Fundamental Mechanisms and Doping Effects in Silicon Infrared Absorption for Temperature Measurement by Infrared Transmission

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ABSTRACT

Infrared absorption in silicon has been investigated at elevated temperatures. The fundamental absorption process in lightly to moderately doped silicon at 1.3 and 1.55 μm have been identified as band-to-band and free carrier mechanisms, respectively. The effects of heavy substrate doping on absorption at elevated temperature have also been studied. Significant deviations (10%) from transmission vs. temperature, as used to measure temperature in a Rapid Thermal Processing system, begin to occur with substrate doping levels of $\sim 10^{18}$ cm^{-3}.

INTRODUCTION

Temperature measurement in Rapid Thermal Processing (RTP) systems, especially in the low-temperature (<900 °C) range, has long been a problematic issue. It has recently been demonstrated, however, that the temperature of silicon wafers can be probed non-invasively in a RTP system by measuring the infrared transmission of the wafer. The method does not require knowledge of the emissivity and has a demonstrated accuracy on the order of a few degrees [1]. The method has also been applied to RTP silicon homoepitaxy and the growth of silicon-germanium strained layers on silicon substrates [2,3]. Details of the technique and the experimental apparatus (fig. 1) can be found in the literature [1-3]. In this paper, the fundamental absorption processes are investigated, and the effect of heavy substrate doping on transmission vs. temperature is presented.

INFRARED ABSORPTION IN SILICON

Near-infrared absorption in silicon proceeds primarily by two processes: electron transitions across the bandgap from the valence band to the conduction band (band-to-band absorption), and free carrier absorption by both electrons and holes. Free carrier absorption is an increasing function of temperature for two reasons. First, the absorption cross section increases with temperature, having roughly a linear dependence up to 400 K [4],

$$\sigma(T) = 1.5\times10^{-20} \cdot T \cdot \lambda^2 \text{ cm}^2 \qquad (1)$$

where σ is the total cross section for electrons and holes, λ is the wavelength in microns, and T is the temperature in K. For the simple modelling in the rest of this paper, we will assume this relationship is true up to 850 °C. Based on the room temperature absorption data of [5], 2/3 of the absorption coefficient will be attributed to electrons, and 1/3 to holes. Second, as the temperature increases, the intrinsic carrier concentration of silicon increases. This will lead to an increased carrier concentration when the intrinsic concentration rises above the doping level. The carrier concentration can easily be calculated using the well known relationships of intrinsic carrier concentration on temperature and bandgap, and the temperature dependence of the bandgap [6]. It should also be pointed out that free carrier absorption has approximately a λ^2 dependence on wavelength, i.e. decreasing as the photon energy increases.

The second dominant absorption mechanism is band-to-band absorption. Because of the indirect nature of the bandgap, such absorption in silicon requires a phonon, and hence increases strongly with temperature. This process also increases at elevated temperature because of the reduction in the bandgap. Macfarlane et al [7] have determined that this process proceeds with both transverse and longitudinal acoustic phonons in the <100> direction, which may either be absorbed or emitted. They developed a quantitative model of the four possible optical absorption processes (transverse or longitudinal acoustical phonon, emission or absorption), which was simplified by Jellison et al [8] to assume parabolic bands. Good agreement with absorption data at 1.15 μm up to 1140 K was found. The details of the model are not repeated here for brevity, but can be found in [8]. Since the density of states increases with distance from the band edge, band-to-band absorption near the band edge increases strongly with the photon energy.

The predictions of the above models for free-carrier and band-to-band absorption were then compared to data to gain insight into the dominant mechanisms at 1.3 and 1.55 μm and to determine the effect of doping on the infrared transmission technique for measuring temperature. It should be stressed that the numerical modelling was done only to gain insight into the physical processes, and not to accurately reproduce the experimental results. Therefore, no parameters were adjusted from the models stated above, and more complicated physical effects, such as absorption by impurity (dopant) levels or heavy doping effects on the bandgap, were not incorporated into the modelling.

