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Analyzing periodical textured silicon solar cells by the TCAD modeling

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Abstract
The most effective way to improve the optical properties of silicon-based solar cells is to form the textures on their surface. In this paper, the authors studied the influence of geometric sizes of periodical pyramidal textures, which are formed on the surface of a silicon-based solar cell, on its photoelectric properties. Through optics theories, it was determined that the angle at the base of the pyramid should be equal to 73°7′12″. But, using the Sentaurus TCAD program, it was found that the angle at the base of pyramid should be 70°21′0″, in order to reach the maximum efficiency. Because the model takes into account all the electric, optic and thermic properties of the solar cell. The modeling identified that the output power of the simple planar silicon-based solar cell was equal to 6.13 mW/cm^2, the output power of the solar cell, which was covered with the pyramidal texture with height of 1.4 μm, was equal to 10.62 mW/cm^2. It was found that the efficiency of the solar cell increases by 1.6 times, when it is covered with pyramids with the angle at the base of pyramid equal to 70°21′0″.

Keywords
texture, solar cell, pyramid, silicon, Ray Tracing, modeling

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УДК 535.4

Анализ периодически текстурированных кремниевых солнечных элементов с использованием технологии моделирования TCAD

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Аннотация
Наиболее эффективный способ улучшения оптических свойств солнечных элементов на основе кремния — формирование текстуры на их фронтальной поверхности. В работе изучено влияние геометрических размеров периодической пирамидальной текстуры, образованной на поверхности солнечного элемента на основе кремния и его фотоэлектрические свойства. При учете оптической теории определено, что оптимальный угол наклона у основания пирамиды составляет 73°7′12″. При использовании программы Sentaurus TCAD обнаружено, что для достижения максимальной эффективности угол наклона у основания пирамиды должен составлять 70°21′0″. Расхождение углов наклона связано с тем, что в модели были учтены электрические, оптические и термические свойства солнечного элемента. Путем моделирования определено, что выходная мощность простого планарного солнечного элемента на основе кремния составляет 6,13 мВт/см^2. Выходная мощность солнечного элемента,

фронтальная поверхность которой покрыта текстурой в виде пирамиды со средней высотой 1,4 мкм, равна 10,62 мВт/см². Таким образом, обнаружено, что эффективность солнечного элемента увеличивается в 1,6 раз, когда его фронтальная поверхность покрыта текстурой в виде пирамиды, у которой угол наклона у основания — 70°21′0″.

Ключевые слова
текстура, солнечный элемент, пирамида, кремний, Ray Tracing, моделирование

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Introduction

Nowadays, various constructions are being manufactured in order to increase the efficiency of a solar cell. According to the Shockley Quessier's theory, the efficiency of a silicon-based solar cell does not exceed 29 % [1]. But the efficiency of industrially produced silicon-based solar cells is approximately 21 % [2]. Optic, electric, and thermic properties of solar cells should be improved to gain the maximum value efficiency. Optical layers are covered and textured on the surface of a solar cell to increase its absorption coefficient [3–5]. Besides, to improve optical and electrical properties of silicon solar cells, various metal nanoparticles are introduced into them [6, 7].

There are a lot of methods to create textures on silicon surface. The most common of these use alkalis and acids [8]. Mainly, NaOH and KOH are used in industry in order to form textures on surface of a silicon-based solar cell [9]. Because surface of a silicon solar cell is etched with alkalis, pyramid-shaped textures are formed on the surface of a silicon solar cell. When it is textured with NaOH, the corner at the base of the pyramids will be 54°42′0″ [10]. Especially in the experiment, random textures with different geometric size are formed. But in the experiment conducted by Zheng Fang, the sizes of textures, which were formed on surface of a solar cell, were standardized when the solar cell was chemically etched during 456 s [11]. This explains that periodical pyramidal textures can be formed on surface. This paper studies the influence of geometric sizes of periodical pyramidal textures, which are formed on the surface of a solar cell, on its properties.

Method

The Sentaurus TCAD program package is commonly used for modeling silicon-based solar cells and includes some instruments. Each instrument has its independent function. Among them are as follows: Sentaurus Structure Editor, Sentaurus Device, Sentaurus Visual and Sentaurus Workbench that are used to simulate solar cells.

