EFFECTS OF GRAIN SIZE ON THE CHARGE CARRIER MOBILITY OF BaSi₂ POLYCRYSTALINE THIN FILM

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I. INTRODUCTION

Polycrystalline semiconductors currently attract much attention because of their potential applications in microelectronics and the production of cheap thin-film solar cells. Their practical utilization depends on the crystal perfection of grains typical of polycrystalline films. Moreover changes of electronic properties at their boundaries should be carefully taken into consideration. Semiconducting silicides being well compatible with conventional silicon technology and promising for various applications are also known as environmentally friendly materials. Barium dislicide ($BaSi_2$) with the band gap of 1.15 – 1.30 eV [1], having rather large values of the absorption coefficient near the absorption edge and a large minority-carrier diffusion length in addition to a long minority-carrier lifetime can be viewed as a potential material for efficient conversion of sun's light to electricity [2]. $BaSi_2$ is also attractive not only for photovoltaic applications but for thermoelectric applications because of the large value of Seebeck coefficient [3]. There are some investigations devoted to the study of $BaSi_2$ basic electronic and optical properties [4], but at the same time there is almost the lack of information on the transport properties of the material under consideration. Thus the main purpose of our paper is to present the theoretical results how grain boundaries affect the carrier mobility in $BaSi_2$ polycrystalline thin films.

II. SIMULATION

Generally in semiconductors there are several standard well-known scattering mechanisms [5]. Each mechanism can be described by the complex function of meaningful physical values which can be treated as an appropriate set of parameters. In our case if one accounts for all the possible scattering mechanisms the resulting mobility according to the Mathiessen's formula is

$$1/\mu = 1/\mu_{AC} + 1/\mu_{NPO} + 1/\mu_{PO} + 1/\mu_{CIM} + 1/\mu_{GB},$$

where μ_{AC}, μ_{NPO}, μ_{PO}, μ_{CIM}, μ_{GB}, are partial mobility due to the carrier scattering on the acoustic phonons, nonpolar and polar optical phonons, charged impurity centers, and grain boundarys respectively. Previously this approach was used for a number of semiconducting silicides [6].

In the case of parabolic bands and nondegenerate charge carriers for each separate mechanism one has [6]

$$\mu_i = \frac{4q}{3m^*(kT)^{5/2}\sqrt{\pi}} \int_0^\infty E^{\frac{3}{2}} \tau_i \, epx\left(-\frac{E}{kT}\right) dE,$$

where m^* in the carrier effective mass (for electrons it to be 0.4 wise $m_{xx}=0.6$; $m_{yy}=0.37$; $m_{zz}=0.3$ in units of the free-electron mass [4]), q is the electron charge, T is the temperature, k is the Boltzmann constant, and τ_i is the momentum relaxation time of the i-th mechanism.

For acoustic phonon scattering the time is [5]

$$\tau_{AC} = \frac{\pi\hbar^4 q^2 \rho v_s^2}{\sqrt{2m^{*3}E}D^2 kT},$$

where ρ is the material density (3.54 g/cm³ [1]), v_s is the mean longitudinal sound velocity (4.1·10⁵ cm/s [3]), and D is a constant defined by the components of the deformation potential tensor. Usually for semiconductors its value varies from 5 to 15 eV [5].

For optical nonpolar phonon scattering the time is [5]

$$\tau_{NPO} = \tau_{AC} \left[C \left(1 + \frac{kT_0}{E} \right)^{\frac{1}{2}} + \exp\left(\frac{T_0}{T}\right)\left(1 - \frac{kT_0}{E} \right)^{\frac{1}{2}} \right]^{-1},$$

where $T_0 = \hbar\omega_o/k$, ω_o is the optical phonon frequency (493 cm^{-1} [7]) is the Debay temperature, $C = \eta/2\left(\frac{T_0}{T}\right)\left(\exp\left(\frac{T_0}{T}\right) - 1 \right)^{-1}$, and $\eta = (D_{NPO}/D_{AC})^2$. The latter ratio of the nonpolar optical deformation potential to the acoustic one is a parameter of our model.

The momentum relaxation time due to polar optical phonon scattering is [5]

$$\tau_{PO} = \sqrt{\frac{2^5 E}{m^*}} \frac{\pi\hbar^2\varepsilon_p}{kT_0q^2} \left\{ n(T_0)\left(1 + \frac{kT_0}{E} \right)^{\frac{1}{2}} + [n(T_0) + 1]\left(1 - \frac{kT_0}{E} \right)^{\frac{1}{2}} \right.$$
$$\left. + \frac{kT_0}{E}\left[(n(T_0) + 1)\operatorname{arcsinh}\left(\frac{E}{kT_0} - 1 \right)^{\frac{1}{2}} - n(T_0)\operatorname{arcsinh}\left(\frac{E}{kT_0} \right)^{\frac{1}{2}} \right] \right\}^{-1},$$

where, $n(\omega_0) = (\exp(\hbar\omega_0/kT_0) - 1)^{-1}$, $\varepsilon_P = (1/\varepsilon_{in} - 1/\varepsilon_0)$, ε_{in} and ε_0 are the high-frequency and the static dielectric constant ($\varepsilon_0 = 14.6$ [4]).