FUNDAMENTAL ABSORPTION PROCESSES IN LIGHTLY DOPED SILICON

To perform measurements of transmission vs. temperature, it is necessary to have an independent measure of temperature. Therefore for the data described in this paper, measurements were not made using the RT-CVD apparatus in fig. 1. Instead, the measurements were made in a conventional furnace which was adapted for infrared transmission measurements. The optical path was perpendicular to the length of the quartz furnace tube, and the temperature was measured as conventionally done with a calibrated thermocouple. The estimated error in temperature was +/- 2 °C. Because of drifts in the optical alignment at high temperature, the error bars in the transmission are +/- 20%. To remove dependences on laser power, detector efficiency, etc, all transmitted signals at elevated temperature are normalized (divided) by their room temperature values where the wafers are virtually 100% transparent, as described in [1]. (For heavy dopings, the wafers are not 100% transparent at room temperature. This is discussed further in the next section.) From this normalized transmission, n(T) (which is by definition less than one), one can easily extract the absorption coefficient at elevated temperature:

$$\alpha(T) = -1/d \cdot \ln(n(T)) \tag{2}$$

where d is the wafer thickness. The results for a lightly doped p-type wafer are shown in fig. 2. Also shown are the predictions of the models for free-carrier, bandgap and total absorption constants. The model results are in excellent agreement with the data. No parameters were adjusted from the models given earlier. It is clear from the model results in fig. 2 that the dominant absorption process at 1.3 μm at elevated temperature is band-to-band absorption. The results are very different at 1.55 μm. Because of the lower photon energy, bandgap absorption at 1.55 μm is practically negligible over the temperature range of interest. Therefore, at 1.55 μm the dominant absorption process in silicon up to 850 °C is free-carrier absorption.

These hypotheses can be confirmed by measuring the wavelength dependence of the absorption coefficient at these two different wavelengths. This was done by changing the temperature of the source lasers to vary the wavelengths by approximately 10 nm. The results are shown in fig. 3. (This data was taken in a furnace in which the thermocouple was not accurately calibrated, and hence should not be directly compared to that of fig. 2). At 1.3 μm, a ~10 nm decrease in the wavelength results in a distinct increase in the absorption coefficient, since the photon energy is now sufficient to promote bandgap absorption at a larger bandgap and hence lower temperature. The dependence of the absorption coefficient at 1.5 μm is much weaker than that at 1.3 μm, but a slight decrease in absorption results as the wavelength is decreased. Such a decrease is consistent with the λ^2 dependence expected for free carrier absorption.

These results are important for the extension of the technique to other wavelength and/or temperature ranges. For example, for temperature measurement in the 800 °C range, the 1.5 μm signal would be used because of the negligible transmission at 1.3 μm (absorption coefficient too high). (See fig. 4, for example). Over 850°C, however, the transmitted signal at 1.55 μm would also be too weak to be of practical use. One might consider then using a different wavelength with weaker absorption at elevated temperature than that at 1.55 μm. Since free-carrier absorption dominates at 1.55 μm, near 1.55 μm lower absorption will occur at shorter, not longer, wavelengths. However, because of the strong dependence of bandgap absorption on wavelength, the total absorption at 1.3 μm is already much greater than that at 1.55 μm. Because of the fairly weak decrease of free carrier absorption with wavelength (λ^2), at most a ~30% decrease in absorption coefficient is expected at some intermediate wavelength between 1.3 and 1.55 μm. Therefore it appears unlikely that the infrared transmission technique for measuring temperature can be extended significantly beyond 850 °C. On the other hand, to extend the method to lower temperatures will require a stronger dependence of transmission on temperature at low temperature than that at 1.3 μm (see fig. 4, for example). This will require a stronger absorption coefficient at low temperature. This can be achieved by increasing the photon energy, leading to increased bandgap absorption at lower temperatures.

DOPING EFFECTS

Ideally, one would like to have a single normalized transmission vs. temperature relationship for all substrates. However, because doping affects carrier concentration vs. temperature, and because heavy doping can lead to significant free-carrrier absorption at room temperature, one expects the transmission vs. temperature relationship to depend on the substrate doping. (For example, at room temperature the 1.3 μm absorption length ($1/\alpha$) in an n-type wafer with doping 3 x 10^{18} cm^{-3} is ~500 μm, roughly the thickness of a typical four-inch wafer.) Normalized transmission vs. temperature data for p-type wafers with doping levels ranging from 9 x 10^{14} to 7 x 10^{18} cm^{-3} are shown in fig. 4. Within the error bars of the measurements (mentioned in the previous section), the normalized transmission of a wafer with moderate doping (4 x 10^{16} cm^{-3}) is indistinguishable from that of a lightly doped wafer, but a large decrease in transmission occurs for a doping level ~10^{19} cm^{-3}. Qualitatively similar results are also predicted by the combined free carrier/bandgap absorption model (fig. 5).