Geometric models of solar cells are formed by the Sentaurus Structure Editor. There are two methods for creating a geometric model; they use standard shapes and write the code in the Tool Command Language (TCL). In this paper, we developed an algorithm in TCL to create a geometric model of textured solar cells. First, some points were defined with 0.5 μm of distance between neighbor points on the surface of a solar cell by the loop operator. Then these points which are located in an odd place were moved as far as to the height of the pyramid by the loop operator in order to cover the entire surface with textures. So, periodical upright pyramidal textures are formed on the surface of silicon-based solar cells. A geometric model of a planar and textured silicon-based solar cell, which was formed with the Sentaurus Structure Editor, was described in Fig. 1. In this paper, the width of the pyramid was not changed, but angle at the base of the pyramid changed by changing the height of the pyramid because the angle at the base of the pyramid depends on its height and width. In the paper, only 2D geometric models of silicon solar cells were used to simulate their properties, as silicon solar cells have high geometric symmetry. So, the obtained results, which were simulated by using 2D model, will be very close to the result of 3D model for a solar cell. In addition, the Sentaurus Device solves this problem by adding area factor. The height of solar cells is considered equal to 1 μm in the Sentaurus Device.

The Sentaurus Device is used in order to simulate processes and give physical properties to the geometric model, which is created with the Sentaurus Structure Editor. The modeling of electrical properties of all the semiconductor devices is the same. So, if it is an equilibrium state, the calculation of the Poisson's equation and charge carriers with the Fermi statistics will be enough to simulate semiconductor device. If it is a nonequilibrium state, the transport of charge carriers will be taken into account too. The transport of charge carriers is formed when an external electric field is set, illuminated

Fig. 1. Three types of 2D geometric model of silicon-based solar cells made by the Sentaurus Structure Editor: the width of pyramid is 1μm, the heights of the pyramid are 0.4 μm and 1 μm, respectively. Solar cells contain four layers: the high concentration of the donor doped $N_D = 10^{18}$ cm^{-3} (*n*++), the donor doped $N_D = 10^{17}$ cm^{-3} (*n*), the acceptor doped $N_A = 10^{15}$ cm^{-3} (*p*) and the high concentration of acceptor doped $N_A = 10^{15}$ cm^{-3} (*p*++) layers. The thickness of *n*++ layer is 0.1 μm, the thickness of *n* layer is 1 μm, the thickness of *p* layer is 10 μm and the thickness of *p*++ layer is 0.5 μm

and heated. The transport of charge carriers is taken into account for modeling solar cells, as the solar cells were illuminated. Physical processes of solar cells are very complicated due to the light effect on solar cells. The modeling of solar cells is done in three phases. At the first stage, the optical properties are identified, the transport of charge carriers and their thermic and electric properties are modeled. The modeling of solar cells is more complicated than of other semiconductor devices as it has optical properties. Among various methods used by the Sentaurus Device to identify optical properties of a solar cell we can name Transfer Matrix Method (TMM), Ray Tracing Method and Beam Propagation Method. Depending on the structural appearance of a solar cell, the calculation methods are selected. The TMM calculates optical properties of multilayer and thin film planar solar cells. The advantage of the TMM is the determination of light absorption, transmission and reflection coefficients in each layer of solar cells. Besides, in the calculation process, this model takes into account an interference phenomenon, which is important in the thin film solar cell. The Ray Tracing Method is used to calculate the optical properties of textured surface structures. And hence, in this model, refractions of light rays are also considered several times. Thus, in this paper, the Ray Tracing Method was used to simulate the textured silicon solar cell.

In the Sentaurus Device, the photogeneration is modeled in 2D and 3D through the Ray Tracing Method. Refraction, transmission, reflections are calculated by geometric optics and special boundary conditions are announced. In the Ray Tracing Method, the complex refraction index of material, which is given in the formula below, is used in order to identify optic properties of a semiconductor device:

$$n_{tot}(\lambda) = n(\lambda) + ik(\lambda),$$

where n_{tot} is a complex refractive index; n is a real part of a complex refractive index; k is an imaginary part of a complex refractive index; λ — the wavelength.

In this method, the polarization theory of light is used like the TMM. Through polarization of light, optical phenomena are identified by the Fresnel coefficients following the Ray Tracing Method.

