The Role of Surface Roughness in Plasmonic-Assisted Internal Photoemission Schottky Photodetectors

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ABSTRACT: Internal photoemission of charged carriers from metal to semiconductors plays an important role in diverse fields such as sub-bandgap photodetectors and catalysis. Typically, the quantum efficiency of this process is relatively low, posing a stringent limitation on its applicability. Here, we show that the efficiency of hot carrier injection from a metal into a semiconductor across a Schottky barrier can be enhanced by as much as an order of magnitude in the presence of surface roughness on the scale of a few atomic layers. Our results are obtained using a simple semianalytical theory and indicate that properly engineered plasmonic-assisted internal photoemission photodetectors can be a viable alternative in silicon photonics. Other applications, such as plasmonic-enhanced photocatalysis, can also benefit from these results.

KEYWORDS: plasmonics, photodetectors, Schottky barrier, internal photoemission, surface enhancement, scattering

Silicon is the material of choice in the microelectronics industry for several decades. In recent years, the use of silicon has been expanded to new areas. In particular, the field of silicon photonics has recently emerged, involving the ability to guide and manipulate light on a chip that is fabricated with a standard complementary metal oxide silicon (CMOS) technology and is based on silicon on insulator structures. Above other advantages, silicon is transparent at the telecom wavelength bands around 1.3 and 1.55 μm. Indeed, a variety of silicon photonics devices have been demonstrated over the years, including waveguides, modulators, splitters, biosensors, and more. Yet, while silicon photonics is a promising platform for optical devices, its quantum efficiency is typically well below 1%, which contradicts several experimental results. Several explanations were proposed, including the high confinement of light, increasing the transmission cross section of the electrons from the metal into the semiconductor, and others. But while all these theories can explain the enhanced rate of hot carrier excitation...
in plasmonic nanoparticles, none of them can remotely account for the hot electron injection efficiency exceeding most theoretical predictions by an order of magnitude.

While the previous models assumed specular reflection of electrons from a flat interface between a metal and semiconductor,30,32 a practical “smooth” interface will always show roughness of at least a few atomic layers.44 Such roughness is expected to play a significant role in altering the probability of electron transfer over the Schottky barrier. Hereby, we analyze the role of surface roughness in enhancing the IPE probability using a perturbative model, which shows that even relatively small roughness can lead to a dramatic increase in the transmission probability of electrons into the semiconductor and therefore resulting in a significant increase in the quantum efficiency of IPE-based photodetectors. Our work can be used to better understand the experimentally observed enhanced IPE efficiency34–36 and to provide guidelines for achieving better IPE-based Schottky photodetectors with higher responsivities, in both free space and guided mode configurations.

**HOT ELECTRON INJECTION ACROSS THE SMOOTH INTERFACE**

We start our analysis by calculating the probability of hot electrons with energy $E$ above the Fermi level to be injected over the effective (i.e., including the effects of image force and reverse bias) potential barrier $\phi_b$ in the absence of roughness (i.e., flat interface). For that, we find the relation between the lateral wavevector $k_{\parallel \text{lm}}$ (continuous across the boundary) and the normal to the interface wavevectors $k_{\text{zm}}$ and $k_{\text{zs}}$ (the wavevectors in metal and semiconductor, respectively)

$$k_{\text{zm}} = \sqrt{k_F^2 - k_{\text{lim}}^2}$$

$$k_{\text{zs}} = \sqrt{k_{\text{max}}^2 - k_{\text{lim}}^2}$$

$$k_{\text{max}}^2(E) = \frac{2m_e}{\hbar^2}(E - \phi_b) = \frac{m_e}{m_0} E - \phi_b k_F^2$$

(1)

where $k_F$ is the Fermi wave vector, $E_F = \hbar^2 k_F^2 / 2m_0$ is the Fermi energy, and $m_0, m_e$ are the mass of the electron in the metal and the effective mass of the electron in the semiconductor, respectively. The wavevectors are all shown in Figure 1.

