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Measurement and Analysis of Scatter from Silicon Wafers*

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Measurement and analysis of scatter from silicon wafers

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ABSTRACT

The measurement of wafer surface roughness has become of increasing interest in the semiconductor industry in the last year. This interest is driven by the need to reduce background "haze" associated with laser scanning particle counters, by the ever decreasing line width requirements and by a recent report that gate oxide breakdown voltage decreases as roughness increases. Scatter measurement offers the potential of being a fast, non-contact method of monitoring roughness; however, the ability to accurately calculate wafer roughness via scatter depends on various wafer surface characteristics. The paper presents data taken on a number of wafers and demonstrates that bare silicon scatters almost exclusively from surface topography and is isotropic over an appropriate spatial bandwidth, thus facilitating scatter measurement. Because silicon proved to be an excellent source of topographic scatter, an experiment was under taken to compare the one dimensional roughness measurements made with an optical profilometer to the two dimensional (area) measurements made via scatter, and these results are also reported.

Keywords: silicon wafers, roughness, microroughness, light scatter, haze

2. INTRODUCTION

Light scatter has been used to map and size particulates on silicon wafers for many years, but, in contrast to the optical industry, only recently has it been seriously considered as a source of micro-roughness characterization in the semiconductor industry. In fact it is only recently that micro-roughness has been considered a serious problem in the semiconductor industry [1-4]. It is interesting that these two industries approached solving the problem of component surface roughness so differently. The optics community started by devising means to measure roughness through profilometry, scatter, etc. and carefully monitored their progress in producing better surfaces. From the mid-1960's to late 1980's the instrumentation, standards and conventions necessary for measurement, communication and specification of optical surface roughness were developed. The means to polish better optical surfaces has never really exceeded the capability to measure them.

Meanwhile, over roughly the same time period, engineers and scientists in the semiconductor industry were producing surfaces so smooth that characterizing roughness was not a major concern. Their attention was focused on a host of other problems associated with increasing yield and quality of products that were rapidly growing in complexity. Compared to a mirror, scatter from the polished side of a clean silicon wafer is barely visible to the eye (Is the laser really on?). It was clear back in the early 1980's that the optics community still had a great deal to learn about polishing surfaces. Of course there is an advantage to having single crystal substrates to work with, but the difference was amazing. Now, in the mid-1990's, the optics community has learned more about producing smooth surfaces, and even tighter device specifications have the semiconductor community suddenly learning how to measure and specify surface roughness. They have the opportunity, as a group, to master the problems of spatial frequencies, surface power spectra, comparison measurements, and ASTM Standards, much faster than the ten to fifteen years spent in the optical community before a consensus was reached.

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Because scatter is a fast, non-contact area measurement, it is an obvious choice for the laboratory, at-line and on-line instrumentation needed to characterize roughness in the semiconductor industry. As will be seen in the following sections, silicon is an ideal material for roughness analysis by scatter. The ever tightening requirements, and the economics associated with producing large quantities of faster, smaller semiconductor products, can be expected to stimulate the development of new capabilities in scatter based instrumentation. The optical industry will also (eventually) benefit from these coming advances in process control instrumentation.

A number of laser based particle scanners have been available for several years that use the sudden increase in scatter signal from a scanning laser beam to map defects and particulates on the wafer surface. These measurements have had their biggest impact as a means of checking and improving process cleanliness in both material and wafer fabrication. Particle scanners play a key role in bringing new production processes up to economically viable yield levels. Surface pits, particulates and subsurface defects can all cause these systems to register the location, and relative scatter signal size of a surface problem. Because of the uncertainty over the cause of a particular signal, they are referred to as "light point defects" (LPD's), or more recently "light scattering events" (LSE's). Most of these systems integrate the scattered signal through collection optics onto one, two or three detectors. Signals are usually expressed in parts per million (PPM), but because the various models available use different angular integration limits, comparison of PPM values from one model to another is pointless.

To date little design attention has been paid to the spatial frequency limits imposed by the collection optics, and in fact the limits often vary during a scan because of incident angle variations and/or relative motion of the scatter source to the collection optics. Thus, the measurements made by these instruments cannot be easily converted to surface roughness information. The background signal measured when an LSE is not illuminated is called "haze." It is just the integrated scatter from whatever is in the illuminated spot (roughness, films, very small particulates, etc.). Haze is also "measured" visually by examining the wafer when illuminated with a broadband light. These evaluations are even more confusing with "brown haze" and "rainbow haze" being reported (but not quantified). The background haze has a lot to do with determining the smallest LSE that can be detected, because it obscures the particle signal. New semiconductor product specifications are forcing the industry to consider wafer roughness as limiting source of noise for particle scanners.