Currently, there are some models describing scattering by charge centers, such as the Brooks – Herring or Conwell – Weisskopf models [5] or recently proposed modified model by N.A. Poklonski at al.[8] But the all give one qualitavly the same results. For scattering by charge centers it was used the following [5]

$$\tau_{CIM} = \left[\frac{\pi N_{CIM}Z^2q^4}{\varepsilon_0^2 E^{\frac{3}{2}}\sqrt{2m^*}} \left\{ \ln(1 + x) - \frac{x}{1 + x} \right\} \right]^{-1},$$

where N_i is the charge centers concentration, Z – is the charge value of the center, $r_0 = (\varepsilon_0 kT/4\pi nq^2)^{1/2}$ – Debay screening radius, n – self carrier concentration ($5\cdot10^{15}$ cm^{-3} [10]).

Mobility in the case of scattering at grain boundaries is determined by expression [9]

$$\mu_{GB} = \frac{qL_D}{\sqrt{8m^*\pi kT}} \exp\left(-\frac{E_{GB}}{kT} \right),$$

where L_D – linear grain size, E_{GB} – value of the barrier at the grain boundaries.

Scattering at the grain boundaries is the dominant scattering mechanism in the low-temperature region with a low level of doping. It was shown in our recent paper [10] that with a relatively large magnitude of the potential barrier ($E_{GB} = 0.1$ eV, $L_D = 250$ nm), the mobility maximum shifts to higher temperatures (Figure 1). The magnitude of the potential grain boundary barrier depends on the concentration of free carriers in the grain, the structure, and the type of a grain. Technologically, it is possible to obtain grains of different sizes. We demonstrate in Figures 2 and 3 how the temperature dependence of the mobility of electrons varies with the grain size and the potential barrier at the boundaries. Thus, with increasing in the grain size, the mobility of electrons increases in absolute values at almost the same temperature of the maximum (Figure 2 a). With a further increase in the grain size the mobility maximum shifts toward lower temperatures (Figure 2 b) due to a decrease in the magnitude of the potential barrier at grain boundaries. At relatively high values of the potential barrier at the grain boundaries the grain size significantly affects the temperature dependence of the mobility of the carriers. As the grain size decreases and the potential barrier increases, the mobility begins decreasing in absolute values (Figure 3).
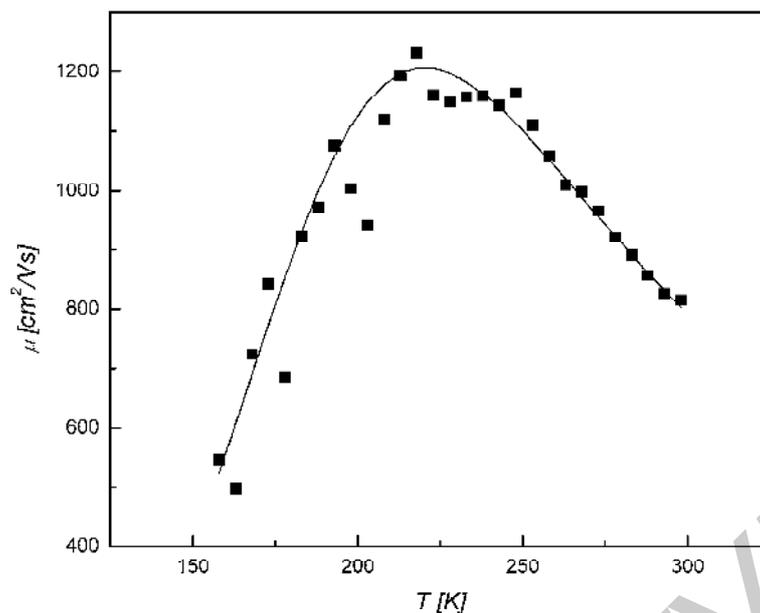
Figure 1 – Mobility versus temperature (experiment – black squares, simulation – the solid line [10])
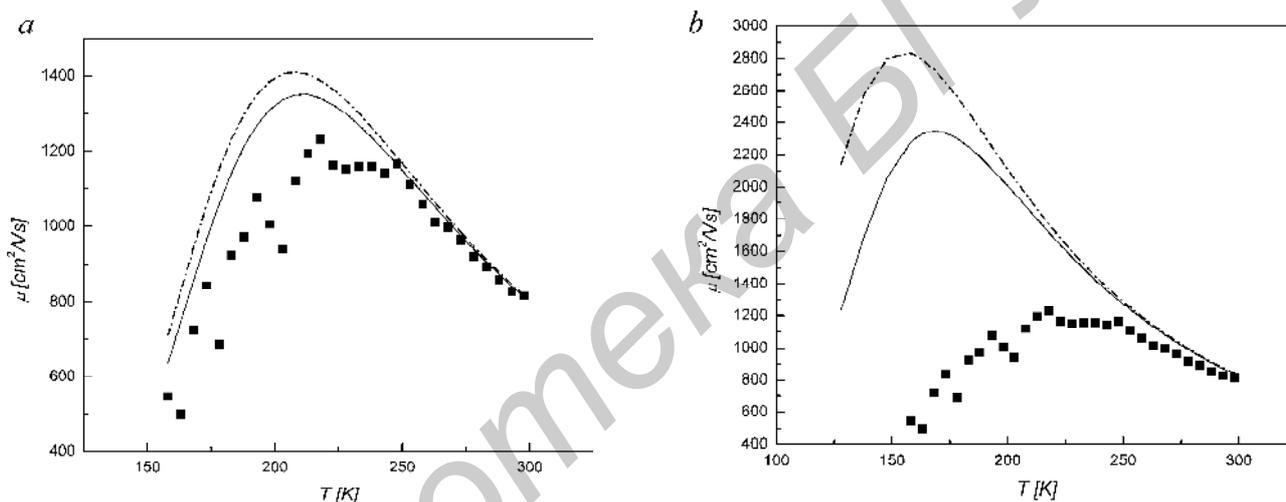

