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Simulation of incoherent radiation absorption in 3C-, 6H- and 4H-SiC at rapid thermal processing

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Abstract. For 3C-, 6H- and 4H-SiC polytypes of different conduction types and with various impurity concentrations we investigated absorption of incoherent radiation from the near IR spectral region at rapid thermal annealing. General regularities of both radiation absorption and sample heating are considered. We evaluated various processing modes; one should take this into account when developing technological procedures based on rapid thermal processing for SiC.

Keywords: rapid thermal processing, silicon carbide, incoherent radiation.

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1. Introduction

At present rapid thermal processing (RTP) with incoherent radiation [1-3] finds expanding applications in manufacturing of SiC-based electronic devices. Among its peculiarities is a possibility to activate chemical reactions at surfaces, as well as form insulating layers with high degree of structural perfection, refractory metal silicides, shallow *p-n* junctions using diffusion from a surface source [4]. Such features as practically complete recrystallization and impurity activation at implanted layers annealing, high efficiency at metallization annealing, simple design, small size and weight of technological equipment and high accuracy of control over processing modes make pulsed thermal processing promising for the silicon carbide technology [5-8].

However, use of RTP in the silicon carbide technology is retarded by the fact that regularities of absorption of incoherent radiation from the near IR region, as well as their effect on the heating modes for different SiC polytypes, are still inadequately studied. The objective of this work was investigation of peculiarities of incoherent radiation absorption by different SiC polytypes, with account made for emission spectrum of radiation sources and concentration of impurities in the substrate.

2. Absorption of radiation in SiC

The main parameter that describes interaction between radiation and semiconductor is the absorption coefficient. It depends on various characteristics of both radiation and material. The special feature of pulsed thermal processing of SiC structures by incoherent radiation is the dependence of radiation intensity ion wavelength (Fig. 1, curve 3). Let us now consider the mechanisms for radiation absorption in SiC.

The principal mechanisms for radiation absorption in semiconductors are as follows: (i) intrinsic absorption; (ii) absorption by free charge carriers; (iii) absorption involving localized states; (iv) excitonic absorption; (v) lattice absorption; (vi) intraband absorption; (vii) plasma absorption. One may neglect the (iv)-(vii) absorption mechanisms because they occur at low temperatures and high photon energies.

Thus, at heating SiC, incoherent radiation is absorbed according to the following three principal mechanisms: charge carrier transitions between the allowed bands; transitions between the localized states and allowed bands; excitation of the free charge carriers in the allowed bands.

When photon energy $h\nu$ is over the semiconductor gap, then intrinsic absorption of radiation occurs. The coefficient of intrinsic absorption α_i depends not only on the radiation wavelength, but also on temperature T, since the gap decreases with temperature. For SiC the corresponding dependence is of the following form:

$$E_g(T) = E_g(0) - bT \ . \qquad (1)$$

Here $E_g(0)$ is the gap value at $T = 0$ K; b is the temperature coefficient of gap [9].

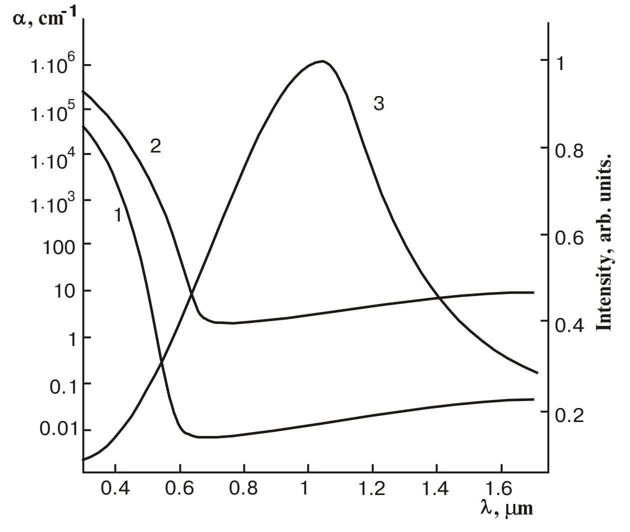

Fig. 1. Spectral dependence of absorption coefficient for nitrogen- doped ($N = 10^{15}$ cm^{-3}) 3C-SiC at 300 (1) and 1300 K (2) (left scale); emission spectrum of a halogen lamp (right scale).