Through the complex light refraction index of the materials given in the formula, the absorption coefficient is calculated:

$$\alpha(\lambda) = \frac{4\pi k}{\lambda},$$

where α is the absorption coefficient.

Through the absorption coefficient, the optical generation is calculated with the formula:

$$G^{opt}(x, y, z, t) = I(x, y, z)[1 - e^{-\alpha L}],$$

where G^{opt} is the optical generation; I is the light intensity; L is the medium thickness; x, y, z are the Cartesian coordinates; t is time.

The value of the complex refractive index for each layer is different. Light intensity decreases and absorbs when it is transmitted from each layer. Optical generation was calculated for each layer. The quantum yield function is used to calculate the optical generation. The energy of each photon is compared to the band gap energy of the material. If the energy of a photon is higher than the band gap energy, the quantum yield function will be equal to 1, otherwise it will be equal to 0. This helps to calculate the number of photons, which are absorbed by each region.

Boundary conditions must be declared for each interface between regions. In the Ray Tracing Method, a boundary condition can be defined by the given exact value to the reflection and transmission coefficients of each interface. Or they are calculated by using the Fresnel coefficients. In this model, the boundary conditions, which are set between the air and texture of silicon, were identified through the Fresnel's laws:

$$\begin{cases} r_{\perp} = \dfrac{n_1\cos\alpha - n_2\cos\gamma}{n_1\cos\alpha + n_2\cos\gamma} \\ t_{\perp} = \dfrac{2n_1\cos\alpha}{n_1\cos\alpha + n_2\cos\gamma} \end{cases}, \quad (1)$$

$$\begin{cases} r_{\parallel} = \dfrac{n_1\cos\gamma - n_2\cos\beta}{n_1\cos\gamma + n_2\cos\beta} \\ t_{\parallel} = \dfrac{2n_1\cos\beta}{n_2\cos\beta + n_1\cos\gamma} \end{cases}, \quad (2)$$

where n_1 and n_2 are the refractive indices of mediums; β — the angle of incident light; γ — the angle of refracted light; r and t — the Fresnel coefficients.

The Fresnel's laws are based on polarization of light in two planes. Natural light is separated into polarized rays which are perpendicular and parallel. The Fresnel coefficient of a perpendicular polarized ray is calculated with the formula (1). The Fresnel coefficient of a parallel polarized ray is calculated with the formula (2).

In the Ray Tracing Method, the total power of light is calculated with the formula:

$$P_{total} = P_{abs} + P_{escape} + P_{stopped},$$

where P_{total} is the power of the total ray; P_{abs} is the power of the absorption rays; P is the power of the escaped rays; $P_{stopped}$ is the power of the stopped rays.

The power of each ray is controlled. If it is less than limited minimum intensity in the model, then the calculation is stopped for this ray. Through this, the risk of unlimited calculation is prevented.

Electrical properties of solar cells are simulated by using the Poisson and continuity equations and Fermi statistics. First, the charge carriers concentration should be calculated by using the Fermi statistics as shown in the formulas:

$$n = N_c F_{1/2}\left(\frac{E_{F,n} - E_c}{kT}\right),$$

$$p = N_V F_{1/2}\left(\frac{E_V - E_{F,p}}{kT}\right),$$

where $F_{1/2}$ — the Fermi half integral; E_c — the conduction band energy; E_V — the valence band energy; $E_{F,n}$ — the quasi Fermi energy for electrons; $E_{F,p}$ — the quasi Fermi energy for holes; T — the absolute temperature; N_c — the density of states in the conduction band; N_V — the density of states in the valence band; k — the Boltzmann constant.

Second, the electric field and potentials are calculated by using charge carriers concentration, which is found by the Fermi statistics, in the Poisson equation:

$$\Delta\varphi = -\frac{q}{\varepsilon}(p - n + N_D + N_A),$$

where ε is the permittivity; n and p are the concentration of electron and holes; N_D and N_A are the donor and acceptor concentration; q is the electron charge, Δ is the Laplace operator.