The detection of much smaller particles is driven by the need to build circuits with smaller features on the wafer. Line widths have dropped below $1\text{ }\mu\text{m}$. It is easy to see that signal scatter from the particle/surface combination is likely to drop much faster. The particle cross-sectional area varies as diameter squared and the Rayleigh scatter varies as diameter to the sixth power. The rule of thumb is that particle diameter must be kept below $1/3$ to $1/10$ the minimum feature size, which means that manufacturers would like to be able to map particles as small as $0.1\text{ }\mu\text{m}$, but they are hoping to cut that almost in half again before the year 2000. To put this into perspective, if the illuminated spot were the size of a basketball court (instead of approximately 0.01 mm^2), then a $0.1\text{ }\mu\text{m}$ particle would be about as large as a golf ball. At a scan rate corresponding to one minute for a 200 mm diameter wafer, you would have 20 microseconds to determine if there was a golf ball on the basketball court. An obvious solution is to reduce the spot size to increase particle scatter. This has been done, but only at the expense of component throughput. Particles in the $0.1\text{ }\mu\text{m}$ range are proving to be difficult to find, and mapping even smaller diameters is going to be very difficult.

A lot of the background haze that limits particle detection comes from surface roughness. If this noise source can be reduced then particle scanner signal to noise will increase. At issue is whether or not wafer roughness is the main source of scatter (haze). If so, this also opens the door to using scatter (haze) measurements as a fast source of non-contact roughness metrology for this industry. A second reason for measuring roughness is that it may be a contributor to other types of device defects. It has been speculated that reducing roughness increases gate oxide breakdown voltage and may be a contributor to problems in other aspects of device fabrication [4]. These potential effects will be documented only with great difficulty because of the number of production

steps (each potentially changing surface roughness) that are required to create features that can be tested (such as a gate oxide capacitor). Even so, it stands to reason that roughness will eventually play a role in component quality as component dimensions shrink. So there may be several production applications where reducing roughness on wafers, or other production process surfaces, is of value. The ability to monitor wafer surface roughness during polishing and other surfaces during production is likely to be of considerable value.

The next section briefly reviews the key issues associated with the relationship between topographic scatter and roughness. Following that is a section presenting a number of wafer BRDF measurements. Finally a brief comparison is made between roughness measurements made via scatter and optical profilometry.

3. REVIEW OF TOPOGRAPHIC SCATTER CONCEPTS

Under certain circumstances, light scattered as a result of surface reflection can be measured and used to determine roughness statistics of the reflector. In particular the calculation of the surface power spectral density function (or PSD) can be found from the measured bidirectional reflectance distribution function (BRDF). In fact, the PSD is the preferred way to evaluate surface topography and compare roughness characteristics of various samples. One of the requirements for calculating the PSD from the BRDF is obviously that most of the scatter be caused by surface topography, as opposed to sources independent of roughness such as surface contamination or bulk defects. The other requirement is that the surface be optically smooth, which is not a problem for measuring the front sides of silicon wafers.

The papers by Church et al [5-7] introduced the vector perturbation approach to the optical scatter literature in the mid-seventies. This approach, which has proved to be very accurate is commonly used in the optics industry [8]. Identical perturbation results (using different notation) were published in 1979, by Elson [9]. The basic relationship, sometimes known as the "Golden Rule" is presented here as Equation 1. It shows that the two dimensional PSD, given as $S_2(f)$, is proportional (within a cosine) to the scatter pattern expressed in BRDF units.

$$BRDF = \frac{16\pi^2}{\lambda^4} \cos\theta_i \cos\theta_s Q S_2(f) \quad (1)$$

There are P_i watts incident on the reflector and dP_s is the scattered power measured through the differential solid angle $d\Omega_s$. The light wavelength is given by λ , and the angles θ_i and θ_s (measured from surface normal) are the incident and scattering angles respectively, Q is the polarization coefficient (which is numerically close to the specular reflectance for many situations). This relationship has been investigated in great detail in the literature [a review appears in reference 8] and has been proven to be very accurate for the case of smooth, clean, front surface reflectors (ie: topographic scatter from an optical surface). One recent experiment utilized a silicon wafer with a single, small step on the surface [8,10]. The step can be measured by profilometry and the BRDF calculated from a slightly modified form of Equation 1. The theoretical and measured BRDF's are almost identical.