Only the hot electrons with lateral wave vectors less than $k_{\text{max}}$ have a finite probability to be injected over the Schottky barrier, i.e., $k_{\parallel \text{lm}} \leq k_{\text{max}}$. This defines a cone of allowed wave vectors of hot electrons that can be injected into the semiconductor.14,23,32,47 The cone angle is given by

$$\sin^2 \theta = \frac{k_{\parallel \text{lm}}^2}{k_F^2}$$

The escape cone can be seen (purple solid cone) in Figure 1c.

Inside the cone, the transmission coefficient of electrons from metal to semiconductor is

$$T(k_{\parallel \text{lm}}) = 1 - \frac{|k_{\text{zm}} - k_{\text{zs}}|^2}{|k_{\text{zm}} + k_{\text{zs}}|^2}$$

(2)

and as we only consider the in-plane wavevectors up to $k_{\text{max}}$ (see Figure 1a), all the wavevectors are real and

$$T(k_{\parallel \text{lm}}) = \frac{4k_{\text{zm}}k_{\text{zs}}}{(k_{\text{zm}} + k_{\text{zs}})^2}$$

(3)

The transmission probability is calculated by integrating eq 3 over all the allowed wave vectors. Before integration, let us make an approximation by assuming the constant density of states in the metal in the vicinity of the Fermi level. Normalizing all the wavevectors to $k_F$, we find the transmission probability via averaging over the lateral wavevector $k_{\parallel \text{lm}}$:

$$T(E) \equiv T(k_{\text{max}}) = \frac{\int_0^{k_{\text{max}}} T(k_{\parallel \text{lm}}) k_{\parallel \text{lm}} \, dk_{\parallel \text{lm}}}{\int_0^{k_{\text{max}}} k_{\parallel \text{lm}} \, dk_{\parallel \text{lm}}} = 8 \int_0^{k_{\text{max}}} \frac{\sqrt{1 - k_{\text{lim}}^2} \sqrt{k_{\text{max}}^2 - k_{\text{lim}}^2}}{\left(\sqrt{1 - k_{\text{lim}}^2} + \sqrt{k_{\text{max}}^2 - k_{\text{lim}}^2}\right)^2} k_{\parallel \text{lm}} \, dk_{\parallel \text{lm}}$$

(4)

To ascertain the importance of finite reflection, we first find out the transmission probability in the absence of reflection within the allowed cone of transmission in the momentum space. This is achieved assuming perfect transmission, i.e., $T(k_{\parallel \text{lm}}) = 1$ in eq 3. Substituting in eq 4, one obtains
Figure 2. (a) Hot electron injection probability from Au into Si as a function of hot electron energy including (solid line, eq 4) and neglecting (dotted line, eq 5) finite reflectivity at the interface. (b) Hot electron injection probability from Au into Si as a function of the incident photon (plasmon) energy including (solid line, eq 7) and neglecting (dotted line, eq 6) finite reflectivity at the interface. In both cases, the finite reflectivity reduces the probability of hot electron injection by as much as a factor of 2.

Next, we calculate the exact result from eq 4, including the effect of the finite transmission within the cone of angles in the momentum space. The result is shown as a solid line in Figure 2(a) for the case of the Au \((E_F = 5.5 \text{ eV}, k_F = 12 \text{ nm}^{-1})\)–Si \((m_s = 0.3m_0)\) interface with the barrier \(\phi = 0.5 \text{ eV}\). As one can see, the finite reflection reduces the probability of hot electron injection by as much as a factor of 2.

We now turn to describe the probability of internal photoemission of a hot electron that is generated by a photon \(\hbar \omega\). In the absence of reflection, this is achieved by integrating eq 5 over all the energies from \(\phi_b\) to \(\hbar \omega\). Doing so, we get

\[
T_0(E) = k_{_\text{max}}^2(E) = \frac{m_s E - \phi}{m_0 E_F},
\]

shown as a dotted line in Figure 2(a).

