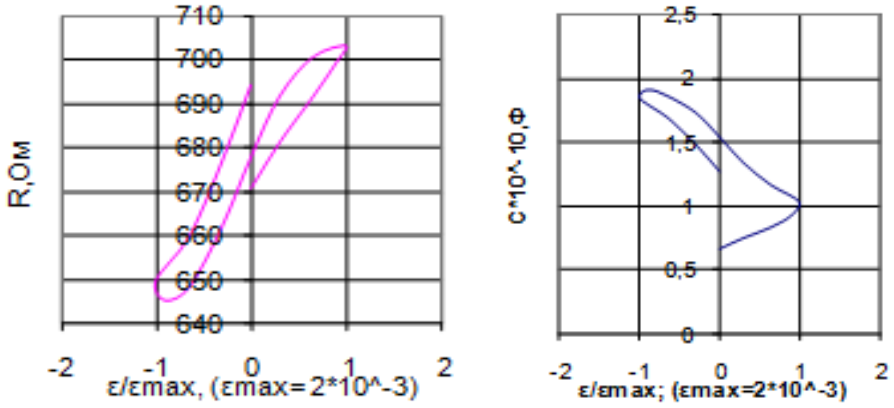
By measuring the frequency dependence of the resistance $R(\omega,\varepsilon_i)$ at n points (n<< N) we get a system of equations used in the linear regression method. n is a limited number of points, which is chosen so as to ensure the coincidence of the experimental data with the approximation formula (7).

We have found n=5 with a deformation interval between the experimental points equal to $\varepsilon_i-\varepsilon_{i-1}=10^{-6}$. This allows, within any five consecutive points, to consider $\Delta F(\varepsilon_i)$ and$b_i(\varepsilon_i)$ independent of the deformation. Outside this interval, $\Delta F(\varepsilon_i)$ and $b_i(\varepsilon_i)$ depend on the strain.

Let us calculate the effective density of surface states N_{ss} for various values of the imposed strain - ε_i. As noted above, to determine the effective density of surface states, it is necessary to find both the change in the Fermi level $\Delta F(\varepsilon_i)$and the change $\Delta Q_{ss}(\varepsilon_i)$ in the effective surface charge density:

$N_{ss}=U\cdot\Delta C(\varepsilon_i)/\Delta F_i(\varepsilon_i)$.

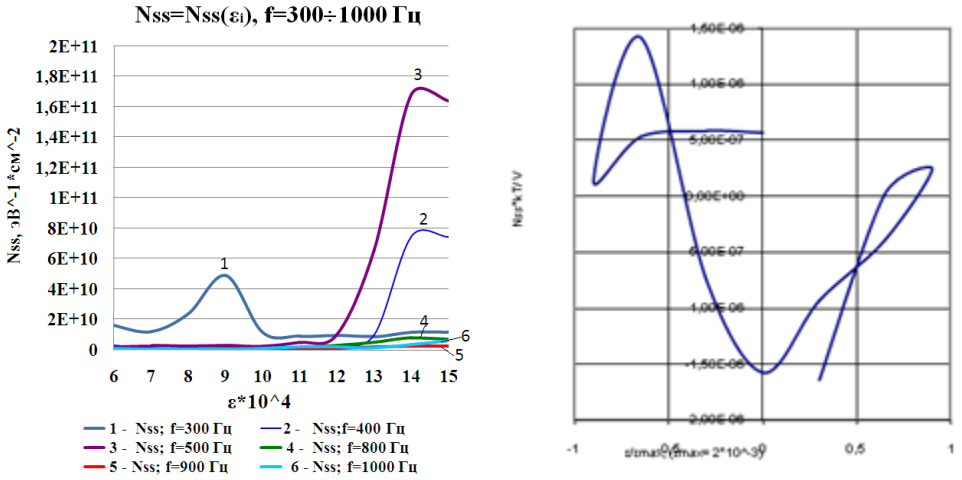
Figure 1 a and b shows the dependences of the resistance $R(\varepsilon_i)$ and capacitance $C(\varepsilon_i)$ of samples of nanocrystalline films of bismuth telluride - antimony, on the imposed deformation (for one full cycle of symmetrical load (stretching - from zero to ε max and then from ε max to zero and back to the compression region) measured for frequency f=240 kHz



а) б)

Fig.1. a) Dependence of resistance and b) capacitance of samples of nanocrystalline films of bismuth-antimony telluride on the imposed strain R(ε), measured for one complete cycle of symmetrical load (extension - from zero to ε max and then from εmax to zero and back to the compression region) at a frequency f = 240 kHz.

Figure 2 shows the dependences of the effective density of electronic surface states $N_{ss}(\varepsilon_i)$ on the imposed strain.



а) б)

Fig.2. Dependence of the effective density of electronic surface states on the imposed deformation $N_{ss}(\varepsilon_i)$, calculated for the frequency a) f=300 Hz , f=300 ÷1000 Hz , and b) f=240 kHz.

DISCUSSION

Above are the calculation methods for studying the dependencies $R(\omega,\varepsilon_i)$ and$C(\omega,\varepsilon_i)$. The resulting formulas were used to compile a calculation program on the IBM PC, with the help of which, using experimental data, the dependences of the resistance and capacitance of the films on frequency and strain were determined - $R(\omega,\varepsilon_i)$ and $C(\omega,\varepsilon_i)$. In addition, using these data, the effective density of electron surface states (ESS) of polycrystalline semiconductor films of bismuth–antimony tellurides was determined from measurements of the deformed (ε_i) and frequency (ω) dependences of their resistances $R(\omega,\varepsilon_i)$ and capacitances $C(\omega,\varepsilon_i)$. The measurements were made on a bench providing the necessary accuracy and speed of measurements. It has been established that the relative values of the ESS of some semiconductor polycrystalline Bi_2Te_3-Sb_2Te_3films vary with the magnitude of the imposed strain. From this, one can judge the irreversibility of heterogeneous structures upon the imposition of deformation, i.e. The electronic structure of a heterogeneous semiconductor film changes strongly when a cyclic deformation is applied. **[8-11]**

CONCLUSION

Thus, from the above results, one can judge the irreversibility of heterogeneous structures upon deformation, i.e., the electronic structure of a nanocrystalline semiconductor film changes strongly when cyclic deformation is applied. It has been established that at sufficiently large

values of deformation ($\sim 2 \cdot 10^{-3}$)and a large number of superimposed deformation cycles, films that have the same $N_{ss}(\varepsilon,N)$ could be used as sensitive elements of low-cycle sensors of accumulated fatigue damage.

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