The decreased normalized transmission for heavy doping is caused by free carrier absorption. The normalization procedure removes the effect of the extra free carriers at low temperature (i.e. near the normalization temperature), but because the free-carrier absorption cross section increases with temperature, the free carriers significantly reduce the normalized transmission at elevated temperature. Based on simulations, these effects are not expected to become significant until doping levels are in 10^{18} cm^{-3} range. When using the infrared transmission technique in practice to measure temperature, one usually operates on the "steep" portion of the normalized transmission curve, i.e. greater than 500 °C for the 1.3 μm signal and greater than 650 °C for the 1.5 μm signal. When using the technique as such, the error in extracted temperature due to substrate doping variations is expected to be less than 3 degrees for substrate dopings up to 5 x 10^{17} cm^{-3}.

SUMMARY

The fundamental absorption modes in silicon at elevated temperature have been identified as band-to-band absorption at 1.3 μm, and free carrier absorption at 1.55 μm. Based on this information, it appears possible to extend the infrared transmission technique for measuring temperature in RTP systems to temperatures under 500 °C, but extension to temperatures significantly in excess of 850 °C appears difficult. High levels of substrate doping decrease the normalized transmission compared to lightly doped wafers due to the temperature dependence of free carrier absorption, but for practical purposes this affect is negligible for substrate doping levels up to 5 x 10^{17} cm^{-3}.

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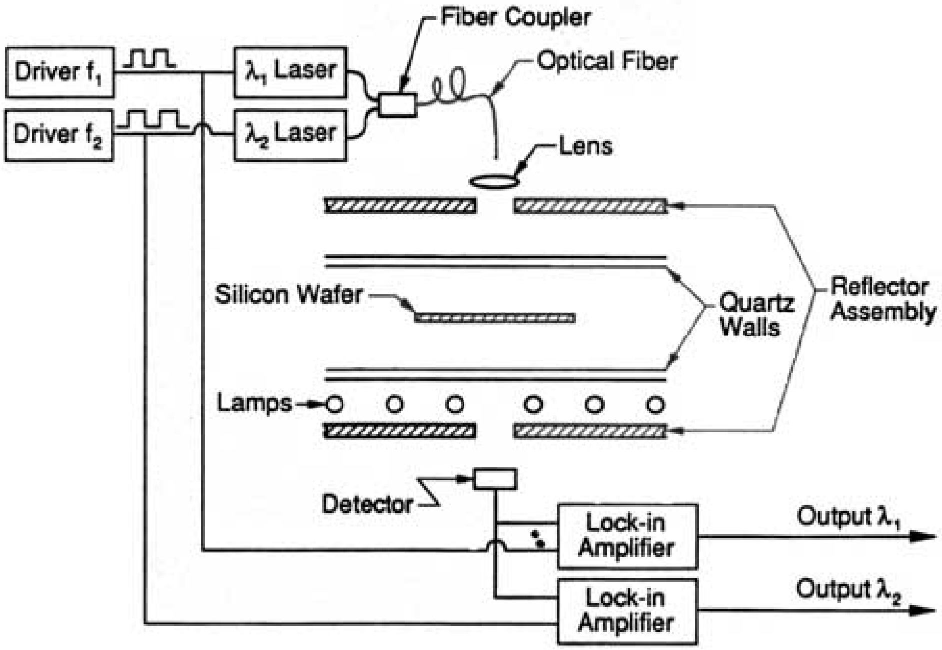

Fig. 1. Experimental RTP chamber modified for temperature measurement by infrared transmission.

