INTENSITY ENHANCEMENT IN TEXTURED OPTICAL SHEETS FOR SOLAR CELLS

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We adopt a statistical mechanical approach toward the optics of textured and inhomogeneous optical sheets. As a general rule, the local light intensity in such a medium will tend to be $2n^2(x)$ times greater than the externally incident light intensity, where $n(x)$ is the local index of refraction in the sheet. This enhancement can contribute toward a $4n^2(x)$ increase in the effective absorption of indirect-gap semiconductors like crystalline silicon. Also it may lead to a voltage increase equal to $KT\log 4n^2$.

I. INTRODUCTION

In the past decade, there have been a number of suggestions for the use of light trapping by total internal reflection to increase the effective absorption in the indirect-gap semiconductor, crystalline silicon. The original suggestions (1), (2) were motivated by the prospect of increasing the response speed of silicon photodiodes while maintaining high quantum efficiency in the near-infrared.

Subsequently, it was suggested (3) that light trapping would have important benefits for solar cells as well. High efficiency could be maintained while reducing the thickness of semiconductor material required. Additionally, the constraints on the quality of the silicon could be relaxed since the diffusion length of minority carriers could be reduced proportionate to the degree of intensity enhancement. With such important advantages, interest in this approach has continued, but progress in this field has been hindered because there was no method available to calculate the degree of enhancement to be expected.

For example, St. John (1) mentions that total internal reflection will result in two or more passes of the light rays with a proportionate intensity enhancement. On the other hand, Redfield (3) regards the number of light passes, or degree of enhancement, as an adjustable parameter which could vary anywhere between 1 and 100 and he plots the collection efficiency as a function of this parameter. In calculating the ideal efficiency of silicon solar cells, Loferski et al. (4) seemed to imply that perfect light trapping might be possible, which corresponds to an infinite degree of enhancement.

It is the purpose of this paper to show that the degree of intensity enhancement to be expected due to total internal reflection is $2n^2$ which for silicon is ≈ 25. In other words, a light ray in silicon may be expected to make 25 passes on average before escaping. With a proper angular average of the longer path length of oblique rays, the "effective" absorption enhancement factor is $4n^2$ over the case of single pass normally incident rays. Also, we will show that the geometrical details of the silicon shape are relatively unimportant. Whether the silicon is simply roughened on one side (1), (2) or whether precisely angled grooves are etched into the surface (3), (4), the overriding tendency will be for an enhancement factor of $4n^2$ provided only that the surface is sufficiently strongly textured. Finally, we will show that in an inhomogeneous sheet, for example a composite, the enhancement will be given by the same formula employing the local index of refraction $n(x)$.

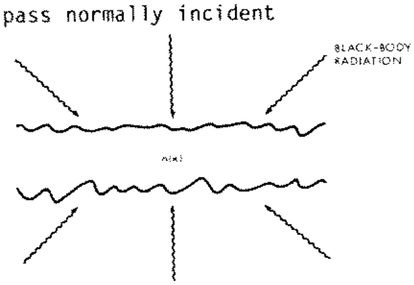

Fig. 1. An inhomogeneous and textured optical sheet with position-dependent index of refraction $n(x)$ immersed in black-body radiation.

This intensity enhancement can translate into either an increase in the short circuit current or in a properly designed solar cell it can lead to a voltage improvement of $KT\log 4n^2$.

Two distinct derivations will be presented in the following two sections. In Chapter 2, we will give a derivation based on statistical mechanics. Such an approach is very powerful

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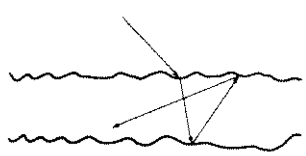
and it can be generalized to situations where geometrical optics is inapplicable (though we will not attempt such a generalization in this paper). In Chapter 3, a geometrical optics derivation will be presented. Its simplicity will permit us to better recognize some of the prerequisites and limitations of this type of intensity enhancement. In Chapter 4, we will show how these considerations are modified in the presence of absorption. Finally, in Chapter 5, we indicate how these effects can lead to a voltage enhancement in addition to a short circuit current improvement.

