Effect of Periodic Microscopic Surface Roughness on the Reflection of Light from Semiconductor Surfaces

Bassam M. Mustafa* and Saud K. Sulaiman

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Abstract

The effect of microscopically periodic rough surfaces on the reflection from semiconductors was studied. The range of wavelengths covered extended from 0.15 to 0.70 microns. A rough surface is called microscopically rough if the length scale of the irregularities is much less than the incident wavelength. Rough surfaces have different topographies. Using models for the periodic surface roughness, such as lamellar grating, low sinusoidal and low symmetric ridge. Computer calculations of the complex reflectance were carried. The lamellar grating was found to have the minimum reflectance. Also different geometrical parameters were studied in order that the lamellar grating will have minimum reflectance. All the calculations were carried for a Silicon substrate, and a minimum reflectance was obtained in the UV region.

1- Introduction

In the derivation of Fresnel laws it was assumed that surfaces are flat (1), but flat surfaces are fictitious concept. This means that surfaces must be rough to some degree. The problem of non-specular reflection from rough surfaces was studied by many researchers (2,3,7), surfaces roughness can be divided into scattering roughness (when the length scale irregularities is comparable with the wavelength of the incident light), and microscopic roughness for length scale much less than (λ). The microscopic roughness does not scatter appreciable light, but instead it decreases the amount of reflected light through the increment of the amount of the transmitted light by softening the dielectric discontinuity between the sample and the ambient. The treatment of microscopic roughness is relatively recent, and the empirical verification of these ideas had to await the development of spectroellipsometry (8,9). The microscopic surface roughness acts as antireflection coating and can be described successfully by the three phase mode (substrate-thin
film-ambient), where the rough surface is represented by thin film having dielectric constant whose value is a blend of the latter for both the substrate and the ambient.

Many researches have been performed in order to improve the transmissivity of solar cells (2), in a particular range of E.M. spectrum in which the device is capable of transferring radiation's into electric energy. The enhancement coating and selective surface technology (12) has been followed in most of solar cell designs.

A recent treatment of optical response of microscopically rough surfaces (13) establishes the direct link between the relative roughness induced change $\Delta r/r$ in $r$ (complex normal incidence reflectance), and the screening or depolarization charge that develops as result of microscopic roughness.

In this paper, we present a new compact approach to reduce the amount of the reflected light from semiconductor surfaces, and hence increasing the share of the transmitted light. This will help in improving the efficiency of photoelectric devices in which the first interaction occurs at the surface during the penetration of light to the bulk of the device material (10,11).

In this paper, we tried to find the effect of microscopically rough surfaces. Therefore we compare different kinds of periodic surface roughness configurations, and find the one with the lowest reflectance, then studying the geometrical factors affecting the reflectance for this surface, using these parameters we try to obtain the minimum reflectance. Finally we make use of the optical properties of Si assuming that it is the most popularly used semiconductor in photoelectric devices. It is important to say that microscopic roughness occurs artificially in some semiconductor (9), also high power laser etching produced periodic microroughness (16).

2- Fresnel Reflection

When a plane harmonic wave is incident upon a plane boundary separating two different media, there will be given reflected and transmitted waves. The reflection and transmission coefficients for normal incidence, from Fresnel equations (1) are, respectively:

$$E_r = \frac{n_a - n_s}{n_a + n_s} E_i$$  \hspace{1cm} (1a)$$

$$E_t = \frac{2n_a}{n_a + n_s} E_i$$  \hspace{1cm} (1b)$$

Where $E_i$, $E_r$, and $E_t$ are the complex amplitudes of the incident, reflected and transmitted electric fields, respectively.

$n_a$ and $n_s$ are the refractive indices of the ambient and the substrate.
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If we assumed the ambient to be air its refractive index is approximately equal to unity, also if we assumed $n_s$ is in its complex from $n+ik$ then, the reflectance of the perfectly smooth surface $R_s$ is given by (14):

$$R_s = \frac{(n - 1)^2 + K^2}{(n + 1)^2 + K^2}$$ (2)

Where $R_s = r^2$, $r = E_r/E_i$ and $(k)$ is the distinction coefficient (6).

And the subscription s here denotes the surface. Eq. (2) is usually appropriate to determine the expected smooth surfaces reflectance for metals and semiconductors (for the case of normal incidence).

3- Reflection from Rough Surfaces

The reflectance of any surface is a sensitive function of its roughness, several experimental investigations of the relation between surface roughness and its reflectance (3,7,10) as the latter is deeply influenced by the perturbation of the ideal case of reflection due to scattering.

Surface roughness always exist in different sizes, when the length scale is much less than the wavelength, then it will be known as microscopic roughness (13), it exists in most of the surfaces of metals and semiconductors, even for those which we consider as smooth surfaces (9). We shall study the effect of microroughness on the complex reflectance.