Finally, the transport of charge carriers is calculated by using the continuity equation. The continuity equation has the following four main models: Drift-Diffusion, Thermodynamic, Hydrodynamic and Monte Carlo. In this paper, to calculate the transport of charge carriers, we used the thermodynamic model, which is given in formulas. Due to the temperature effect, the electrical and optical properties have been taken account into:

$$\vec{J}_n = -nq\mu_n(\nabla\Phi_n + P_n\nabla T),$$
$$\vec{J}_p = -pq\mu_p(\nabla\Phi_p + P_p\nabla T),$$

where μ_n, μ_p are mobility of electron and holes; Φ_n, Φ_p are the electron and hole quasi-Fermi potentials; P_n, P_p are the thermoelectric power of electron and holes; T is the absolute temperature; ∇ is the Del operator; $\vec{J}_p$ is the hole current; $\vec{J}_n$ is the electron current.

To use the thermodynamic model in calculating the transport of charge carriers with effect of temperature, the lattice temperature should be calculated by using the formula:

$$\frac{\partial}{\partial t}(c_L T) - \nabla(k\nabla T) = -\nabla[(P_n T + F_n)\vec{J}_n + (P_p T + F_p)\vec{J}_p] - \\ -\frac{1}{q}\left(E_c + \frac{3}{2}kT\right)(\nabla\vec{J}_n - qR_{net,n}) - \\ -\frac{1}{q}\left(E_v + \frac{3}{2}kT\right)(-\nabla\vec{J}_p - qR_{net,n}) + \hbar\omega G^{opt} - \\ -\frac{1}{q}\left(E_v + \frac{3}{2}kT\right)(-\nabla\vec{J}_p - qR_{net,n}) + \hbar\omega G^{opt}, \quad (3)$$

where k is the heat conductance; c_L is the heat capacity; E_c is the minimum energy of the conduction band; E_v is the maximum energy of the valence band; G^{opt} is the optical generation; $R_{net,n}$ and $R_{net,p}$ are the net recombination.

If the lattice temperature is not calculated with the formula (3), the thermodynamic model will work as a drift-diffusion model, since the latter is simple, so it does not take into account the effect of temperature on the transport of charge carriers. Besides, the thermodynamic model also calculates the heat power, which is formed due to recombination and scattering phenomena.

In this research work, the finite element method has been used to simulate a solar cell. The size of meshes was considered flexible through the solar cell. So, in the contact and p-n junction region, the meshes were formed smaller than other regions of the solar cell. The minimum size of meshes is 0.005 μm and maximum one is 0.05 μm. So, the relative error was smaller than 10^{-6}.

Results and discussion

In the Sentaurus TCAD, the solar cell which was covered with planar textures in different heights is modeled. The height of textures, which covered the surface of the solar cell, varies from 0 μm to 1.8 μm, its width is 1 μm. Fig. 2 shows the absorbed photon density distribution through the thickness of solar cells, which are planar (Fig. 2, *a*), pyramidal texture with 0.4 μm (Fig. 2, *b*) and 1.6 μm (Fig. 2, *c*) of height. As the height of the textures increases, the depth of light absorption decreases. So, more rays were absorbed in the part close to the surface. It can be accounted for the following two reasons.

The first reason implies the enlargement of the surface of a solar cell. So, if N photons fall on the S surface and absorb in the d depth, the surface of the solar cell increases to 2S when the textures are formed, whereas the number of incoming photons remains unchanged. But they are distributed on larger surface and thus, the absorption depth decreases. Secondly, a light ray which falls on the smooth surface, refracts only once, but it refracts more times in textured surface, depending on the angle of textures. Besides, the path of the light ray in a solar cell increases. This is also caused by the increase of the absorption coefficient [12].