II. STATISTICAL MECHANICAL DERIVATION

Consider an inhomogeneous optical slab with position-dependent index of refraction $n(x)$ as illustrated in Figure 1. Let the index of refraction vary sufficiently slowly in space, so that a density of electromagnetic modes may be defined, at least locally inside the sheet.

Now place the optical medium into a region of space which is filled with black-body radiation in a frequency band $d\omega$ at a temperature T. When the electromagnetic radiation inside the medium approaches equilibrium with the external black-body radiation, the electromagnetic energy denisty (5) is



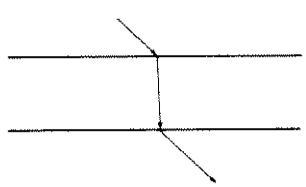


Fig. 2. Two optical sheets with qualitatively different surface textures. (a) Angular randomization and intensity enhancement do occur. (b) In a plane-parallel slab, there is no angular randomization and no intensity enhancement.

$$U = \frac{h\omega}{\exp\{h\omega/KT\} - 1} \frac{2d\Omega\, k^2\, dk}{(2\pi)^3} \tag{1}$$

This is the standard Planck formula for black-body radiation in a vacuum, but as Landau and Lifshitz show (5), it can be adapted to any optical medium by making $k = n\omega/c$. In addition, the energy density may be changed to an intensity I (power per unit area), by multiplying (1) by the group velocity $v_g = d\omega/dk$. Making both changes in (1) we obtain

$$I \equiv Uv_g = \frac{h\omega}{\exp\{h\omega/KT\} - 1} \frac{2d\Omega n^2}{(2\pi)^3} \frac{\omega^2}{c^2} d\omega \tag{2}$$

This differs from the vacuum black-body intensity simply by the factor n^2. Therefore, the intensity of light in a medium which is in equilibrium with external black-body (bb) radiation is n^2 times greater

$$I_{int}(\omega,x) = n^2(\omega,x) I^{bb}_{ext}(\omega) \tag{3}$$

This factor comes about simply due to the fact that the density of states in such a medium is proportional to n^2 and the equipartition theorem guarantees equal occupation of the states, internal as well as external.

Now let us decide whether or to what degree the situation changes when an arbitrary external radiation field replaces the black-body radiation. Since we are considering a transparent medium, inelastic events such as absorption and reemission at another frequency are not permitted. Therefore, each spectral component may be considered individually. In this circumstance, departure of the external field from an exact black-body frequency distribution will not affect Equation (3), which will remain valid separately at each frequency ω.

A much more serious question, which will be the main focus of this paper, is: What happens when the external radiation field departs from the isotropic distribution of black-body radiation? This situation is illustrated in Figure 2(a), where the external light is shown to be collimated. If the surface of the optical sheet is quite irregular in shape, then the light rays, upon entering the medium, will lose all memory of the external incident angle after the first, or at most the second, scattering from a surface. In other words, all correlation with the external angle will be lost almost immediately upon refraction or total internal reflection, especially when averaged over the illuminated surface of the sheet. If this condition is satisfied, then a collimated incident beam of intensity I_{ext} will produce, inside the optical sheet, a random angular distribution of light, no matter which direction the beam happens to be coming from. Therefore, a collimated beam, when subdivided so that it illuminates the optical medium equally from all directions produces identical internal light distributions under those respective conditions. The condition of isotropic illumination is, however, equivalent to that of black-body illumination. Therefore, Equation (3) remains valid whether the external field is isotropic as in the black-body case or whether it is collimated.

$$I_{int}(\omega,x) = n^2(\omega,x) I_{ext}(\omega) \tag{4}$$

Equation (4) will be corrected for certain surface transmission factors in Section 3, but it is a key formula in this paper. It rests on the assumption that all correlation of the internal rays with the external angle of incidence is lost almost immediately upon entering the medium and/or upon averaging over the illuminated surface. Even optical sheets with ordered surface textures will show the type of randomization we are discussing here. The reasons are as follows:

a) If light randomization does not occur upon the entering refraction, it can occur on the first internal reflection.

b) If not on the first reflection, then on the second.

c) If not then, it can still be the result of a spatial average over the illuminated surface area.

d) If not even then, it can still result from angular averaging due to motion of the source, like the sun moving through the sky.