![Fig (1): a cross section of rough surface](image)

The rough surface is represented by a thin layer separating a substrate $(s)$ and an ambient $(a)$ as in Fig.1, both of them are homogeneous, isotropic and locally responded. The ambient is assumed to be transparent, i.e. $\text{Im}(\varepsilon_a)=0$, and the substrate is absorbing, i.e. $\text{Im}(\varepsilon_s)\neq0$, where $\varepsilon_a$ and $\varepsilon_s$ are the dielectric constants of the substrate and the ambient, respectively. The effect of microroughness is described by the following equation derived by Aspnes (13):
\[ \frac{\Delta r^4 \pi n_a}{r} \frac{\lambda E_O \Omega}{\Omega} \left\{ \int dr \cdot \hat{x} \cdot \hat{n}(r_s) \phi_1(r_s) \right\} \]

(3)

Where: \( L \) is the surface periodicity, \( \Omega \) is the projection of the illuminated spot on the z-plane, \( n_a \) is the refractive index of the ambient, \( \lambda \) is the incident wavelength, \( \hat{x} \) is the unit vector pointing along the direction of the incident electric field, \( \hat{n}(r_s) \) is the unit outward vector at the position \( r_s \) in the interface.

This equation is based on the scalar potential \( \phi_1(r_s) \) arising from the polarizing charge due to microstructure.

This equation does not hold unless the electric field has a perpendicular component to the interface, which is represented by the term \( \hat{x} \cdot \hat{n}(r_s) \), which means that the effect of micro-roughness on the reflectance vanishes if the electric field is everywhere parallel to the interface as in the case shown in Fig. 2.

**Fig (2):** A unidirectional stepped surface, the polarization is parallel to the steps

To solve eq.(3), we must find the mathematical form of the local potential \( \phi(r_s) \), which is related to the shape of the surface's features, this can be obtained either by symmetry (16) or by conformal mapping (17). By applying the symmetry method to evaluate eq.(3) for the lamellar grating, which is shown in Fig. 3. We get an expression for the relative change in complex reflectance (13) due to the model of surface roughness (lamellar grating) with spatial periodicity \( L=2t \) (4).

**Fig. (3):** A cross section of the lamellar grating surface
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\[ \frac{\Delta r}{r} = \frac{4 \pi n a}{\lambda} \left[ 1 - \frac{2 \varepsilon a}{\varepsilon_s} \right] \]

If \(|\varepsilon_s|\) is large and the microstructure varies spatially in only two dimensions \(\phi_1(x)\) is obtained by conformal mapping (17). If we apply this method to evaluate eq. (3) for a rough surface with sinusoidal cross section which is shown in Fig. 4 we get for:

\[ \frac{\Delta r}{r} = \frac{4 \pi n a}{\lambda} \left[ 1 - \frac{2 \varepsilon a}{\varepsilon_s} \right] \frac{\pi d}{2L} \]

This equation gives us the relative change of the complex normal-incidence reflectance.

Fig. (4): the low sinusoidal grating

Fig. (5): The low symmetric ridge

Fig. (6): the isolated low step
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For the roughness model, the ridge which is shown in Fig.5 and the step which shown in Fig.(6) we get:

\[
\frac{\Delta r}{r} = \frac{4\pi l}{\lambda L} \left[ 1 - \frac{2\varepsilon_s}{\varepsilon_s} \right] \frac{d^2}{\pi} \left[ 1/2 + \ln4 + \ln(L/d) \right]
\]  

(6)

For the ridge

\[
\frac{\Delta r}{r} = \frac{4\pi l}{\lambda} \left[ 1 - \frac{2\varepsilon_s}{\varepsilon_s} \right] \frac{d^2}{\pi} \left[ 1/2 + \ln \pi + \ln(L/d) \right]
\]

(7)

Calculations and results

The reflectance of the microscopically rough surfaces \( R_s \) is related and is directly proportional to the reflectance of the equivalent smooth surface \( R_e \) and \( R_s \) is obtained from the following relations (18):

\[
\frac{\Delta R}{R} = 2 \text{Re}\left( \frac{\Delta r}{r} \right)
\]

(8)

where

\[
\frac{\Delta R}{R} = \frac{R_s R_s}{R_r R_r}
\]

so that

\[
R_r = R_s \left( 1 + \frac{\Delta R}{R} \right)
\]

(9)

The dielectric constant is a complex value, therefore \( \Delta r/r \) in turn, is complex, hence, we must separate its real value to obtain \( \Delta R/R \). Assuming that:

\[
\varepsilon_s = \varepsilon_1 + \varepsilon_2
\]

(10)

Fig.(7): the reflectance of a smooth and a microscopically rough surfaces maximum values of reflectivity at (0.30 and 0.40 μm).
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To specify the surface with the lowest reflectance, the equations (4), (5), (6) and (7) were applied using another computer program. The latter determines $R_e$ and compares it for the four rough surfaces in this program had the same dimensions ($L$ and $d$). It was found that the lamellar grating surface is the one with the lowest reflectance as shown in Fig.8. Therefore the rest of the calculation's will be done on this profile, these calculations include the geometrical parameters of the surface.

