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EMISSIVITY OF ROUGH SILICON SURFACES: MEASUREMENT AND CALCULATIONS

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ABSTRACT

The directional reflectance and approximate emissivity of rough silicon wafers were measured by reflection measurements using a single point detector and a broad area illumination source. Experiments were also performed to determine the cone angle of the incident light required to properly measure the emissivity of rough backsides. Based on surface roughness parameters acquired with an Atomic Force Microscope, reflectance calculations were performed within the framework of the Beckmann-Spizzichino model. The results are qualitatively consistent with experimental observations.

INTRODUCTION

The rapid and practical measurement of the emissivity of rough wafer backsides is important for RTP applications. As the emissivity depends on many parameters which generally vary during the processing, it is critical to measure the emissivity *in situ*. Such *in situ* measurements have been made possible by the recently developed ripple technique [1, 2]. With this technique, the reflectance of a surface and the thermal radiation can be simultaneously measured. These two quantities can then be used to infer the emissivity and temperature [3]. In contrast to a polished surface, to measure the emissivity correctly for a rough surface, ideally an extended probe beam with constant radiance covering the whole hemisphere over the sample is needed [3]. However, in real RTP systems, such an ideal scheme is impossible to realize. Instead, it is always replaced with extended probe beams with a solid angle smaller than that of an hemispheric light source, which is 2π. As a result, the measured reflectivity is only an approximation of the hemispheric reflectivity. Presumably, as the surface becomes rougher, a larger solid angle of the probe beam is required to make the measured reflectivity a good approximation of the hemispheric reflectivity. For both practical and fundamental reasons, it is very important to find out how the required solid angle changes as the roughness changes. In this work, we have done a series of surface reflectance and Atomic Force Microscope (AFM) experiments. The experimental observations, together with reflectivity calculations, indicate that, when a proper measure of the surface roughness is used, both the required probe beam solid angle and the approximate emissivity increase as the surface becomes rougher.

REFLECTION MEASUREMENT AND ROUGHNESS CHARACTERIZATION

In the reflectance measurement, the reflectance of both polished and rough sides of silicon wafers were measured as a function of the probe beam solid angle. Fig.1 shows the schematic of the experimental set-up on an optical table. A frosted flood lamp with a 12 cm diameter was used as an extended probe beam. The lamp was covered with a white cloth to make the light more like a "gray body", i.e., a diffusive light source. Optical measurements indicate that the light from the lamp is quite diffusive and the radiance variation from the center to the edge is ~20%, with a brighter center. In the reflection result to be shown later, such radial variation of radiance has been compensated. The light passes through an orifice with a variable diameter. The solid angle of the probe light source is controlled by the size of the orifice. In the following, we will express the solid angle in the center-to-side cone angle θ_{cone}, as shown in Fig.1. A silicon photo-diode with 100 mm^2 reception area was used to detect the reflected light. This detector is covered with a thin slice of polished GaAs wafer (20 mil thick, doped with ~10^{17} cm^{-3} silicon). Thus, the wavelength of the detected light will be essentially within 0.8–1.1 µm. A convex lens with a 15 cm focal length was installed between the detector and the sample so that a small area on the sample was sharply imaged on the detector. As shown in Fig.1, the center line of the detector is 60° off the sample surface. Thus, the detected light was emitted from a small sample area (~120 mm^2) at a 60° reflection angle.

The reflectance measurements of all the samples were measured at room temperature in air.

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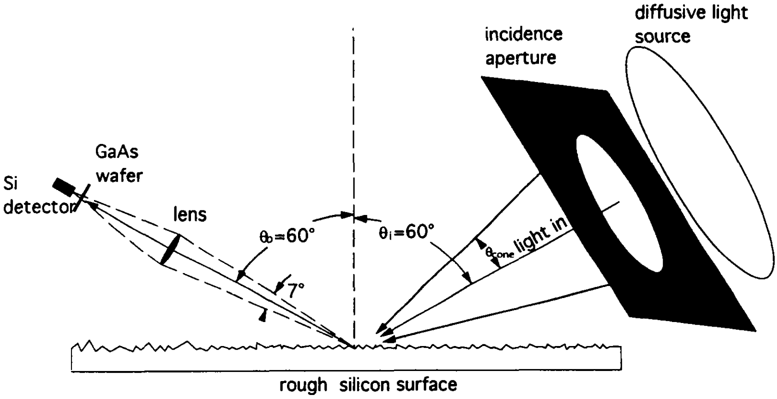

Fig. 1. Experimental set-up of the reflectance measurement on rough surfaces using a single detector and a broad area radiation source.