The expression for the dependence of intrinsic absorption coefficient on photon energy and temperature (allowing for phonons) is as follows:

$$\alpha_i(h\nu,T)=A\left[\frac{\left(h\nu-E_g(T)-E_p\right)^2}{1-\exp\left(-E_p/kT\right)}+\frac{\left(h\nu-E_g(T)+E_p\right)^2}{\exp\left(-E_p/kT\right)-1}\right]$$

for $h\nu > E_g(T)+E_p$,

$$\alpha_i(h\nu,T)=A\left[\frac{\left(h\nu-E_g(T)+E_p\right)^2}{\exp\left(-E_p/kT\right)-1}\right]$$

for $E_g(T)-E_p < h\nu < E_g(T)+E_p, \alpha_i(h\nu,T)=0$

for $h\nu < E_g(T)-E_p$. (2)

Here E_p is the phonon energy; A is a constant. The phonon energy values for different SiC polytypes are given in [9].

The coefficient of radiation absorption by free charge carriers, α_e, is of the form [11]:

$$\alpha_e(h\nu,T,N)=\frac{n(N,T)e^3\lambda^2}{4\pi^2\left(m^*\right)^2\varepsilon_o n^* c^3\mu(N,T)}. \tag{3}$$

Here $n(N, T)$ is the free charge carrier concentration; N is the impurity concentration; m^* and $\mu(N, T)$ are the charge carrier effective mass and mobility, respectively; n^* is the refractive index; ε_0 is the permittivity; e is the elementary charge; c is the speed of light. The coefficient of radiation absorption by free charge carriers depends on T, since the charge carrier concentration grows with temperature [12]. For SiC the charge carrier mobility is determined predominantly by their scattering on acoustic phonons and ionized impurity atoms; it decreases with temperature [9,13].

The expression for the coefficient α_d of radiation absorption at localized states (taking into account that in SiC the principal localized states are those due to impurity atoms) is of the following form [10]:

$$a_d(h\nu,T,N)=B\frac{N}{E_I}\left[\frac{E_I}{h\nu}\right]^4\times$$
$$\times\frac{\exp[4(1-E_I/h\nu)]\arctan(1-E_I/h\nu)}{1-\exp[2\pi(E_I/h\nu-1)]}. \tag{4}$$

Here E_I is the impurity ionization energy (its values for different impurities are given in [9]); B is a constant.

The general expression for radiation absorption coefficient in SiC is a sum of expressions (2)-(4). As an example we show in Fig. 1 the calculated (using the above technique) spectral dependence of the radiation absorption coefficient for 3C-SiC doped with nitrogen ($N = 10^{15}$ cm^{-3}) at temperatures of 300 and 1300 K. An analysis showed that the results of calculations agree with the known regularities in behavior of the spectral dependence of the radiation absorption coefficient for semiconductors: when temperature and impurity concentration grow, then the intrinsic absorption edge shifts to longer wavelengths and absorption intensity increases (that is most pronounced beyond the intrinsic absorption edge).

An analysis of regularities in the absorption of incoherent radiation is complicated by the fact that emission intensity of the radiation sources used (halogen lamps at RTP) depends on the radiation wavelength (see Fig. 1), so its spectral dependence should be taken into account. To this end an integral absorption coefficient was introduced in [14] for radiation absorption in a semiconductor wafer. It is of the following form:

$$A_t(T,N)=\frac{\int_{\lambda_1}^{\lambda_2}(1-R)(1-\exp[-\alpha(\lambda,T,N)D])I(\lambda)d\lambda}{\int_{\lambda_1}^{\lambda_2}I(\lambda)d\lambda}. \tag{5}$$

Here R is the reflection coefficient (for the wavelength range considered, λ_1-λ_2, we took $R = 0.22$ [9]); $\alpha(\lambda, T, N)$ is the absorption coefficient; D is the wafer thickness (we took $D = 0.033$ cm); $I(\lambda)$ is the spectral dependence of the incoherent emission intensity for a radiation source.

Using the above model, we calculated the temperature dependency of the integral absorption coefficient for different SiC polytypes (3C, 6H and 4H) with different conduction types and various impurity concentrations.

Nitrogen (boron) was taken to be the donor (acceptor) impurity. The results of calculations are given in Figs. 2-4.