In other words, there is a rather overwhelming tendency toward randomization in the angular distribution of light and toward the validity of Equation (4), but it is not always satisfied.

Consider the simple plane-parallel slab shown in Figure 2(b). Clearly, there is no intensity enhancement in that case.[1] To distinguish between the class of geometries for which Equation (4) is valid and the class of geometries in which it is invalid is a problem in ergodic theory and in measure theory. We will not attempt in this paper to distinguish between these two classes mathematically in the measure theory sense. Instead, we will assume that the statistical approach is valid except in those few geometries where a cursory inspection shows that randomization cannot occur under any of the circumstances listed earlier, a) to d). Equation (4) will be valid provided any of those prerequisites, a) to d), is satisfied.

Now consider the situation shown in Figure 3. In that geometry, the light is confined to a half space by the presence of a white reflective plane. In effect, the light intensity external to the optical sheet has been doubled by virtue of reflection from the white surface. The total intensity enhancement will then be given by

$$I_{int}(\omega,x)=2n^2(\omega,x)I_{inc}(\omega) \qquad (5)$$

where $I_{inc}(\omega)$ is the incident light intensity.

One of the key implicit assumptions that we have not emphasized earlier is that there be no absorption, either within the volume or on the surface of the medium. Optical absorption effects will be treated in Section 4.

The main conclusion of this section is that a statistical mechanical approach results in the intensity enhancement given in Equation (5). The factor $2n^2$ can be quite substantial; i.e., approximately 25 for silicon and approximately 15 for TiO_2. Even conventional glass with an index of 1.5 has an enhancement factor equal to 4.5. In view of the importance of this result, we give an alternative derivation based on geometrical optics in the next section.

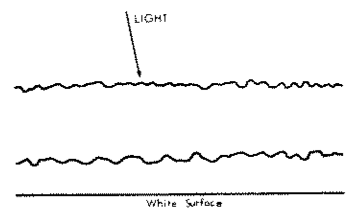


Fig. 3. A white reflective surface effectively doubles the external intensity and increases the enhancement factor to $2n^2$.

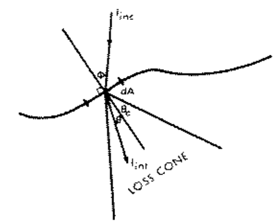


Fig. 4. The balance between incoming and outgoint radiation determines the internal intensity I_{int}.

III. GEOMETRICAL OPTICS DERIVATION

Our approach is based on "Detailed Balancing" of the light which is incident on a small area element dA, and the light in the loss cone which escapes from it. Consider the geometry shown in Figure 4. Let I_{inc} be the incident radiation power per area element dA. A fraction T_{inc} (ϕ) of this light will be transmitted through the incoming interface, where ϕ is the angle of incidence. This must be balanced by the internal radiation which escapes. Let us assume that the internal radiation is isotropic due to the randomizing influence of refraction and reflection from the textured interfaces as discussed in the previous section. Let B_{int} be the internal intensity per unit internal solid angle. The internal intensity I_{int} on both sides of an area element dA is given by

$$I_{int}= \int B_{int}\cos\theta \, d\Omega$$

where $\cos\theta$ is the reduction of intensity on the area element due to oblique incidence. In this paper we will follow the convention that internal intensity I_{int} is bidirectional while the incident intensity I_{inc} is unidirectional. Therefore

$$I_{int} = 2 \times 2\pi \int_0^{\pi} B_{int}\cos\theta \sin\theta \, d\theta$$

$$I_{int} = 2\pi B_{int}$$

Only a small fraction of this power per unit area will escape, since the loss cone solid angle is much less than 4π steradians. The intensity which escapes is

$$I_{esc} = 2\pi \int_0^{\theta_c} \frac{I_{int}}{2\pi} T_{esc}(\theta) \cos(\theta) \sin\theta \, d\theta \quad (6)$$

where $n \sin\theta_c = 1$ and θ is the internal angle of incidence. If we substitute a weighted average transmission factor $\overline{T_{esc}}$ for the angle-dependent surface transmission factor $T_{esc}(\theta)$, then the integral in Equation (6) may be easily computed.

