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Simulation of single and double anti-reflective film for solar cell

Simulación de una y doble película antirreflectante para celda solar

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Abstract

This work presents the analysis of the Fresnel reflection and transmission coefficients at normal incidence to determine an equation for the reflectivity of single and double thin films that are deposited on the reflective surface of a solar cell. The resulting expressions are simulated in the Matlab software, and it is shown how by having such a thin layer, zero reflection can be achieved at a desired wavelength and the zero reflection bandwidth can increase considerably by having a thin double layer.

Thin films, Anti reflective coatings, Fresnel coefficients

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Resumen

En este trabajo se presenta el análisis de los coeficientes de reflexión y transmisión de Fresnel a incidencia normal para determinar una ecuación para la reflectividad de una y doble película delgada que está depositada sobre la superficie reflectante de una celda solar. Las expresiones resultantes son simuladas en el software de Matlab y se muestra como al tener una capa tan delgada se puede lograr una reflexión cero a una longitud de onda deseada y el ancho de banda de reflexión cero puede aumentar considerablemente al tener una doble capa delgada.

Películas delgadas, Recubrimientos antirreflectante, Coeficientes de Fresnel

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Introduction

Anti-reflective (AR) films are crucial for improving the efficiency of solar cells. In a solar cell, the amount of sunlight absorbed directly affects its ability to generate electricity. However, a significant part of the incident light can be reflected from the cell surface, which reduces its efficiency. Decreasing reflection losses at material interfaces represents one approach to increase the efficiency of photovoltaic modules [\(Deubener et al. 2019\)](https://doi.org/10.1016/j.jeurceramsoc.2008.08.009) and other systems for solar energy conversion [\(Raut](file:///C:/Users/TIC-BENITO/Downloads/DOI%09https:/doi.org/10.1039/C1EE01297E) [et al. 2011\)](file:///C:/Users/TIC-BENITO/Downloads/DOI%09https:/doi.org/10.1039/C1EE01297E).

Anti-reflective films are used to minimise this loss of reflected light and maximise the amount of light absorbed by the cell. Single-layer anti-reflection (SLAR) coatings have emerged as an effective approach to reduce reflections on substrates such as glass. These coatings can achieve high transmission rates of up to 98.5% [\(Menezes et al., 2014\)](https://doi.org/10.4236/msa.2014.511078) or even 99.4% in some cases [\(Ghazaryan et al.,](https://doi.org/10.1002/adem.201801229) [2019\)](https://doi.org/10.1002/adem.201801229). However, multilayer coatings offer better performance over a wider wavelength range. These coatings can be modelled and optimised by systematically adding layers and adjusting their thickness and refractive indices [\(Asghar &](http://dspace.nbuv.gov.ua/handle/123456789/118077) [Naseem, 2003\)](http://dspace.nbuv.gov.ua/handle/123456789/118077).

In solar cell applications, multilayer antireflective coatings (ARCs) have shown a significant reduction in optical losses; a 6-layer coating achieves reflectivity as low as 1.05 % on textured surfaces [\(Sahouane et al., 2018\)](https://doi.org/10.1088/2053-1591/aaca16). For ultrathin gallium indium copper selenide (CIGS) solar cells, multilayer ARCs serve as light traps in the red and near-infrared regions, resulting in substantial increases in short-circuit current density [\(Rajan et al., 2013\)](https://doi.org/10.1109/PVSC.2013.6744870). These studies demonstrate the versatility and effectiveness of multilayer ARCs in various optical applications.

Operating principles of an AR

AR films operate on the principle of optical interference. By applying a film with the appropriate thickness and refractive index to the surface of the solar cell, reflections on the top surface of the film and at the interface between the film and the substrate cancel each other out, thereby reducing the amount of reflected light.

To achieve destructive interference, the film thickness is usually a fraction of the wavelength of the incident light, typically $\lambda/4$, where λ is the wavelength of the light. This causes the reflected waves from different interfaces to phase shift and cancel each other, as depicted in figure 1.

