Temperature Measurement of Metal-Coated Silicon Wafers by Double-Pass Infrared Transmission

Charles W. Cullen and James C. Sturm, Member IEEE

Abstract—We report the measurement of the temperature of metal-coated silicon wafers by a double-pass infrared transmission technique. Infrared light incident on the backside of the wafer passes through the wafer, and is re-emitted out the backside after reflecting off the metal surface on the front side of the wafer. The temperature is inferred by the change in the re-emitted signal due to absorption in the wafer. The work has been demonstrated on double-polished wafers from 100°C to 550°C using wavelengths from 1.1 to 1.55 μm. A method for overcoming limitations of the present arrangement for wafers with a rough backside is proposed.

I. INTRODUCTION

The measurement of the temperature of a silicon wafer is crucial for accurate control of integrated circuit manufacturing processes. This problem is especially difficult in nonequilibrium environments, such as inside a rapid thermal processing (RTP) tool. Thermocouples do not provide a good measure of the wafer temperature unless intimately attached to the wafer, and hence are not practical for large-scale manufacturing. Pyrometry depends on accurate knowledge of the emissivity, which depends on wavelength, temperature itself, wafer polish, substrate doping, and surface coatings such as field oxides [1], [2]. Errors well over 50°C are easily possible [3]. In addition, in an RTP tool, pyrometry is further complicated by interference from the heating lamps and emission from warm windows into the process chamber. In this paper a new technique, temperature measurement by double-pass infrared (IR) transmission, is presented for the temperature measurement of wafers which are blanket-coated with metal. The first experimental results of the technique are reported, and the capabilities and potential limitations of the technique are discussed.

Because of the strong dependence of the optical absorption of silicon on temperature in the near-infrared, it has been demonstrated that the temperature of a silicon wafer can be measured by monitoring the transmission of 1.3 μm and 1.55 μm light through the wafer inside an RTP reactor from 550°C to 800°C with an accuracy on the order of 1°C [4], [5]. By high frequency modulation of the semiconductor laser light sources and the use of lock-in amplifiers, the effect of lamp interference on the measurement is avoided. The effect of the scattering on the light due to the rough wafer backside was overcome by normalizing the measurements on each wafer to the initial "cold" (i.e., room temperature) transmission through the wafer. The independence of this normalization on the exact "cold" temperature is discussed in Section II.D. Due to the increase of both the interband (bandgap) and the intraband (free-carrier) absorption at high temperatures, so little light was transmitted through the wafer at any wavelength above 850°C that the technique was not practical above this temperature [6]. However, by moving to shorter wavelengths and larger bandgap absorption, in principle the technique is extendable to temperatures below room temperature [7]. The initial work on this IR transmission technique was performed on bare silicon wafers (or wafers with patterned oxide holes) and was applied to blanket or selective silicon or silicon-germanium epitaxy.

In industrial manufacturing, however, epitaxy is rarely performed under 800°C, and many thermal processing steps below 800°C involve metal layers. In such steps, like a Self-Aligned silicid (SALicid) formation process, there is often a blanket (unpatterned) layer of metal on the wafer. Such a blanket layer of metal will prevent any photons from an IR probe beam from being transmitted through the wafer, with the result that the IR transmission technique described above cannot be used to measure the wafer temperature. We therefore have developed a modified version of the technique, double-pass infrared transmission, to apply to such situations.

II. TEMPERATURE MEASUREMENT EXPERIMENTS

A schematic diagram which illustrates the double-pass technique is shown in Fig. 1. The probe beam is incident on the wafer backside, while the frontside is coated with metal. Part of the incident beam is reflected from the surface (an undesired parasitic in our work) and part is transmitted into the wafer. The beam inside the wafer will be reflected by the metallized top surface of the wafer, and transmitted back through the
wafer to re-emerge out the backside. The strength of this double-pass signal re-emitted out the back of the wafer as a function of temperature $T$, $t_{DP}(T)$, can be modeled by

$$t_{DP}(T) = K \cdot R_{M}(T) \cdot T_H(T) \cdot e^{-\alpha(T) \cdot l}$$

(1)