For a flat interface between the metal and the semiconductor, an electron having a parallel momentum, \(k_{_\text{im}} > k_{_\text{max}}\) (outside of the transmission cone), will be reflected and thus cannot be transported into the semiconductor. However, surface roughness can assist in relaxing the momentum mismatch and provide a path for the electron to be transmitted into the semiconductor. In the limit of the perturbation theory (small roughness), the probability of surface roughness scattering of the electron incident onto the interface with a lateral wavevector \(k_{_\text{im}} > k_{_\text{max}}\) into the state in the semiconductor with the lateral wavevector \(k_{_\text{is}}\) can be evaluated according to the Fermi golden rule as

\[
P(E, k_{im}, k_{is}) = \frac{2\pi}{\hbar} |\langle \Psi_m(E, k_{im})|H_{fl}|\Psi_s(E, k_{is})\rangle|^2 \times \rho(E, k_{is})
\]

Here the wave function of the incident electron includes contributions of the incident, reflected, and evanescent waves,

\[
\Psi_m(E, k_{im}) = \begin{cases} 
1 & \text{if } z \leq 0 \\
\frac{2k_{zm}}{k_{zm} + jq_z} e^{-j\eta_z} & \text{if } z > 0 
\end{cases}
\]

where \(k_{zs} = \sqrt{k_{zm}^2 - k_{z\text{max}}^2}\), \(q_z\) is the wavevector in the semiconductor, and the wave function has been normalized to the electron velocity in the metal, \(\nu_{zm} = h k_{zm}/m_{mp}\) as it is commonly done in current probability calculations. The wave function in the semiconductor involves incident and reflected waves as well as the wave transmitted into the metal and propagating with the wavevector \(k_{z\text{1m}} = \sqrt{k_{p}^2 - k_{zs}^2}\),

\[
\Psi_s(E, k_{is}) = \begin{cases} 
\frac{e^{-j\eta_z}}{k_{zs} + k_{z1m}} & \text{if } z > 0 \\
\frac{2k_{zs}}{k_{zs} + k_{z1m}} e^{-j\eta_z} & \text{if } \eta_z \leq 0 
\end{cases}
\]

where \(L\) is the normalization distance and \(a \approx 2\) for \(k_{zs} \ll 1\). The density of final states is the one-dimensional density of states for one spin multiplied by a factor of 2 for the valley degeneracy factor since the only states in Si into which a hot carrier can tunnel are two X-valleys located along the [001] direction.

\[
\rho(E, k_{is}) = \frac{2L}{\pi \hbar k_{zs}} = \frac{2\eta_z L}{\pi \hbar k_{zs}}
\]
Finally, the interface roughness $h(r)$ is described by the mean square height $h_0^2$ and correlation length $\Lambda$, and its Fourier power spectrum is

$$l(h(k_{gr}))^2 = \pi h_0^2 \Lambda^2 \exp(-k_{gr}^2 \Lambda^2/4)$$ (12)

We use the subscript "gr" for the wave vector because eq 12 represents the rough surface as a superposition of gratings with grating wavevector $k_{gr}$ providing momentum-matching between the electronic state in the metal $|\Psi_m\rangle$ whose lateral wavevector $k_{\parallel m}$ is outside the escape cone and the electronic state in the semiconductor $|\Psi_s\rangle$ whose lateral wavevector $k_{\parallel s}$ is inside the escape cone (Figure 1a,c). In this respect, the role played by interface roughness as the "randomized grating for electrons" is identical to the role played by the roughened surface acting as a grating that allows photons to avoid total internal reflection when they emerge from the optically dense medium into the air, a fact used to enhance external efficiency of light-emitting diodes.

Examples of a typical interface roughness profile for $h_0 = 0.0033$ nm and different correlation lengths are shown in Figure 3.

From the power spectrum of the roughness we can derive the Hamiltonian as

$$H_R(k_{||}) = E_R h(k_{||}) \delta(z)$$ (13)

Substituting eq 13 in eq 8 one obtains

$$P(E, k_{||m}, k_{||s}) = \frac{2\pi}{\hbar} \frac{h_0^2 \Lambda^2}{\pi n_0} \exp(-\Delta k_{||}^2 \Lambda^2/4) \times |\Psi_m(E, k_{||m}, 0)|^2 |\Psi_s(E, k_{||s}, 0)|^2 \times \frac{2m_e \hbar^4 k_{||}^4}{\pi^2 \hbar^2 k_{gr}^2 m_0^2}$$ (14)

where the scattering wave vector $\Delta k_{||} = (k_{||m} - k_{||s})^2$.