Figure 2 – Mobility versus temperature (experiment – black squares, simulation – the solid and dashed lines; a – L_D = 350 nm (the solid line), 400 nm (the dashed line), E_{GB} = 0.1 eV, b – L_D = 600 nm and E_{GB} = 0.08 eV (the solid line), L_D = 700 nm and E_{GB} = 0.073 eV (the dashed line)).
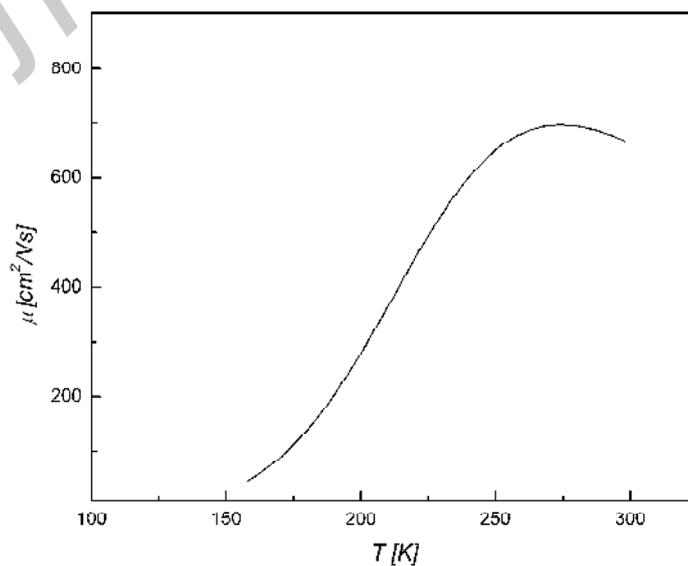

Figure 3 – Mobility versus temperature (L_D =200 nm, E_{GB} = 0.13 eV)

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III. CONCLUSIONS

Since it is technologically possible to control the gain size by varying doping concentration and deposition ratio of Ba and Si atomic fluxes, we suggest the grain size at room temperatures does not significantly affect values of electron mobility. The size of grains should be carefully considered only at low temperature. From the other side, the potential barrier at grain boundaries crucially decreases the maximum mobility values at the whole temperature range. We suppose the same tendencies to be observed in the case of hole as main carriers.

ACKNOWLEGMENTS

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AB INITIO SIMULATION OF GRAPHENE INTERACTION WITH SiO$_2$ SUBSTRATE FOR NANOELECTRONICS APPLICATION

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I. INTRODUCTION

Graphene is a promising material with high charge mobility [1-3]. The substrate material has a significant negative influence on the charge carriers mobility. Quartz well established as substrate in graphene technology. However, the mobility of charge carriers in such systems is worse than the theoretical calculations of a pure graphene sheet [2, 3]. The space charge inhomogeneity (so-called charge puddle) leads to degradation of the graphene electronic properties [4-6]. Physical characteristics leading to the occurrence of electron-hole puddles not identified uniquely [1, 4, 7]. Possible reasons for the formation of a charge puddle: open dangling bonds [8], point defects in the graphene layer [9-11], and charged impurities [12, 13].

The results of experimental work [14] prove that the presence of dangling bonds on the surface of the SiO$_2$ quartz substrate during the fabrication of the device may be the main reason for the occurrence of an electron-hole puddle in graphene.

Amorphous SiO$_2$ has various types of surface species. Therefore, impact of amorphous SiO$_2$ surface variety on the structure and electronic properties of graphene has been study in present theoretical investigation.

The α-quartz is the most stable polymorphic modification of SiO$_2$, and its most stable surface is (001) [15, 16]. Two typical quartz substrates were chosen for simulation. Ones have been with open oxygen (O$_{unsat}$) or silicon (Si$_{unsat}$) dangling bonds.

It is possible to passivate the broken bonds by substrate surface adsorbed hydrogen atoms for each of these types of bonds (Si$_{sat}$ and O$_{sat}$). In theoretical work [17] have been determined that the most stable is surface α-SiO$_2$ with the atomic configuration (0001) (O$_{sat}$). Calculations were performed by quantum-