Overall, three types of silicon wafers samples were used. For each of them, both polished and rough sides were measured. These samples are 15–26 mil thick and are moderately doped (typical resistivity = 7–70 Ω cm). Naked eye observation indicates that their backsides have different reflectance. In a typical measurement, a silicon surface's reflectance is measured as the cone angle θ_{cone} changes from 0° to ~30°. Care was taken so that the positions of the lamp, sample and detector remained the same during the measurement for each sample. Thus, the reading of the detector is proportional to the reflectance of the surface at a certain cone angle.

For the wavelength in this experiment (0.8–1.1 μm), the silicon surface is opaque [4]. Thus, the emissivity can be inferred from the hemispheric reflectivity according to $\varepsilon = 1 - R_{h.s.}$, where ε is the emissivity, and $R_{h.s.}$ is the hemispheric reflectivity [3]. $R_{h.s.}$ can be further expressed as

$$R_{h.s.}(\vec{\theta}_o) = \int_{(2\pi)} d\vec{\theta}_i \cos\theta_i \, r(\vec{\theta}_i,\vec{\theta}_o) \ , \qquad (1)$$

where $\vec{\theta}_i = (\theta_i, \varphi_i)$ and $\vec{\theta} = (\theta_o, \varphi_o)$ represent the directions of the incidence and reflected light, respectively; θ_i and θ_o are polar angles of the incident and reflected light as shown in Fig.1; φ_i and φ_o are the associated azimuth angles; $d\vec{\theta}_i$ is the solid angle of incident light; and $r(\vec{\theta}_i, \vec{\theta}_o)$ is the bi-directional reflection function. The integration of the solid angle, $d\vec{\theta}_i$ is over 2π, or, the whole upper hemisphere [4].

In the following reflection experiment, the actually measured reflectance is

$$R_{msr}(\vec{\theta}_o) = \int_{(cone)} d\vec{\theta}_i \cos\theta_i \, r(\vec{\theta}_i,\vec{\theta}_o) \ . \qquad (2)$$

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As it is defined, R_{msr} should increase as the solid angle of integration increases and would eventually approach $R_{h.s.}$ as the cone is close to 2π.

Fig.2 shows the measured reflectance (R_{msr}) versus the cone angle (θ_{cone}) of the probe light beam for all the wafer surfaces. The error bars are not shown in the figures. A good estimate of the error is ~5%. The center-edge variation of the light source radiance has been corrected. The $R_{msr}(\theta_{cone})$ curves for the three polished surfaces are very close to each other. For all of them, the reflectance starts to saturate at a cone angle of $\theta_{cone} = 5°$ and becomes nearly flat at $\theta_{cone} = 30°$. Thus, the reflectance at $\theta_{cone} = 30°$ should be very close to the hemisphere reflectivity. In the following, we will assume the reflectance at this angle to be the calculated reflectivity of a smooth silicon surface (R), which is about 0.32 for incidence light with isotropic polarization and a 60° incidence angle. In addition, we will refer the θ_{cone} at which the saturation starts as the saturation cone angle, or, θ_{sat}. Thus, $\theta_{sat} = 5°$ for polished surfaces. For perfectly "mirror-like" reflections on an ideally smooth surface, θ_{sat} should be close to zero. The considerably bigger θ_{sat} observed here is attributed to the non-zero size of the detector and the convex lens, and, to a lesser degree, the residual roughness of the polished surfaces.