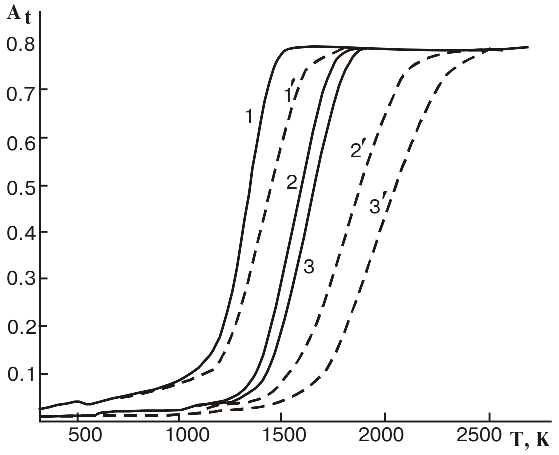

Fig. 2. Temperature dependence of the integral absorption coefficient for *n*- (1, 2, 3) and *p*-type (1′, 2′, 3′) wafers: 1, 1′ – 3C-SiC; 2, 2′ – 6H-SiC; 3, 3′ – 4H-SiC. (Impurity concentration $N = 10^{15}$ cm^{-3}.)

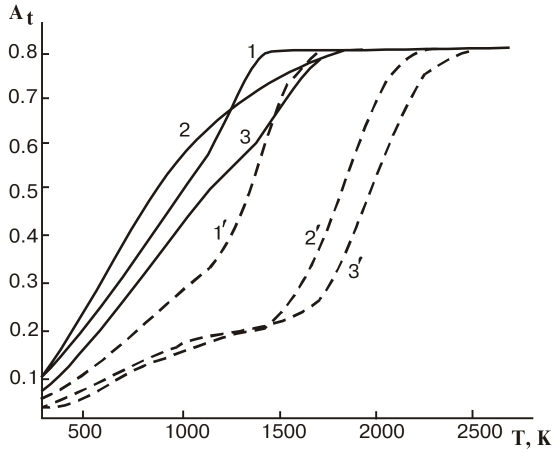

Fig. 3. The same as in Fig. 2 but at $N = 10^{17}$ cm^{-3}.

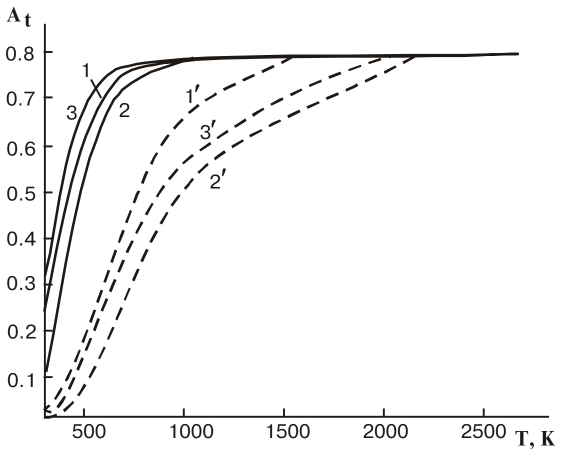

Fig. 4. The same as in Fig. 2 but at $N = 10^{18}$ cm^{-3}.

3. SiC heating with incoherent radiation

Absorption of incoherent radiation by a semiconductor wafer is accompanied with material heating. When considering it, one should take into account losses due to radiation and convective heat transfer. At long-term (over 10^{-2} s) processing the temperature is uniformly distributed over the wafer thickness [4,5,8]. The maximum temperature value may be estimated from the heat balance equation:

$$DC(T)\rho\frac{dT}{dt} = WA_t(T,N) - 2\sigma\varepsilon\left(T^4 - T_0^4\right) - 2\alpha(T - T_0). \qquad (6)$$

Here D, $C(T)$, ρ, ε, α and σ are the wafer thickness, specific heat, density, emissivity, coefficient of convective heat transfer and the Stefan-Boltzmann constant, respectively [9, 15]; W is the radiation power density of the radiation source; T_0 is the ambient temperature.

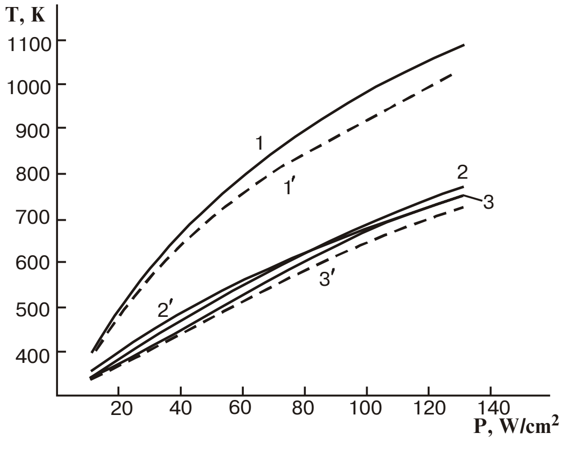

Fig. 5. Heating temperature vs radiating power density for *n*- (1, 2, 3) and *p*-type (1′, 2′, 3′) wafers: 1, 1′ - 3C-SiC; 2, 2′ - 6H-SiC; 3, 3′ - 4H-SiC. (Impurity concentration $N = 10^{15}$ cm^{-3}.)