In this paper, the I-V characteristic of a silicon solar cell, which was covered with different textures, is identified. In Fig. 3, the I-V characteristic of a silicon solar cell, which is

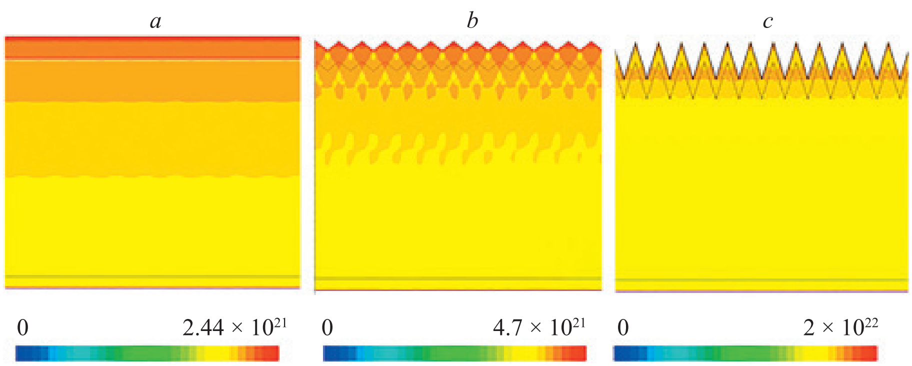

Fig. 2. Distribution of photons which are absorbed in silicon-based solar cell: planar (*a*), the width is 1μm and the height is h = 0.4 μm (*b*), h = 1.6 μm (*c*)

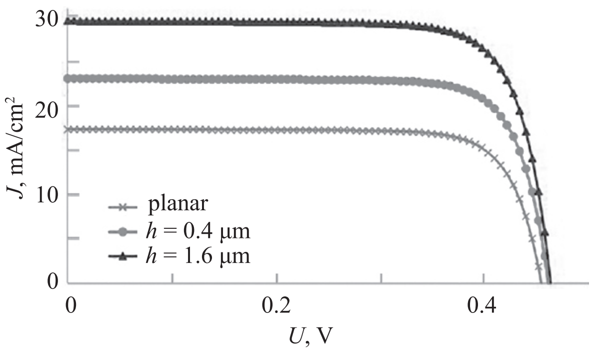

Fig. 3. I-V characteristic of the silicon-based solar cell, which is covered with planar pyramids (width is 1 μm, h = 0.4 μm and 1.6 μm)

covered with planar pyramids (width is 1 μm, h = 0.4 μm and 1,6 μm), is shown.

As can be seen in Fig. 3, the height of texture does not affect the open-circuit voltage. But the short-circuit current increased 1.33 times, when the height of pyramid was $h = 0.4$. The short-circuit current increased 1.7 times, when the height of pyramid was $h = 1.6$ [12]. In the study, which was conducted by Soonwoo Kwon, the short-circuit current increased 1.1 times, when the surface of the silicon-based solar cell was treated with KOH [13]. The difference with the result obtained in the model was due to inability to control the size and periodicity of texture in the experiment. But through modeling, the increase of short-circuit current 1.6 times was identified by Rahul Devan, when periodicity textures were formed on the surface of the silicon solar cell [14]. This result is very close to the results which we obtained. Fig. 4 presents the I-V characteristic of the silicon solar cell, which is covered with planar pyramids (h = 0.4 μm and 1,6 μm). So, the maximum output power of the silicon solar cell was dP_{mpp} = 2.08 mW/cm^2, when its surface was covered with the pyramidal texture (height is h = 0.4 μm). If the height is h = 1.6 μm, the output power will increase to dP_{mpp} = 4.49 mW/cm^2. In the model of the silicon-solar cell, which was formed by Hamid Heidarzadeh, the maximum efficiency is identified in the pyramidal texture at a height of 8 μm. The efficiency of the silicon-based solar cell, which width is 50 μm, increased 1.25 times, through textures formed on the surface [15].

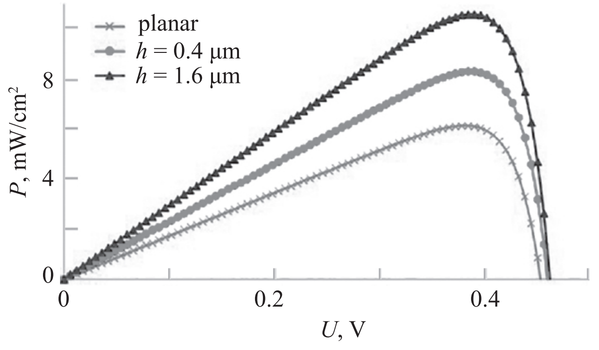

Fig. 4. Volt-power characteristic of the silicon-based solar cell covered with planar pyramids (width is 1 μm, h = 0.4 μm and 1.6 μm)

Fig. 5 presents the graph of the dependence of the output power of the solar cell on the height of texture on the surface. The value of the angle at the base of pyramid was identified, through its height h, width w and the formula:

$$\theta = \tan^{-1}\left(\frac{2h}{w}\right),$$

where h is the height of the pyramid; w is the width of the pyramid and θ is the angle of the pyramid substrate.