where $R_{M}(T)$ is the reflectivity at the top metal surface, $T_H(T)$ is the power transmission coefficient of the back air-silicon interface, $l$ is the path length through the wafer, and $\alpha(T)$ is the absorption coefficient, and $K$ is a constant which represents the laser power, any scattering at the back interface due to a rough surface, and other factors which are not a function of temperature. It can easily be shown by Snell’s law that the path length through the wafer, $l$, is

$$l = 2 \cdot d \cdot \left[1 - \frac{\sin^2(\theta_{inc})}{n^2}\right]^{-1/2}$$

(2)

where $d$ is the wafer thickness, $\theta_{inc}$ is the angle of incidence of the probe beam, and $n$ is the index of refraction of the silicon wafer. This double-pass signal $t_{DP}$ will be a strong function of temperature due to the temperature dependence of the absorption. However, the direct reflection of the original probe beam from the wafer backside, $r_{dir}$, will only be a very weak function of temperature, due to the relatively small dependence of $n$ (and hence the reflection coefficient) on temperature [8]. The detector will sense both the undesired direct reflection $r_{dir}$ which minimizes the directly reflected beam.

One might choose to minimize the directly reflected beam by an anti-reflection coating. However this complicates manufacturing, and the design of such a coating might be difficult if multiple wavelength probe beams were used. Therefore we have chosen to minimize the directly reflected beam by using polarized incident light (or a polarizer in front of the detector) and incidence at Brewster’s angle ($\theta_B = \arctan(n)$). On a polished surface, the reflection coefficient for p-polarized light is thus zero. In the near infrared ($\lambda \approx 1.3 \mu m$), the index of refraction of silicon is 3.50 [8], corresponding to $\theta_B = 74^\circ$. In this case the path length of the transmitted beam inside the wafer becomes $l = 2.08 \cdot d$. Note that under such operating conditions to minimize the reflection at the back silicon-air interface, the neglect of multiple reflections of the probe beam inside the wafer is justified, as was implicitly done in (1).

Nearly all our experiments were performed in an apparatus as shown in Fig. 2. The edges of the silicon sample (typically 525-μm thick and about 50 mm across) rested on top of small quartz rods of ~1 mm diameter, which in turn rested on top of a resistive heater inside a vacuum chamber. The wafers were p-type with a resistivity of 10-50 Ω-cm with a (100) orientation. The metallized frontside of the wafer was placed face-down onto the quartz rods toward the heater. A small hole in the resistive heater (~2 mm diameter) and borosilicate glass windows in the top and bottom of the chamber allowed for transmission measurements at normal incidence, which were not used in this study. Borosilicate glass windows on the sides of the chamber were used for the double pass experiments described in this paper. Semiconductor laser sources were used at 1.18, 1.3, and 1.55 (±0.01) μm, and were all modulated near 10 KHz. Each had a power on the order of 100 μW. The lasers were all coupled into a single multimode optical fiber. A collimating lens merged into the fiber was used to project the light onto the wafer, with a far-field divergence of under 1°. The distance of the fiber lens and the detector from the wafer was about 20 cm. A single InGaAs semiconductor detector and a broad-band infrared polarizer were used. Lock-in amplifiers were used to independently recover the signals from each source laser. The actual wafer temperature was measured by a thermocouple attached to the wafer by high temperature epoxy at a point about 10 mm away from the point being probed. The repeatability of the temperature measurement was about ±8°C, and the error in the measurement of the detected optical signal was about ±15%. Over the “steep” part of curves of normalized transmission versus temperature in Fig. 3, this ±15% would cause an error in the inferred temperature of ±5°C.