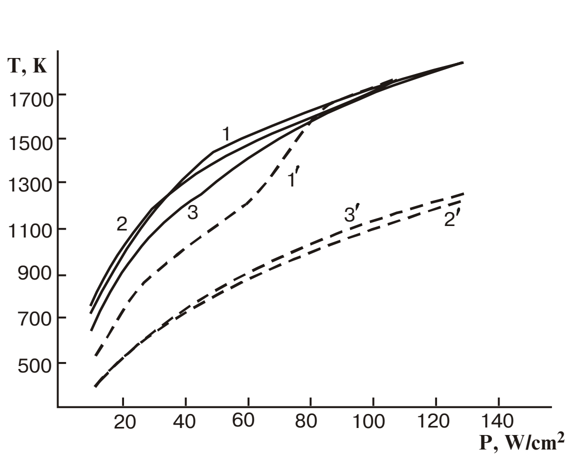

Fig. 6. The same as in Fig. 5 but at $N = 10^{17}$ cm^{-3}.

The results of our calculations of heating temperature at RTP made for a SiC wafer 0.033 cm thick are shown in Figs. 5-7. The calculations were performed for the heat balance mode. Different source specific power

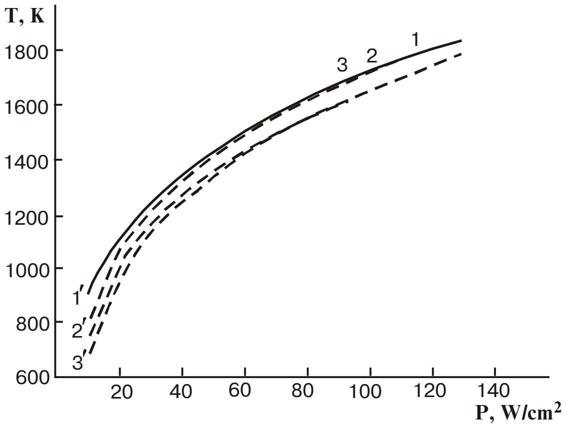

Fig. 7. The same as in Fig. 5 but at $N = 10^{18}$ cm^{-3}.

values were used; this enabled us to change the heating rate from 10^0 up to 10^2 K/s.

4. Discussion of results

From an analysis of the results of calculations made for the wavelength range studied one may conclude that:

- for low-doped SiC the absorption of incoherent radiation from the near IR region at early stages of heating is insignificant and depends on temperature but slightly. An abrupt increase in absorption is observed at temperatures over 1100 K due to a growth of the free charge carrier concentration and gap decrease;
- as the dopant concentration is increased, the absorption of incoherent radiation grows at early stages of heating;
- the temperature dependence of the charge carrier concentration strongly affects absorption of incoherent radiation in SiC at RTP;
- at high temperatures the wafer transmission coefficient approaches zero. The temperature, at which the maximum absorption begins, decreases with charge carrier concentration in the wafer;
- absorption in *n*-SiC is bigger than that in *p*-SiC. The explanation is that activation energy of donor impurities in SiC is lower than that of acceptor impurities, and so at early stages of heating the charge carrier concentration in *n*-SiC is higher than in *p*-SiC [9];
- absorption of incoherent radiation in b-SiC is over that in a-SiC. Absorption of incoherent radiation in 6H-SiC is over that in 4H-SiC. This is due to smaller gap width (and so higher charge carrier concentration) [9];
- for SiC wafers with doping level below 10^{17} cm^{-3} both impurity type and concentration, as well as polytype, strongly affect the heating temperature. At higher doping levels this effect becomes small.

Conclusion

An analysis of the results obtained shows that, when developing new technological procedures involving RTP for SiC, one should take into account the integral absorption coefficient of the SiC polytype used, radiation wavelength, type of conduction and impurity concentration in the wafer. This will enable one to retain crystal structure and phase composition, as well as circumvent extra stresses in SiC structures at RTP.

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