Next we normalize all the wavevectors to $k_F$ and both $h_0$ and $\Lambda$ to $k_F^{-1}$ (i.e., introduce $k' = k/k_F$, $h_0' = h_0 k_F$ and $\Lambda' = \Lambda k_F$ and later drop the "prime"). Then we calculate the probability of scattering from a particular state in the metal by performing integration over the whole range of the wavevectors in the silicon ($k_s$), which in our case would mean to do the integral

$$\int_{-1/4}^{1/4} \int_0^{k_{||m}} dk_{||} \int_0^{k_{||s}} dk_{||}$$

where $1/4 \pi^2$ is the density of states in $k$ space to obtain

$$P(E, k_{||m}, k_{||s}) = \frac{2m_e}{\pi n_0} \sqrt{1 - k_{||m}^2} h_0^2 \Lambda^2 \exp(-\Delta k_{||}^2 \Lambda^2/4) \times \int_0^{k_{||m}} \sqrt{1 - k_{||}^2} e^{-i k_{||} \Lambda z/\hbar} \int_0^{k_{||s}} e^{-i k_{||} \Lambda z/\hbar} \int_0^{k_{||m} - k_{||s}} e^{-i k_{||} \Lambda z/\hbar}$$ (15)

Using the relation

$$\int_0^{2\pi} e^{-i k_{||} \Lambda z/\hbar} d\theta = 2\pi I_0(k_{||} \Lambda z/2)$$ (16)
Ek m

which makes the re-

m

it is expected to make the impact of roughness only stronger, as

the band structure near X valleys is neglected in this work, but

correlation length; (b) versus electron energy. The injection e

in a single valley,

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square roughness of

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ow (saturation) yields

This result is obtained in the small perturbation approx-

imation, which assumes that there is no reverse

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sion for the smooth interface is shown as a dashed line.

where $I_0$ is the modified Bessel function of the first kind (or

hyperbolic Bessel function), one obtains

$$
P(E, k_{\|m}) = 4 \frac{m}{m_0} \frac{\sqrt{1 - k_{\|m}^2}}{1 - k_{\max}^2} \frac{\lambda_h}{2} e^{-\lambda_h} k_{\|m}^{\lambda_h / 4}$$

$$
\times \int_{k_{\max}}^{k_{\max}} \frac{k_{\max}^2 - k_{\|m}^2}{(\sqrt{k_{\max}^2 - k_{\|m}^2} + \sqrt{1 - k_{\|m}^2})^2}$$

$$
\times I_0(k_{\|m}^2/2)e^{-k_{\|m}^2/4}dk_{\|m}$$

(17)

This result is obtained in the small perturbation approx-

imation, which assumes that there is no reverse flow from the

sider interaction with photons). Correcting for this reverse

ow (saturation) yields

$$
P'(E, k_{\|m}) = \frac{P(E, k_{\|m})}{1 + 2P(E, k_{\|m})}$$

(18)

Finally, we average over the all possible incidence angles in the

etal, i.e., integrate over $k_{\|m}$ normalize by

\int_{k_{\max}}^{k_{\max}} k_{\|m} dk_{\|m} = 1/2
to obtain

$$
P_E(E, h_0, \Lambda) = 2 \int_{k_{\max}}^{k_{\max}} P'(k_{\|m}) k_{\|m} dk_{\|m}$$

(19)

RESULTS AND DISCUSSIONS

We assume the aforementioned Au–Si interface with a mean

square roughness of $h_0 = 0.33$ nm and wide range of

correlation lengths shown in Figure 3. In the absence of
detailed analysis of the interface available to us these shapes

with a roughness between one and two atomic layers appears

to be reasonable $^{45,46,51,52}$ Furthermore, in relative units $h_0 k_{\max} \ll \pi$ and the small perturbation analysis is justified. The

effective mass is taken to be the effective density of state mass

in a single valley, $m_e \approx 0.3 m_0$. The effect of strong anisotropy of the band structure near X valleys is neglected in this work, but

it is expected to make the impact of roughness only stronger, as

it is the large longitudinal effective mass that would appear in

eq 17.