The first set of experiments was performed on double-polished wafers, i.e., with a polished backside. Brewster’s angle was experimentally determined by minimizing the detected signal from a wafer without a metal coating, so that there would be no strong reflection of the double pass signal from the metal on the wafer front side. Direct reflectivities from the wafer backside (compared to direct reflection from a metal surface) as low as 10^{-4} were achieved, with typical values in experiments less than 10^{-3}. This means that the contribution
of the undesired direct reflection to the desired double-pass signal was at most 10% even when the desired signal was reduced to 0.01 of its low temperature value to absorption at high temperature. The metal layers used for the experiments were either aluminum (0.15 μm) or platinum (0.2 μm). A few measurements were made at 1.1 μm using a different experimental arrangement. The 1.1 μm radiation was obtained by filtering a broad-band IR source (heated filament) with a monochromator. Due to the uncertainty in the monochromator calibration (±0.05 μm), these data points are not as reliable as those at the longer wavelengths.

The data of the double-pass transmitted signal versus temperature from 100°C to 550°C for wavelengths of 1.1 to 1.55 μm are shown in Fig. 3. The actual detected signal is normalized by its low temperature value to give a "normalized transmission," n(T). The laser power, etc., (represented by K in (1)) are not a function of temperature, and the transmission and reflection coefficients at an air–silicon interface are also a very weak function of temperature due to the weak dependence of the index of refraction of silicon on temperature [8]. If one assumes that the metal reflectivity RM is also a constant (discussed in Section III), n(T) depends only on the absorption coefficient

\[ n(T) = e^{-2.08 \cdot \alpha(T) \cdot d}. \]  

Note that the normalized detected signal decreases strongly at high temperature at all wavelengths, and also decreases sharply as the wavelength is decreased. Since the dominant absorption for wavelengths 1.18 and 1.3 μm is absorption across the bandgap, which increases strongly as wavelength is decreased, these results qualitatively support the fact that we are indeed measuring the desired double-pass transmission and not some parasitic reflection. Further evidence of this result was obtained by numerically modeling the double pass transmission using (3) and the model for absorption coefficients as a function of temperature and wavelength [6], which has been shown to accurately model single pass normalized transmission at 1.3 and 1.55 μm [6]. The modeling (with no adjustable parameters) is shown in Fig. 3 along with the data. Good agreement is obtained, confirming that the desired double-pass signal is indeed being measured.

By varying the probe wavelength from 1.1 μm to 1.55 μm, our experiments demonstrated the capability of measuring temperature in the range of 100–550°C. The upper temperature was limited by our experimental apparatus. As implemented, the technique is limited to a normalized transmission greater than 10^{-2} because of concerns about the significance of direct reflection. Based on the absorption coefficient model [6], by using 1.55 μm (the wavelength at which absorption at high temperature is a minimum) and our experience at 1.55 μm with single-pass measurements [4], one should be able to extend the upper temperature limit of the technique to 720°C. Over a large part of the range of data, at each wavelength the dependence of the normalized transmission on temperature is 2%/°C or greater. Therefore detecting a 1°C change in temperature requires observing a 2% relative change in the normalized signal, easily within the range of the technique.

### III. Practical Concerns

The previous section demonstrated the feasibility of measuring the temperature of double-polished metal-coated silicon wafers by double-pass infrared transmission in benchtop experiments. In this section we examine various practical concerns, encountered when extending the technique to a practical implementation inside a rapid thermal processor. These issues include lamp interference, substrate doping and thickness, optical alignment concerns, variation of the metal reflectivity, rough wafer backsides, and a comparison to other methods.

#### A. Lamp Interference, Substrate Doping and Thickness, Optical Alignment, and Metal Reflectivity

In a RTP, the heating lamps emit light in the same wavelength range as that used by the probe beams, and some lamp radiation will probably reach the detector even if shielding is implemented. However, because of the low frequency of the lamp variations compared to the modulation frequency of the lasers (10 KHz), one can easily separate these signals. This has indeed been demonstrated in a single-pass system in routine use for rapid thermal chemical vapor deposition [4], [5].