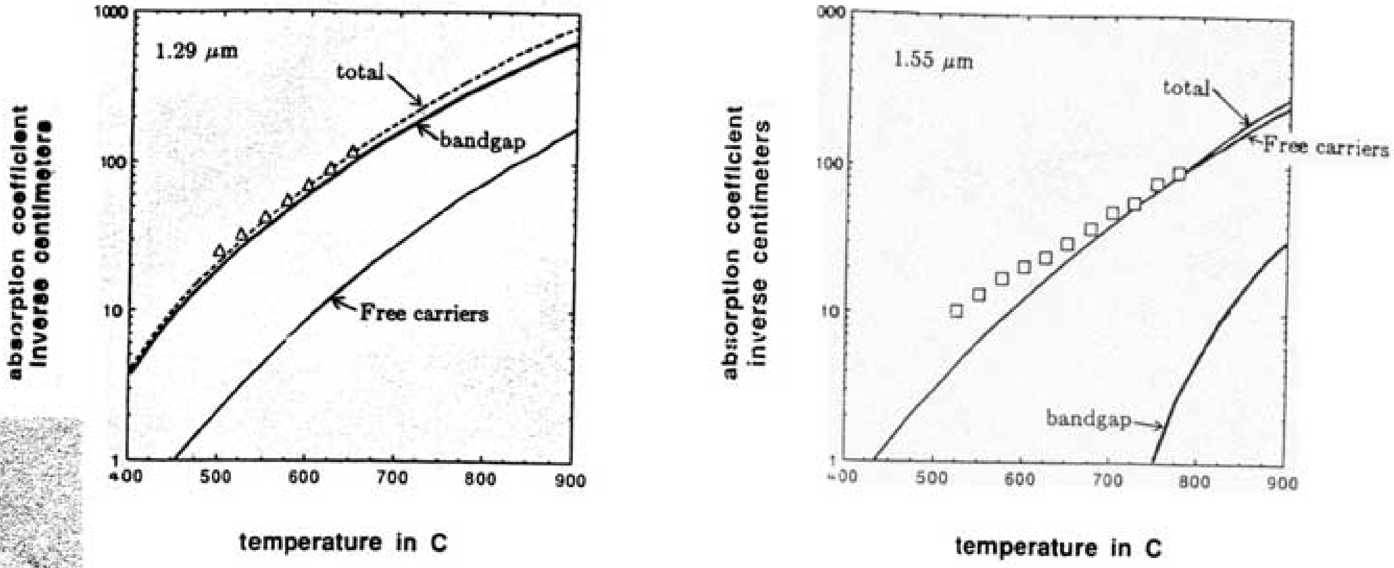

Fig. 2. Data for absorption coefficient in a lightly doped p-type wafer (10-50 Ω-cm) and model results for free carrier and bandgap absorption at (a) 1.30 μm and (b) 1.55 μm.

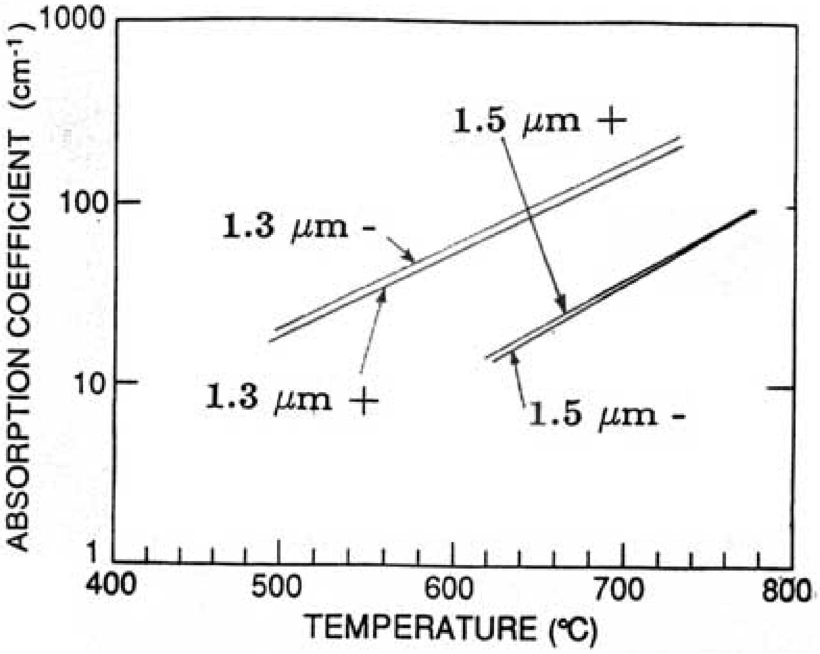

Fig. 3. Absorption coefficient vs. temperature for a lightly doped p-type wafer for small (~10nm) shifts in wavelength. Subscripts + and - indicate larger and smaller wavelengths, respectively.