These investigations make use of a property of Equation 1 referred to as wavelength scaling [8,11]. Because $S_2(f)$ depends only on the surface, its computed value will not change as a function of light wavelength if the measured BRDF is caused only by surface topography meeting the smooth surface requirement. This has been determined for many materials by simply comparing the PSD's calculated from BRDF measurements at different wavelengths. Often materials that scale in the visible do not do so in the mid-IR where the greater skin depth, or other effects, create non-topographic scatter. If silicon wavelength scales, then producing smoother wafers will result in haze reductions that can be predicted by Equation 1, and BRDF measurement instrumentation can be built to quantify and

map roughness on the wafer surface. The data of the next section confirm these convenient properties.

The various types of roughness measurement can be compared to each other if attention is paid to several important details. The best method is to compare the computed PSD's directly. This method removes any doubt about problems due to different spatial bandwidths creeping into rms roughness calculations [8]. Even when PSD's are compared some care must be taken. Profilometers produce a one dimensional trace on the two dimensional surface. This is most often used to calculate a one dimensional PSD (with units of length cubed). On the other hand, scatterometers inherently calculate a two dimensional PSD (with units of length to the fourth). In order for the two of them to be accurately compared, one must be converted to the format of the other. This can be accomplished if the surface is isotropic (so that the one dimensional trace can be used to represent the full surface), and the conversion is greatly facilitated if the PSD fits the ABC form of the K-correlation model [12,13]. The current situation is further complicated by the fact that basic differences exist in the PSD calculations made by various vendors and labs. Thus the current situation for comparison is difficult at best. Solutions are coming. An ASTM Sub-Committee is producing a standard PSD calculation. Comparisons from 1-D to 2-D data sets are being successfully made at several labs. Section 5 presents such a comparison.

4. SCATTERING CHARACTERISTICS OF SILICON

Figure 1 shows the PSD's calculated from BRDF measurements taken at several wavelengths in the near IR to near UV on a bare silicon wafer. Figure 2 shows a similar result for a wafer with an epitaxial layer of silicon over the polished wafer. The agreement in the calculated PSD's for both cases is excellent. This close agreement has been observed many times for wafers manufactured by different processes and different manufacturers. Wavelength scaling for silicon sputtered on fused silica has been previously reported [11]. Figure 3 compares the measured BRDF of wafer of Figure 1 with different rotations about surface normal. The lack of variation between scans demonstrates that this wafer is isotropic. Hundreds of wafers have now been measured for a variety of industry, ASTM and SEMI studies. As long as clean, uncoated wafers are used the answer seems to be that silicon exhibits qualities that make it an excellent candidate for roughness characterization by light scatter measurement. For these situations, where scatter from the bare wafer surface is topographic, haze can be reduced (and thus smaller particles detected) by further reducing surface roughness.

Notice that the PSD's of the various wafers shown in Figures 1-3 do not always have the same shape. Many wafers have a nearly straight line form with slope of -1 to -3 on a log-log plot. This implies a fractal, or $S_2(1)/f^n$ behavior [14]. The analysis of near fractal behavior is further examined in Section 5. Other wafers have more complicated PSD shapes that require a three parameter (ABC) fit [12,13]. In some cases the shape of the PSD can be obtained from the summation of more than one of these generic forms. The various power law forms have been found in the PSD's of many surfaces (both industrial and natural). When the PSD of a manufactured surface can be modeled by the summation of two or more power law expressions, the implication is that more than one separable mechanism is at work. For example, would the use of two different grit sizes in the polishing process show up in this manner? There is still a lot to be learned about the relationship of the PSD shape to the manufacturing process.

An example of a silicon PSD changing dramatically with process parameters is the epitaxial wafer of Figure 2. The addition of this layer to the substrate produces changes that increase the high frequency roughness and decrease the low frequency roughness. These characteristics emphasize the need to pay attention to bandwidth (or angle) limits when comparisons are made. For example, if the rms roughness found via profilometer (which would typically start at about $f=0.01\mu\text{m}^{-1}$) were used to investigate the effects of epitaxial growth, the conclusion would be that the surface gets smoother during the epitaxial process because the roughness measurement (integral of the PSD) is dominated

COMPARE PSD

Figure 1 The same PSD is found from BRDF data taken at two wavelengths from this silicon wafer. This result is common for smooth, clean, uncoated wafers.

COMPARE PSD

Figure 2 Epitaxial silicon also "wavelength scales," but the resulting PSD differs from the underlying silicon substrate.

Figure 3 The PSD of this wafer is isotropic in that its calculated form is independent of rotation about surface normal.