The measurements presented here were performed on lightly-doped substrates. We have previously shown in single-pass transmission experiments (without metal) that the IR transmission is independent of substrate doping up to substrate doping levels of ~10^{18} cm^{-3} [6]. Wafers which are heavily doped, such as those used in p^+ substrate/p^+ epi applications, have a significantly higher absorption than lightly doped substrates at room temperature due to free carrier absorption. Even after normalization, the normalized transmission versus temperature curves for these wafers are substantially different than that for lightly doped substrates [6]. Therefore, a universal normalized transmission versus temperature curve cannot be used for substrates with doping over 10^{18} cm^{-3}. n^+ or p^+ surface layers were found to have little effect, however.

The technique of temperature measurement by IR transmission of course depends on the knowledge of the substrate thickness. From (3) it is clear that the relationship between an error in the wafer thickness (Δd) and the error in the inferred absorption coefficient (Δα) is

\[ \frac{\Delta \alpha}{\alpha} = -\frac{\Delta d}{d}. \]  

By examining the data for absorption coefficient versus temperature [6], in the range of interest α(T) has the general form

\[ \alpha(T) \approx C_1 e^{\frac{T}{C_2}} \]  

where C_2 \approx 90°C. Using (4) and (5) one can show the error in the inferred temperature (ΔT) is

\[ \Delta T = -\frac{C_2 \Delta d}{d}. \]  

That is, the error in temperature is linear with the fractional error in wafer thickness, with a 1% error in wafer thickness causing a ~1°C error in temperature.
Maintaining a low direct reflection is crucial for the success of the technique as presently implemented. To keep the direct reflection coefficient below $10^{-2}$, it is straightforward to show that a misalignment of the angle of incidence of $\pm 1.0^\circ$ may be tolerated. At a temperature where the normalized transmission has dropped to $\sim10^{-2}$ of its cold value, which in practice is a upper temperature limit to our method, this would cause a relative change in the normalized transmission of $\sim10\%$. By examining Fig. 3, it can easily be shown that this would induce a temperature error of $\sim3^\circ$C. Furthermore, Brewster's angle changes slightly at elevated temperature due to the change in index of refraction of silicon [9]. Using the measured change in index of refraction at $1.3 \mu m$ from room temperature to $500^\circ$C, one would expect Brewster's angle to change by about $0.5^\circ$, which is not significant.

If the reflectivity of the metal/silicon interface changes as a function of temperature, the double-pass transmission signal would of course also change. Such a change could occur from a silicidation reaction between metal and silicon, or from a phase change in metal on top of field oxide (such as Ti reacting with a nitrogen ambient to form TiN during the TiSi$_2$ formation process). The effect an uncorrected reflectivity change would have on the inferred temperature depends where on the normalized transmission curve one was. Near a normalized transmission of 0.1, for example, a 25% change in the average reflectivity of the surface would induce a $\sim10^\circ$ error in temperature. This change in the metal/silicon reflectivity could be independently measured by using an additional wavelength where little change in $\mu(T)$ is expected with temperature in the temperature range of interest (e.g., $1.55 \mu m$ near $500^\circ$C) along with the primary wavelength used to measure the temperature. One thus might be able to monitor the progress of a metal reaction process in situ. To date, however, we have not studied changes in the metal reflectivity as a function of time. In our experiments the “cold” reflectivity after an experiment was generally within 15% of the starting reflectivity. It should also be pointed out that our method would not be directly applicable to an RTP metal CVD process in which the wafer initially was not covered by metal.

### B. Backside Roughness Effects

The above results were for wafers with a polished backside. However, other methods, already exist for measuring the temperature of wafers with polished backsides, as will be discussed in Section III.D. In practice, however, most wafers in manufacturing have rough backsides, and thus it would be desirable to extend our work to rough backsides. A rough backside may affect the double-pass technique through an increase in the undesired direct reflection, or through a reduction in the desired double-pass signal (through scattering). Note that the undesired direct reflection encounters a rough surface only once, but the desired signal is scattered twice by the rough surface: once on the way into the wafer and once on the way out. We performed experiments on a wafer having a typical backside roughness (rms roughness measured by a surface profilometer of $\sim4 \mu m$). The effect of the rough surface on the direct reflection and double-pass components of the detected signal were separated by comparing results on wafers with and without metal-coated front surfaces. The results are presented in Table I, and are contrasted to those on wafers with polished backsides. Note that the rough backside reduced the double-pass signal from 200 mV to only 0.3 mV, while the direct reflection actually increased by a factor of two, from 0.18 to 0.36 mV. The ratio of the desired double-pass to undesired direct reflection thus decreased from roughly $10^3$ to 1. In temperature measurement experiments on wafers with rough backsides, at high temperatures the detected signal only decreased by $\sim50\%$, corresponding to the double-pass signal becoming very small but the direct reflection changing little. On different wafers the direct reflection changed slightly, but was of the same order of magnitude. Because it was not possible to separate the desired double-pass signal from the direct reflection, an accurate measure of the sample temperature by a double-pass infrared transmission technique was not successfully achieved.