In Figure 4a we show the probability of the interface

rownness assisted hot electron injection for $h_0 = 0.33$ nm with

four different values of energy versus the correlation length $\Lambda$. Clearly, there exists an optimum value of $k_F \Lambda \approx 4$ at which

he injection is optimal. It can be shown that the mean value of the

attering wavevector ($\Delta k_{\|} = k_{\|}$) is on the scale of $k_F/\sqrt{2}$. It

can also be shown that eq 12 peaks at $k_{\|} \Lambda = 2$. Thus, one would expect that the strongest transmission

ould then take place in the vicinity $k_{\|} \Lambda \approx 3$

$\left(k_{\|} \Lambda = 2 \rightarrow k_{\|} \Lambda = 2 \rightarrow k_{\|} \Lambda \approx 3\right)$, which makes the re-

ults in Figure 4a perfectly reasonable considering the

ymmetric shape of eq 12. In Figure 4b the transmission

ression efficiency) versus hot electron energy is shown

or different $\Lambda$’s. Also the injection efficiency for a smooth

ace is shown as a dashed line in Figure 2(a). Clearly,

hancement by nearly 1 order of magnitude due to interface

oughness is possible for the realistic interface roughness

iles shown in Figure 3.

Next, we calculate the transmission probability as a function

of the photon (plasmon) energy $\hbar \omega$. This is achieved by using

eq 7 while adding the perturbation term from eq 19 and

tegrating over the energies from $\phi_{\|}$ to $\hbar \omega$.

$$
P_{\text{t}}(\hbar \omega, h_0, \Lambda) = \frac{1}{\hbar \omega} \int_{\phi_{\|}}^{\hbar \omega} [P_E(E, h_0, \Lambda) + T(E)] dE$$

(20)

where we added the hot electron injection probability through

the escape cone ($T(E)$ of eq 4) to the roughness-assisted

jection from the outside of the escape cone. The results are

own in Figure 5a.

One can see once again that with totally realistic roughness

les of Figure 3 a substantial enhancement is attained for

atively small (a few interatomic spaces) correlation lengths.

The enhancement $P_{\text{t}}(\hbar \omega, h_0, \Lambda)/T(\hbar \omega)$ is plotted in Figure

b. As one can see, the enhancement can reach an order of magnitude, especially at longer wavelengths, illustrating the

rt role played by the roughness. In view of these

culations it appears that the somewhat puzzling high

jection efficiencies reported in refs 34–36 can be explained,
At least partially, by the mechanism of interface roughness scattering. In order to obtain a better estimate, one needs to measure interface roughness parameters $h_0$ and $\lambda$ with a good degree of precision due to very strong dependence of the injection efficiency on these parameters obtained here. Nevertheless, according to our theory, the injection efficiencies measured in tens of percent rather than single percent can be obtained with properly roughened surfaces, leading, for example, to Schottky detectors with responsivities of up to a 100 mA/W.

Before making conclusions, we shall stress that while our analysis is focused on the transport of hot electrons assuming (100) crystal orientation, the same model is valid also for different crystal orientations as well as for the internal photoemission of holes. That being said, different degeneracy of the bands should be taken into account. It can also be valid for cases where a thin native oxide layer is present, by adding a correction term that takes tunneling though the oxide into account.

**CONCLUSIONS**

In this work, we investigated the role of surface roughness in enhancing the transmission probability (and thus injection efficiency) of hot electrons across the Schottky barrier. To do so, we introduce a model in which the roughness is considered as a perturbation. Assigning a Hamiltonian to this perturbation allows linking the initial states in the metal which are outside of the escape cone to allowed final states in the silicon. A large (up to an order of magnitude relative to the smooth interface) enhancement can be achieved, and this enhancement strongly depends on both mean height and correlation length of the roughness. According to our model, the roughness has a crucial role in increasing the transmission across a Schottky contact to values exceeding 10% in a few angstroms RMS roughness and higher for larger roughness. While in the absence of the detailed experimental data of the roughness structure the model is not precise, it nevertheless provides a plausible explanation for experimental observation of the high efficiency of the injection in refs 34–36 and can help pave the way to high-efficiency sub-bandgap photodetectors in the telecom regime.

**REFERENCES**

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