In contrast to polished surfaces, the reflectances of the rough surfaces saturate in different ways, depending on the roughness of the surface. In general, a rougher surface exhibits a larger θ_{sat} and a lower reflectance at any θ_{cone} in this experiment (0°–30°). At $\theta_{cone} = 30°$, the reflectance of sample #1, #2 and #3 are 0.32, 0.21, and 0.19, respectively. All three $R_{msr}(\theta_{cone})$ curves show signs of saturation at $\theta_{cone} = 30°$. However, from the slope of the curves, one can see that the saturation of the rough surface reflectances is less complete than that of the polished surfaces. That is, the difference between the reflectance at $\theta_{cone} = 30°$ and the hemisphereic reflectivity may be bigger for rough surfaces than for polished surfaces. Approximately, if one assumes the reflectance at $\theta_{cone} = 30°$ is nearly the same as the hemispheric reflectivity, then the approximate emissivity of the rough surfaces are 0.68 (sample #1), 0.79 (sample #2) and 0.81 (sample #3), respectively. These differences of emissivity, or reflectance, reflect the differences of surface roughness. Since the curves of $R_{msr}(\theta_{cone})$ for rough surfaces are not fully saturated at $\theta_{cone} = 30°$, the actual differences of emissivity should be smaller.

To quantitatively characterize the surface roughness, we have examined the surface using a commercial AFM (Digital Instruments). The results indicate that sample #1 is the least rough, while #3 is the most rough. Typically, a sample area of 50μm x 50μm was surveyed. Fig.3 is a typical line-cut of an AFM image of 50μm x 50μm. The surface morphology data contained in the images were then processed to generate the lateral correlation length (T) and the standard deviation of surface height (σ) [5]. As far as reflection is concerned, these two quantities are both important measures of surface roughness: a bigger σ, or a smaller T, indicates a rougher surface [5]. The numerical values of σ and T generated from the AFM images, together with θ_{sat}, R_{msr} at $\theta_{cone}=30°$, and the approximate emissivity from the reflection experiments are summarised in Table I.

Table I. Measured parameters of rough silicon surfaces: Standard deviation (σ); lateral correlation length (T); saturation cone angle θ_{sat}; measured reflectance (R_{msr}) at $\theta_{cone}=30°$; and the inferred emissivity.

Silicon surfaces	σ (μm)	T (μm)	σ/T	θ_{sat}	$R_{msr}(\theta_{cone}=30°)$	$\varepsilon \approx 1-R_{msr}(\theta_{cone}=30°)$
rough #1	0.62	12.5	0.05	~30°	0.32	~ 0.68
rough #2	0.45	3.3	0.137	>30°	0.21	~ 0.79
rough #3	0.56	3.6	0.156	>30°	0.19	~ 0.81

Obviously, all of the surfaces satisfy $2\pi\sigma > \lambda$. We will interpret the results in the limit of $2\pi\sigma >> \lambda$. In this limit, it can be shown [5] that the effect of surface roughness on the reflection qualitatively scale as σ/T, i.e., σ/T is the proper measure of roughness. Of the three rough surfaces, sample #1 has the smallest σ/T, while sample #3 has the biggest σ/T. That is, sample #1 is the least rough surface, while #3 is the roughest. Combining the reflection and AFM results, we can conclude that the reflectance of a smoother surface saturates at a smaller θ_{cone}. In addition, the reflectance at any cone angle decreases as the surface roughness increases. The approximate emissivity is up to 0.1 bigger for the roughest surface (σ/T=0.156) than that of the polished surface..

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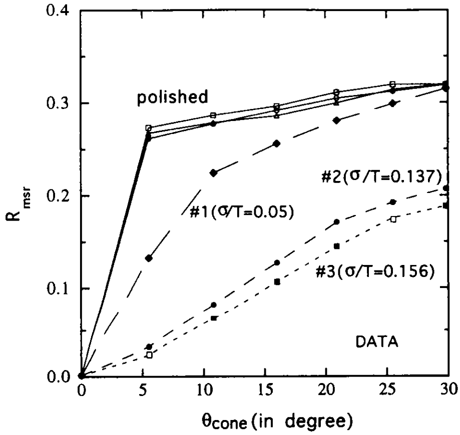

Fig. 2. Measured reflectance as a function of the cone angle of the incidence aperture (θ_{cone}), for different silicon wafer surfaces. Data points for the rough surfaces are represented by solid symbols and dashed lines, while those for smooth surfaces are represented by hollow symbols and solid lines. The rough sides of wafers are labeled as #1, #2 and #3, with increasing roughness. Values of σ/T are taken from Table I.