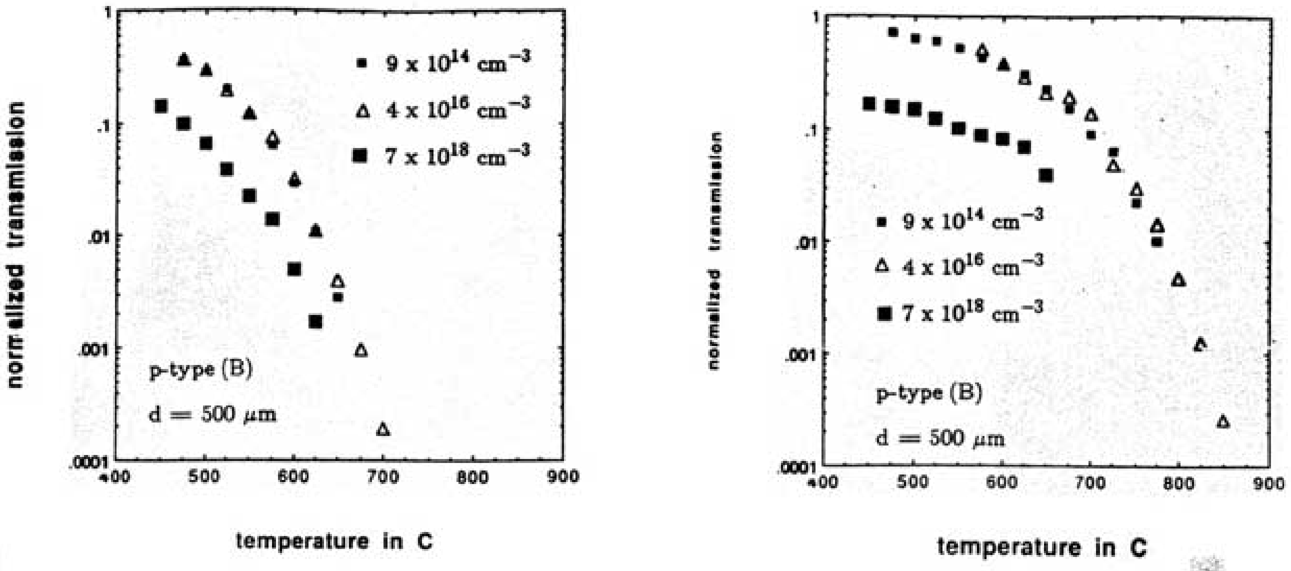

Fig. 4. Normalized transmission vs. temperature data for various p-type substrate dopings at (a) 1.3 μm and (b) 1.5 μm. The data has been corrected to reflect a 500-μm wafer thickness, and the normalization temperature is 50 °C.

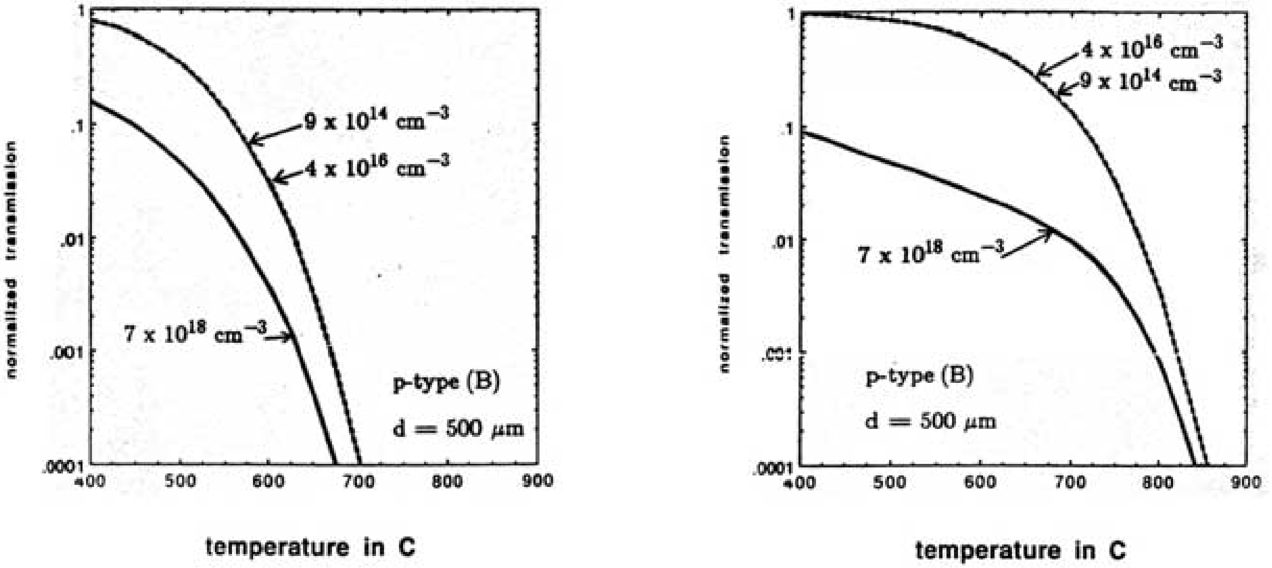

Fig. 5. Modeled normalized transmission vs. temperature for 500-μm p-type wafers with various substrate dopings.