In general the reflectance in semiconductors is less than that of metals: Fig.7 shows the reflectivity of smooth and rough surfaces of silicon. The intermediate value of the reflectivity is due to the absorption by the impurity levels in the semiconductor, which increases the absorption and decreases reflection. The peaks in the reflectance are due to the absence of impurity levels, which are excited by the corresponding wavelengths. The decrease of reflectance by the rough surface due to the increase in the interacted surface area by the E.M. radiation, vertical interfaces in particular. This behaviour is understood on the bases of the derived equations, eq.(4) to eq.(7), these equations show that reflectance is inversely proportional to the wavelength $\lambda$.

![Graph](image)

Fig.(8): Comparison between the styles of microscopically rough surfaces

**Geometrical Parameters**

The geometrical parameters in microscopically rough surfaces are the dimensions of the protrusions of the microstructure, and is represented by the height of the laminations ($d$), or the thickness of the rough layer, and the surface periodicity ($L$), which is the distance between tow consequent protrusions, as well as the thickness of the laminations for the lamellar grating surface ($t$).
1- The effect of changing (d)

The height of the surface protrusions is a basic parameter whether the surface was scattering (3) or microscopically rough surface (1), and the scattering rough surface is that with scale length of irregularities of the order of the incident wavelength.

For microscopic periodic-rough surfaces, the increment of (d) makes the interacted areas of the vertical interfaces become greater, which enhances the polarized charges at the surface, and hence the induced electric field will increase, and the reflectance will be reduced. The reflectance was calculated for several values of d (200, 300 & 400Å), in a computer program. Fig. 9 shows the result of this program. It is clear that increasing the height of the protrusions reduces the reflectance as is proportional to 1/d especially in the UV region of the EM spectrum. Here the reflectance drops to about 0.08 at λ=0.15 µm while the reflectance curve coincide with that of the smooth surface at the visible region (beyond λ=0.4µm) respectively.

![Fig.9: the effect of changing (d) for the lamellar grating](image)

11-The effect of the periodicity (L)

When the periodicity of the surface roughness is changed, this will change the distance between each two consequent vertical interfaces, as in the lamellar grating, therefore the induced electric field will be changed in turn, so that if (L) is reduced then induced electric field will increase as E ∝ 1/x, where E is the electric field between any two conductors, and x is the distance between them. Fig.10 shows that, when (L) is changed to (0.6, 1.4 & 1.2 µm) the reflectance was reduced, respectively.

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Fig.(10): the effect of changing (L) for the lamellar grating

111- The effect of the thickness of lamination (t)

It is a special parameter for the lamellar grating, and it does not exist in the other types of rough surfaces, this singularity makes the reflectance more controllable. As we mentioned before, when the distance between two consequent faced interfaces is reduced, the induced electric field is enhanced, therefore increasing (t) will increase the induced electric field, i.e. the reflectance will be reduced. Fig. (11) shows that the reflectance of the lamellar grating surface was reduced when (t) had the values (0.2, 0.4 & 0.6 µm), respectively.

Fig. 11 The effect of changing (t) for the lamellar grating

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Conclusions

The reflectance is reduced if the surface was microscopically rough, especially at the UV region. This effect vanishes at larger wavelengths.

The lamellar grating surface has the lowest reflectance among the other types of microscopically rough surfaces.

The increment of the height of surface protrusions reduces the reflectance of the rough surface.

The reduction of the surface periodicity reduces the reflectance of the rough surface.

For the lamellar grating surface, when the thickness of the laminations is increased the reflectance of the rough surface is reduced.

Appendix The real and the imaginary parts of the dielectric constant of Si (After, Willardson, 1986)

<table>
<thead>
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<th>( \lambda / \mu m )</th>
<th>( \varepsilon_1 )</th>
<th>( \varepsilon_2 )</th>
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<tr>
<td>0.15</td>
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<td>2.18</td>
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<tr>
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تأثير الخشونة المسطحية الدورية المجهري على الانعكاس من السطح شبه الموصل

بسام مصطفى و سعود سليمان

المختص

درس تأثير السطوح الخشونة المجهريه الدورية على الانعكاس من سطوح أشباه الموصلات. علمًا أن الطيف قيد الدراسة يغطي الأطوال الموجية من 0.15 إلى 0.70 ميكرون. والخشنة يعني بذلك السطح الذي تكون أبعاد الخشونة السطحية أقل من طول موجة الضوء الساقط، وهذه السطوح أنواع مختلفة من التضاريس. باستخدام نماذج من هذه السطوح الخشونة الدورية مثل المحرز الصفيحي والسطح الجيبي المنخفض أو السطح اليدري المنخفض. فضلاً بإجراء الحسابات بالحاسوب للانعكاسية المعقدة لهذه السطوح وقد وجدنا أن المحرز الصفيحي ذو أذرع إمكانيتين بين النماذج الأخرى. ولذلك درست كل المعلم الهندسي التي تجعل المحرز الصفيحي يمكن من يمكن من الأشعة الساقطة عليه وجميع الحسابات أجريت على أرضية من السيليكون وقد حصلنا على نهاية صفرية للانعكاس في المنطقة فوق البنفسجية.

References