$$I_{esc} = I_{int} \frac{\overline{T_{esc}}}{2n^2}$$

If we now apply the principle of "Detailed Balancing", the entering intensity is made equal to the escaping intensity

$$T_{inc}(\phi) I_{inc} = I_{int} \times \frac{\overline{T_{esc}}}{2n^2}$$

Therefore

$$I_{int} = 2n^2 \times \frac{T_{inc}(\phi)}{\overline{T_{esc}}} \times I_{inc} \quad (7)$$

As Equation (7) shows, the enhancement may be increased beyond $2n^2$ if $T_{inc}(\phi)$, the transmission factor into the medium, is greater than $\overline{T_{esc}}$ the average transmission factor out of the medium. Of course, time-reversal invariance guarantees that $T_{inc}(\phi) = T_{esc}(\theta)$. If the incident radiation is isotropic then the ratio $\overline{T_{inc}}/\overline{T_{esc}} = 1$ would appear in Equation (7), ensuring that the enhancement factor is $2n^2$ as it must be for black-body radiation. For collimated radiation, an additional small enhancement $T_{inc}(\phi)/\overline{T_{esc}}$ is possible, but this comes at the expense of angular selectivity. This is fully consistent with the ordinary "Brightness Theorem" of geometric optics (6), which states that intensity increases must come at the expense of angular selectivity. Because of the tendencies toward angular averaging described in Section II, the factor $T_{inc}(\phi)/\overline{T_{esc}}$ will be approximated as unity and, for most purposes, Equation (7) can be rewritten

$$I_{int} = 2n^2 \times I_{inc} \quad (8)$$

It is interesting that Equation (8) itself could also have been derived directly from the "Brightness Theorem" (6) by taking note of the fact that the brightness defined in a medium differs from that in a vacuum simply by the factor n^2.

The intensity decreases discussed thus far in this paper do not necessarily translate directly into absorption enhancements. This will be the subject of the following section.

IV. ABSORPTION ENHANCEMENT

Two types of absorption can modify the results we have presented this far; volume absorption in the textured optical sheet and surface absorption. In general, both types may be expected to be present. For example, in a semiconductor solar cell material, there would be absorption in the semiconductor itself and also at the surfaces due to absorption in the "transparent" electrodes, and due to imperfect reflectors at the rear surface. In this section, we will model the intensity-enhancement effects allowing for absorption. First we will set up a general method. Then we will model a specific geometry that might be of interest for solar cells.

The approach we will follow is to balance the input of light from external sources with the loss of light from the optical medium by absorption and refraction through the escape cone. The light input is $A_{inc} I_{inc} T_{inc}$, where A_{inc} is the surface area on which light is incident and the other symbols have the same meaning as before. To estimate the loss of light, we will proceed along the same lines as in Section 3. We will assume that the light internal to the medium is isotropic due to the randomizing influence of refraction and reflection. There will be three contributions to light which is lost:

1) Light will escape through the escape cone at the rate

$$\frac{A_{esc} I_{int} \overline{T_{esc}}}{2n^2}$$

where A_{esc} is the surface area from which light can escape, which is not necessarily equal to A_{inc}, and the other symbols have the same meaning as before.

2) Light may be absorbed due to imperfect reflection from the boundaries

$$\int_0^{\pi/2} \eta A_{refl} I_{int} \cos\theta \sin\theta \, d\theta = \frac{\eta A_{refl} I_{int}}{2}$$

where η is the fractional absorption due to imperfect reflection at the boundaries and A_{refl} is the surface area of imperfect reflection.

3) Finally, there may be absorption within the bulk

$$\int \frac{\alpha I_{int}}{2\pi} dV\, d\Omega \approx \alpha \ell I_{int} A_{inc} \int_0^{\pi} \sin\phi \, d\phi = 2\alpha\ell I_{int} A_{inc} \quad (9)$$

where dV is a volume element in the bulk, α is the absorption coefficient, and Equation (9) may be regarded as a definition of the effective thickness ℓ. This will be approximately the mean thickness of the sheet. Equation (9) implicitly assumes that the bulk absorption is sufficiently weak that I_{int} is uniform throughout the volume.