Figure 4 Deposition of a nitride coating on this wafer results in the loss of wavelength scaling. This is interpreted as an indicator of non-topographic scatter from the coated wafer.

by the low frequency contributions. Conversely, a haze measurement which starts at five to ten degrees from specular (or about $f=0.2\mu\text{m}^{-1}$), would indicate just the opposite. This general behavior has been observed in epitaxial wafers from more than one source.

There are some exceptions to the isotropic nature of polished silicon surfaces. Wafers cut at a small angle from the crystalline plane have been shown, via atomic force microscopy, to exhibit a periodic stepped surface [15,16]. For many wafers, this periodicity is at a high enough frequency (generally above $5\mu\text{m}^{-1}$) that the effect is not seen in the spatial bandwidth available to many scatter measurements, which has a theoretical maximum less than $2/\lambda\mu\text{m}^{-1}$ and a practical maximum often closer to $1/\lambda\mu\text{m}^{-1}$. The presence of these diffraction peaks has been reported [reference unavailable] for the case of low frequency steps.

The usual topographic nature of silicon wafer scatter over the near IR to UV range can be lost when the wafer is coated. Figure 4 shows a failure to wavelength scale on a wafer with a nitride coating. Whether other coatings exhibit similar properties and to what extent these measurements can be exploited to characterize coatings remains to be seen.

5. COMPARISON OF PROFILE AND SCATTER GENERATED ROUGHNESS STATISTICS

As a further demonstration that the PSD's found from the BRDF actually provide surface statistics, the PSD's found by profilometry and BRDF measurements taken from the same location on a silicon wafer were compared. The BRDF of the wafer was measured, and the resulting two dimensional PSD was fit, on a log-log scale, with a straight line as shown in Figure 5. The relationship between $S_2(f)$ and $S_1(f_x)$, which is the one dimensional PSD found from a line profile, is shown below for the special case of an isotropic surface.

$$S_1(f_x) = S_1(1)/f_x^n \quad (2)$$

$$S_2(f) = S_2(1)/f^{n+1} = \frac{\Gamma\left(\frac{n+1}{2}\right) S_1(1)}{2\sqrt{\pi} \Gamma\left(\frac{n}{2}\right) f^{n+1}} \quad (3)$$

$S_1(1)$ is obviously a constant, $-n$ is the slope of $S_1(f_x)$, and Γ denotes the gamma function. A complete description of this calculation (and the slightly more complicated situation when the PSD requires a three constant (ABC) fit) may be found in reference [8], and in Church's original publications [12,13], using slightly different notation. The value $S_2(1)$ and the slope $-(n+1)$ are found graphically from Figure 5 to be $10^{-2} \text{ A}^2\mu\text{m}^2$ and -3.13 respectively. The value $S_1(1)$ is found from (3) above and the result is

$$S_1(f_x) = 3.85 \times 10^{-10}/f_x^{2.13} \quad (4)$$

which is plotted in Figure 6 along with one dimensional PSD's found by optical profilometry over two bandwidths. The units of the PSD have changed from $\text{A}^2\mu\text{m}^2$ to μm^3 introducing a factor of 10^8 that must be taken into account. The profilometer measurements were taken at two different magnifications (as indicated), which results in two different bandwidths for those measurements. The PSD's were found from the profile data according to the recipe's in the references [8,12,13]. As can be seen, the comparison of the two techniques is excellent. The conclusion is that the BRDF measurement can be used to provide surface statistics that are compatible with more conventional surface characterization techniques. These two measurement techniques are compatible, and should be viewed as complimentary (not contradictory) metrologies, to be used as needed for various lab and process control measurements.

Figure 5 A straight line is fit to the PSD of this wafer. After conversion via Equation 3, it is replotted as a one dimensional PSD in Figure 6.

Figure 6 The one dimensional PSD, found from the two dimensional data of Figure 5, is compared to the one dimensional PSD's found via optical profilometry on the same polished wafer.

6. SUMMARY

Wavelength scaling data has been presented showing that smooth, clean silicon wafers scatter mostly from their surface topography. These characteristics hold for both substrate and epitaxial silicon surfaces; although, the addition of the epitaxial layer does change the roughness statistics. The measurement process has been further confirmed by a favorable comparison of BRDF generated PSD's to those found from optical profilometry. The implication is that haze can be reduced from these surfaces if the roughness is reduced, and conversely, that scatter measurements can be used as a reliable source of surface roughness characterization. Thus profilometry and scatterometry are complimentary metrologies - each with their own advantages and uses. Scatter data was presented from one coated silicon surface that did not wavelength scale. In this case, scatter may not be used to find surface topography, but the implication is that the BRDF does contain information about the coating.

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