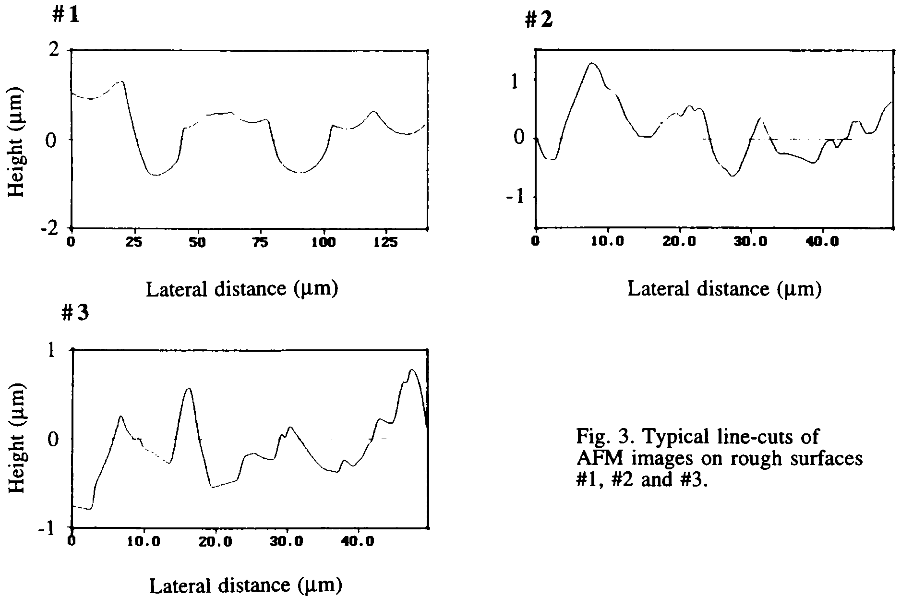

Fig. 3. Typical line-cuts of AFM images on rough surfaces #1, #2 and #3.

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MODELING

To further understand the experimental observations as discussed above, we performed reflectance calculations using the Beckmann-Spizzichino model [5, 6]. In this model, for a rough surface, the reflectance can be expressed as a function of the θ_{cone}, σ and T. Again, we treat only in the limit of $2\pi\sigma >> \lambda$.

Using the definitions of the various radiometric terms in ref. 3, with the reflection-induced depolarization ignored and $2\pi\sigma >> \lambda$, for an incidence beam of light with isotropic polarization, the bi-directional reflectivity function $r(\theta_i, \varphi_i; \theta_o=\pi/3, \varphi_o=0)$ can be expressed as:

$$r(\theta_i, \varphi_i; \theta_o=\frac{\pi}{3}, \varphi_o=0) \approx R\,\frac{T^2}{4\pi\sigma^2}\,\frac{\left(1+\frac{1}{2}\cos\theta_i - \frac{\sqrt{3}}{2}\sin\theta_i\cos\varphi_i\right)^2}{\frac{1}{2}\cos\theta_i(\cos\theta_i+\frac{1}{2})^4}\exp\left(-\frac{k_{xy}^2T^2}{4\,k_z^2\sigma^2}\right), \quad (3)$$

where θ_i and θ_o, φ_i and φ_o, T and σ are as defined in the previous section; λ is the wavelength of the light; R is the reflectivity of the perfectly smooth silicon surface (~0.32); and

$$k_{xy} = \frac{2\pi}{\lambda}\sqrt{\left(\sin\theta_i\cos\varphi_i - \frac{\sqrt{3}}{2}\right)^2 + \left(\sin\theta_i\sin\varphi_i\right)^2},$$

$$k_z = \frac{2\pi}{\lambda}\left(\cos\theta_i + \frac{1}{2}\right).$$

As it is defined in eq. (1), at $\theta_o = \pi/3 = 60°$, $\varphi_o=0$, the hemispheric reflectivity

$$R_{h.s.} = \int_0^{\pi} d\theta_i \int_0^{2\pi} d\varphi_i \sin\theta_i \cos\theta_i\, r(\theta_i, \varphi_i; \theta_o = \frac{\pi}{3}, \varphi_o=0)\,. \quad (4)$$