Equating the light gained to the light lost

$$A_{inc} T_{inc} I_{inc} = \left\{ \frac{A_{esc}\overline{T_{esc}}}{2n^2} + \frac{nA_{refl}}{2} + 2\alpha\ell A_{inc} \right\} I_{int} \quad (10)$$

Regarding I_{int} as the unknown, the expression may be rewritten

$$I_{int} = \frac{T_{inc} I_{inc}}{\{(A_{esc}/A_{inc})(\overline{T_{esc}}/2n^2)+(n/2)(A_{refl}/A_{inc})+2\alpha\ell\}} \quad (11)$$

Although Equation (11) is much more complex than Equation (7) and Equation (8), there are many realistic situations where the simpler expressions are adequate approximations.

One of the main questions we have in this paper is the extent to which the effects we have

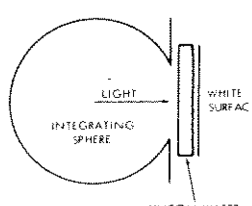


Fig. 5. The integrating sphere was used to determine the light absorbed in the silicon wafer. A comparison is made between the reflectivity of a wafer with a rough ground rear surface (as shown) and with a polished rear surface. In the former case, there was some light lost out the edges of the silicon wafer as well as by absorption.

been discussing will act to enhance volume absorption. Using Equation (11) the volume absorption may be written

$$2\alpha\ell A_{inc} I_{int} = \frac{2\alpha\ell A_{inc} T_{inc} I_{inc}}{\{(A_{esc}/A_{inc})(\overline{T_{esc}}/2n^2)+(n/2)(A_{refl}/A_{inc})+2\alpha\ell\}}$$

The fraction of the incoming light which is absorbed in the volume is

$$f_{vol} \equiv \frac{2\alpha\ell A_{inc} I_{int}}{A_{inc} I_{inc}} = \frac{2\alpha\ell T_{inc}}{\{(A_{esc}/A_{inc})(\overline{T_{esc}}/2n^2)+(n/2)(A_{refl}/A_{inc})+2\alpha\ell\}} \quad (12)$$

This reduces simply to the transmission factor T_{inc} of the incoming light in the limit of very high absorption coefficient α.

A corresponding expression may be written for the total fraction absorbed, including absorption due to imperfect reflection at the surfaces

$$f_{tot} = \frac{2\alpha\ell+(n/2)(A_{refl}/A_{inc})}{(A_{esc}/A_{inc})(\overline{T_{esc}}/2n^2)+(n/2)(A_{refl}/A_{inc})+2\alpha\ell} T_{inc} \quad (13)$$

The absorption enhancement in Equation (12) and Equation (13) is of direct interest for weakly absorbing indirect-gap semiconductors like crystalline silicon. As Equation (12) shows, volume absorption can be very substantial even when $\alpha\ell$ is only $1/4n^2$ which is 1/50 for silicon. The absorption enhancement factor is twice the intensity enhancement factor due to angle averaging effects. The use of these formulas is best illustrated by some specific examples.

Consider the reflectivity of a silicon wafer as measured on an integrating sphere, which is shown in Figure 5. For these measurements, a white reflective medium was placed behind the wafer. The front surface of the wafer was polished. The main idea is to compare the overall reflectivity when the rear surface is either ground rough or polished smooth. The comparison is made in Figure 6. With both surfaces polished, we have a plane parallel plate, the situation described in Figure 2(b) where angular randomization within the silicon does not occur. The light simply makes a round trip in the wafer.

On the other hand, if the rear surface of the silicon is ground rough, internal angular randomization does occur. We may apply Equation (12) and Equation (13) to this situation. The Fresnel transmission of the silicon front surface T_{inc} is about 0.68. The areas A_{esc} and A_{inc} are the same and equal to the front surface area. The rear surface was covered with $MgCO_3$ an almost perfect white reflector, which is frequently used as a reference of whiteness. In the geometry of Figure 5, the edges of the silicon wafer are actually external to the intergrating sphere. Some of the internally trapped light, therefore, escapes across the cylindrical surface defined by the periphery of the round opening in the integrating sphere.