To determine whether the low value of the double-pass signal from a wafer with a rough backside was truly due to roughness, and not due to some unknown factor, the scattering of a collimated laser beam with a wavelength of $1.3 \mu m$ transmitted through a wafer was quantitatively studied. The experiments were performed at a normal angle of incidence, and the transmitted light was measured as a function of the scattering angle. The results for scattering through both one wafer (one rough surface) and two wafers (two rough surfaces) for the same wafers used in the above temperature
measurement experiments are shown in Fig. 4, along with the profile of the original incident laser beam. In all cases the beam profiles were fit to a Gaussian profile

$$I(\theta) = I_{\text{peak}} \cdot e^{(-\theta/\theta_{\text{width}})^2}.$$  

(7)

The beam powers were normalized to the peak power at the center of the original unscattered beam. The original beam with \(\theta_{\text{width}}\) of \(\sim 0.3^\circ\) was scattered by one interface to a much wider beam with \(\theta_{\text{width}} = 9^\circ\), with a reduction in peak intensity of \(1.6 \times 10^{-3}\). A second rough surface increased the \(\theta_{\text{width}}\) to \(16^\circ\) and decreased the intensity by a further factor of 5 to \(3 \times 10^{-4}\) of the original beam intensity. Assuming a factor of 30% power reflection at each interface, for the case of scattering from two rough interfaces (and going through two smooth interfaces) one would estimate that the scattering itself from two rough interfaces would decrease the peak intensity of the original beam by \(1.2 \times 10^{-3}\). This is very close to our experimentally observed reduction in the desired signal due to scattering of \(10^{-3}\) (Table I). Although the scattering experiment was done at normal incidence, and the temperature measurements were done at Brewster’s angle, from this correlation between the two results we conclude that the reduction in the desired double-pass signal in the temperature measurement experiments on rough surfaces is indeed due to excess surface scattering.

C. Proposed Method for Rough Surfaces

The above problem with rough surfaces could be overcome if one could devise a measurement principle which would be sensitive only to the desired double-pass transmitted signal and not the direct reflection. A process for such a measurement is now proposed in Fig. 5. Suppose that the wavelength of the incident probe beam were modulated between two wavelengths, one being the wavelength desired for the temperature measurement (e.g., 1.2 \(\mu\)m), and the second a wavelength at which the transmission and double-pass signal is essentially zero (e.g., 1.0 \(\mu\)m). This could be achieved by using an electro-optic switch to choose one of two input beams to be routed to an output fiber. The desired double-pass signal would then be modulated on and off at the wavelength modulation frequency. If the two laser powers were adjusted inversely to the direct reflection coefficient at their respective wavelengths, the direct reflected signal would be constant (Fig. 5). The total detected signal would have a modulated component corresponding only to the desired double-pass signal, not to the undesired direct reflection. Using a lock-in amplifier, one could then directly detect the double-pass signal without having to worry about subtraction of the direct reflection. In principle, this technique would not require a low direction reflection coefficient, and might not be restricted to Brewster’s angle of incidence. A critical issue will be maintaining the relative power stability of the two light sources so that any ac component of reflection could be avoided. Efforts to implement this arrangement are in progress.