Similarly, as defined in eq. (2), for $\theta_{cone}<\pi/6 = 30°$, R_{msr} is

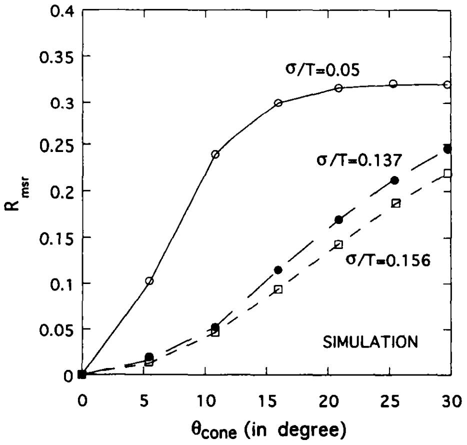

Fig. 4. Calculated reflectance as a function of the cone angle of the incidence aperture (θ_{cone}), for silicon wafer surfaces with same σ/T as the rough sides of #1, #2 and #3. Values of σ and T are taken from Table I.

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$$R_{msr}\,(\theta_{cone}) = \int_{\frac{\pi}{3}-\theta_{cone}}^{\frac{\pi}{3}+\theta_{cone}} d\theta_i \int_{(cone)} d\varphi_i \sin\theta_i \cos\theta_i\, r(\theta_i, \varphi_i; \theta_o = \frac{\pi}{3}, \varphi_o{=}0) \quad . \qquad (5)$$

By substituting eq. (3) into eq. (5), $R_{msr}(\theta = \pi/3, \theta_{cone})$ can be numerically evaluated as a function of θ_{cone} for θ_{cone} up to 30°. The result of the calculations are shown in the $R_{msr}(\theta_{cone})$ plot in Fig. 4. The roughness parameters σ and T are taken Table I. Clearly, as σ/T increases, or, as the surface becomes rougher, the reflectance saturates at a bigger θ_{cone}. In addition, the reflectance at any θ_{cone} decreases as the roughness increases. These results are quite consistent with the reflection results in Fig. 2. Indeed, both results indicate that for rough surfaces with $\sigma/T > 0.05$, a cone angle of at least 30° is needed to have the measured reflectivity (R_{msr}) a good approximation of the hemispheric reflectivity ($R_{h.s.}$). In addition, at any θ_{cone} less than 30°, the reflectance of these surfaces decreases as the roughness increases. Finally, the agreement between experiment and calculations implies that σ/T is a proper measure of surface roughness.

It should be pointed out that saturation behavior of $R_{msr}(\theta_{cone})$ curves from experiments (Fig. 2) are a little different from those from calculations (Fig. 4). Compared with the calculated results, the experimental reflectance data for samples #2 and #3 start to saturate at smaller θ_{cone}; while for sample #1, the reverse is true. In fact, for #2 and #3, the calculated $R_{h.s.}$ are 0.315 for #2 and 0.31 for #3. These values are considerably bigger than the calculated $R_{msr}(\theta_{cone}{=}30°)$, which is 0.25 for #2 and 0.22 for #3. Thus, unlike experimental observations, the calculated $R_{msr}(\theta_{cone})$ curves for #2 and #3 are far from saturation at θ_{cone}=30°. Such differences are not surprising, since the calculations contain quite a few assumptions and simplifications which are not necessarily true in real surfaces. For example, it is assumed that the surface height deviation of the silicon surfaces follows a Gaussian distribution and the depolarization of the incident light in the reflection can be ignored. Also, features of the surface slopes are not included in the model. Further modeling and measurements are needed to determine the true emissivities of very rough surfaces ($\sigma/T > 0.1$).

CONCLUSION

It was found that for very rough backsides ($\sigma/T > 0.1$) of silicon wafers, a cone angle (θ_{cone}) of at least 30° is needed for the measured reflectance (R_{msr}) to be a good approximation of the hemispheric reflectivity ($R_{h.s.}$). At θ_{cone} =30°, the approximate emissivity of rough silicon surfaces (up to $\sigma/T = 0.156$) can be as much as 0.1 larger than that of a polished surface. Results of the Beckmann-Spizzichino model calculations of $R_{msr}(\theta_{cone})$ are qualitatively consistent with reflection measurements. Further effort is needed to improve the modeling and measurement of very rough surfaces ($\sigma/T > 0.1$). Support from SRC is gratefully acknowledged.

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