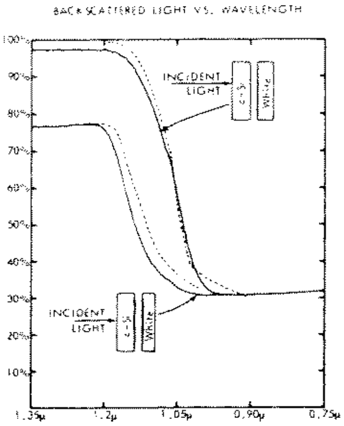


Fig. 6. The reflectivity of a silicon wafer whose rear surface is either ground rough or smoothly polished. Smooth lines are experiment. The dashed lines are theory. The theory for the rough ground surface is (13) in the text. The theory for the smooth polished surface assumes simple round-trip absorption.

This cylindrical surface in the silicon can be regarded as an imperfect reflector of area $A_{refl} = 2\pi r\ell$ where r is the radius of the opening in the integrating sphere. Therefore

$$A_{refl}/A_{inc} = 2\pi r\ell/\pi r^2 = 2\ell/r$$

The parameters in this experiment were r=1 cm and ℓ = 0.025 cm. The quantity η which represents the departure from unit reflectivity at this edge is difficult to estimate a priori, since it depends on the details of the roughness. The value η = 0.82 describes well the wavelength-independent backscattered light in Figure 6 in the transparent region between 1.2 and 1.35 μm. With these values for parameters and the known wavelength-dependent (7) absorption coefficient, a fairly good fit is obtained between $(1 - f_{tot})$ from Equation (13) and experiment through the band-edge transition wavelengths (dashed and smooth lines, respectively, in Figure 6).

The geometry described in Figures 5 and 6 is a very favorable one for solar cells and was first described (1), (2) some time ago. Figure 6 shows clearly the shift of the effective absorption edge toward the infrared for the light-trapping case.

V. OPEN CIRCUIT VOLTAGE ENHANCEMENT

It is obvious that any improvement in the "effective" absorption of a semiconductor sheet would result in an increased infrared photoresponse by a solar cell. This would produce an improvement in the short circuit current. It is important to point out that improved current is not the only way in which these intensity enhancement effects can manifest themselves. If the thickness of the semiconductor layer were reduced proportionate to the improved effective absorption, then the short circuit current would be unchanged, but the open circuit voltage could be increased.

Such a voltage improvement is not automatic by any means. But if the voltage is limited by recombination in the active region, then a reduction in thickness of the active region could result in a voltage improvement. If, on the other hand diffusion current limits the voltage, as is often the case, then thickness reduction would not have a significant effect on the open circuit voltage.

The open circuit voltage of a solar cell is given by

$$V_{oc} = KT \log (J_{sc}/J_{rec})$$

where J_{sc} is the short circuit and J_{rec} is the recombination current in the dark. This may be due to nonradiative recombination at defects in the semiconductor, or more fundamentally due to unavoidable radiative recombination. Shockley and Quiesser (8) took the semiconductor layer to be surrounded non-absorbing material. They included only that recombination radiation which was in the loss cone, and only the light escaping from one of the two surfaces. These are the most favourable assumptions, as is appropriate for calculating an upper limit. They obtained:

$$J_{rec} = \frac{2\pi e}{c^2} \int_{\nu_g}^{\infty} [\exp (h\nu/KT)-1]^{-1} \nu^2 d\nu \qquad (14)$$

where ν_g is the band gap frequency. If on the other hand, one or both surfaces of the semiconductor are absorbing, then all internally emitted light counts as nonradiative recombination. If in addition the semiconductor is optically thin to its own luminescence then Equation (14) must be re-written as:

$$J_{rec} = \frac{8\pi n^2 e}{c^2} \int_0^{\infty} [\exp (h\nu/KT)-1]^{-1} \nu^2 \alpha(\nu)\ell d\nu \qquad (15)$$

An optically enhanced solar cell satisfies the requirements of Equation (14) and is in principle capable of an increase in V_{oc} = KTlog $4n^2$ or about 100 mV for the index of crystalline silicon.

An optically unenhanced solar cell, such as one with absorbing electrodes, potentially pays a 100 mV penalty. Of course, in today's solar cells radiative recombination in the volume of the cell is not the limit on voltage performance. Whether the recombination is radiative or not, as long as it is determined by the volume of the active material, a thin solar cell will have a KTlog $4n^2$ voltage advantage over a thick cell. If on the other hand diffusion current to

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