D. Comparison to Other Methods

In this section we will comment briefly on the relative merits and disadvantages of the double-pass transmission method vs. other methods for measuring the temperature of metallized wafers. Pyrometry with in-situ emissivity correction is an extremely powerful technique [9]. The method in principle compensates for the effects of surface roughness on emissivity. Because of problems with the substrate becoming transparent (and hence making emissivity measurement difficult) and due to problems with lamp interference, such work has mostly been applied to temperatures in excess of 650°C (using 1.5 \(\mu\)m) on heavily-doped substrates. Lightly-doped substrates would require a shorter wavelength and have a higher temperature limit. On double-polished wafers, one can also infer the temperature by observing changes in the reflection of a normally incident laser beam (due to Fabry–Perot effects) as the index of refraction and thickness of the substrate vary slightly with temperature [10]. This method could also be applied to wafers with metallized surfaces, although it is not clear what the upper temperature limit would be and if oscillations would occur in an absorbing heavily-doped substrate. Furthermore, this interference method and other thermal expansion methods are only a relative measure of temperature, not an absolute method. Although the infrared transmission technique does require a normalization to a “cold” value, the method is insensitive to the exact cold value used. This is because the absorption for lightly doped wafers from 1.2 to 1.5 \(\mu\)m is virtually zero (see Fig. 3) for temperatures under 75°C. Performing a “cold” measurement anywhere under 75°C will then just measure fixed factors such as detector efficiency, laser power, etc. which do not depend on temperature. In independent measurements in an RTP-CVD system, we have also confirmed that there was no (<5%) discernable change in the transmission at high processing temperature (1000°C) due to a change in the transmission through the quartz reactor walls. The IR transmission method would in principle be susceptible to process-induced changes in the backside roughness (affecting scattering), such as crystallization of amorphous silicon to polycrystalline silicon, but this has not yet been characterized.

IV. CONCLUSION

A double-pass infrared transmission technique has been demonstrated to measure the temperature of double-polished silicon wafers which were blanket-coated with metal. Using wavelengths from 1.1 to 1.55 \(\mu\)m, a temperature range from
100°C to 550°C was demonstrated. The technique should be extendable over 700°C. A critical issue is the separation of the direct surface reflection from the desired double-pass signal. The excessive scattering of the desired double-pass reflection prevents the use of the technique as it was implemented in our experiments on wafers with rough backsides. An implementation based on wavelength switching to overcome this limitation was proposed.

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REFERENCES


Charles W. Cullen was born in Meadville, PA, on June 30, 1972. He received the B.S.E. degree in electrical engineering from Princeton University, NJ, in 1994. His undergraduate thesis was on the temperature measurement of silicon wafers by infrared transmission techniques. He is presently employed as a systems analyst by Andersen Consulting, Florham Park, NJ. Mr. Cullen is a member of MRS.

James C. Sturm (S'81-M'85) was born in Berkeley Heights, NJ, in 1957. He received the B.S.E. degree in electrical engineering and engineering physics from Princeton University, Princeton, NJ, in 1979, and the M.S.E.E. as well as Ph.D. degrees from Stanford University, Stanford, CA, in 1981 and 1985, respectively.

In 1979 he joined Intel Corporation as a microprocessor design engineer for one year. In 1981 he was a visiting engineer at Siemens Co., Munich, Germany. In 1986 he joined the faculty of Princeton University as an assistant professor in the Department of Electrical Engineering, where he has been an associate professor since 1992. From 1994 to 1995, he was a von Humboldt Fellow at the Institut für HalbleiterTechnik at the University of Stuttgart, Germany. He has worked in the fields of laser processing of semiconductors, thin epitaxial films, silicon-on-insulator, and three-dimensional integration. His current research interests include silicon-based heterojunctions, silicon-germanium growth and applications, silicon-based optoelectronics, rapid thermal chemical vapor deposition, and organic semiconductors. He has served on the organizing committee of IEDM (from 1988 to 1992), as a symposium leader for the Materials Research Society (1987, 1995) and on the SOS/SOI, DRC, and EMC Conference committees.

Dr. Sturm is a member of the American Physical Society, Materials Research Society, and was a National Science Foundation Presidential Young Investigator.