The number of refractions between two pyramids was depends on the angle at the base of the pyramid. If the angle at the base of the pyramid is larger than 64°, the rays are refracted 4 times between two pyramids. This corresponds to the height of the pyramid between 1 and 1.8 μm. Through optics theories, it was determined that the angle at the base of the pyramid should be equal to 73°7′12″ to gain the maximum absorption coefficient and minimum reflection coefficient. But by the Sentaurus TCAD program it was found that the angle at the base of pyramid should be 70°21′0″, in order to reach the maximum efficiency. Because all the electric, optic and thermic properties of solar cells were taken into account in this model. If the width and height of periodical pyramidal textures on the surface of the silicon-based solar cell was 1 μm and 1.4 μm, it showed the maximum power.

The fill factor indicates the quality of the solar cell. Fig. 6 describes the dependence of the fill factor of a solar

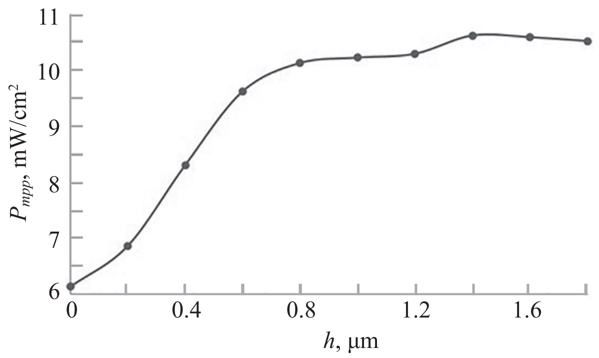

Fig. 5. Dependence of the output power of the solar cell, which was covered with regular pyramidal textures, on the height of pyramid (the width of the pyramid's base is 1 μm)

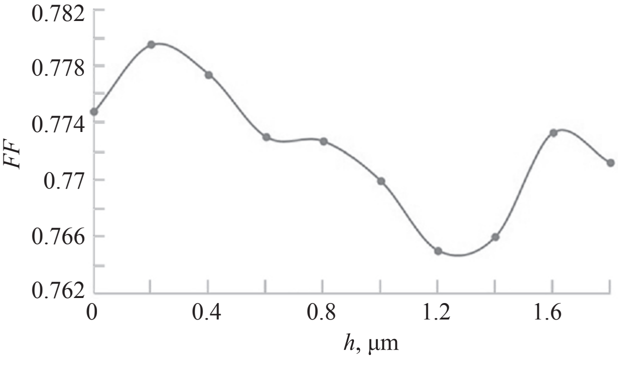

Fig. 6. Dependence of the fill factor of the solar cell, which was covered with regular pyramidal textures, on the height of pyramid (the width of the pyramid's base is 1 μm)

cell on the height of pyramid. The fill factor of the solar cell was calculated by the formula:

$$FF = \frac{J_{mpp}U_{mpp}}{J_{sc}U_{oc}},$$

where FF is the fill factor; J_{mpp} is the current density on the maximum power point; U_{mpp} is the voltage on maximum power point; J_{sc} is the short-circuit current; U_{oc} is the open-circuit voltage.

It was found, that its fill factor reaches the maximum value when the height of the pyramid is 0.2 μm. The value of the fill factor is mainly affected by resistive losses and recombination because they degrade the quality of the I-V characteristic.

Conclusion

The most effective way to improve the optical properties of silicon-based solar cells is to form textures on their surface. This paper studied the influence of geometric sizes of regular pyramidal textures, which are formed on the surface of a silicon-based solar cell, on its photoelectric properties. It was found that the angle at the base of the pyramid should be 73°7′12″ in order to reach the maximum efficiency. This value is only valid for the silicon-based solar cell. Values might be different for other cells. Covering the surface of solar cells with regular pyramids with the angle at the base of pyramids equal to 70°21′0″ increases the energy, which was taken in solar cells, to 1.6 times.

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