Schematic diagram of an anti-reflective film

Source: own elaboration

Analysis of the reflectance and transmittance coefficients at normal incidence of a single wave

Within the study of the basic functioning of an AR, it is crucial to understand the behaviour of light when it strikes between two media with different refractive index (Malacara, 2015). Fresnel transmission and reflection coefficients (Pedrotti et al., 2018) are fundamental to understanding how light behaves when passing from one medium to another, especially in the context of antireflective films.

Irradiance, also known as power density or radiation intensity, is the amount of electromagnetic energy incident on a unit area per unit time. In terms of the Poynting vector (\vec{S}) (Jackson, 1998), irradiance *I* can be expressed as the average magnitude of the Poynting vector over a period of time:

$$
I = \langle \|\vec{S}\|\rangle \tag{1}
$$

For an electromagnetic wave, the magnitude of the vector \vec{S} is:

$$
\vec{S} = c^2 \in_{0} \left| \vec{E} \times \vec{B} \right| \tag{2}
$$

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Where:

 \tilde{c} is the speed of light in a vacuum.

 ϵ_0 is the vacuum permittivity.

 \vec{E} is the electric field vector.

 \vec{B} is the magnetic field vector.

Given that \vec{E} and \vec{B} are perpendicular to each other in an electromagnetic wave $|\vec{E} \times \vec{B}|$ = EB.

Simplifying the equation [2],

$$
\vec{S} = c^2 \in_0 EB \tag{3}
$$

In an electromagnetic wave in a vacuum, the relationship between the electric and magnetic fields is $E = c$. Using this relationship, one has:

$$
\langle ||\vec{S}|| \rangle = c^2 \in_0 E\left(\frac{E}{c}\right) = c \in_0 E^2
$$
 [4]

To obtain the average irradiance, the mean value of the square of the electric field is considered. $\langle E^2 \rangle$, which for a sinusoidal electromagnetic wave is related to the peak value E₀ of the electric field as $\langle E^2 \rangle = \frac{E_0^2}{2}$ $\frac{20}{2}$, therefore the irradiance is:

$$
I = \langle ||\vec{S}|| \rangle = \frac{c \in_{0} E_{0}^{2}}{2}
$$
 [5]

According to (Hecht, 2001) it is considered that the incident flux densities I_i , reflected I_r and transmitted I_t , impinging on an interface with refractive index n_i pain the case of the first interface, which may be air and n_t in the second one considering an AR as shown in figure 2. Then the cross-sectional areas of the incident, reflected and transmitted rays will be respectively, A cos θ_i , A cos θ_r y A cos θ_t . According to the above the incident power is I_i A cos θ_i y represents the energy per unit time flowing in the incident beam and, therefore, the power reaching the surface A. Similarly, $I_rA \cos$ θ_r is the power in the reflected beam, e I_t A cos θ_t is the power that is transmitted through the A.

Box 2

Figure 2 Reflection and transmission of an incident wave *Source: (Hecht, 2001)*

Reflectance R is defined as the quotient of the reflected power and the incident power, i.e.

$$
R \equiv \frac{I_r \text{ A} \cos \theta_r}{I_i \text{ A} \cos \theta_i} = \frac{I_r}{I_i}
$$
 [6]

Similarly, the transmittance T is defined as the quotient between the transmitted flux and the incident flux and is given by,

$$
T \equiv \frac{I_t \text{ A} \cos \theta_t}{I_i \text{ A} \cos \theta_t} = \frac{I_t}{I_i}
$$
 [7]

Consuming that the quotient I_r/I_i is equal to *I^r* and given that the incident and reflected wave are in the same medium the reflectance is:

$$
R = \left(\frac{E_{or}}{E_{oi}}\right)^2 = r^2
$$
 [8]

Normal incidence which is a situation of interest for this work, $\theta_t = \theta_i = 0$, and transmittance (equation 7), like reflectance (equation 6), is the quotient of the appropriate irradiances. Accordingly, transmittance can be expressed in terms of the refractive indices,

$$
T = \frac{n_t \cos \theta_r}{n_i \cos \theta_i} \left(\frac{E_{or}}{E_{oi}}\right)^2 = \left(\frac{n_t \cos \theta_r}{n_i \cos \theta_i}\right) t^2 \qquad [9]
$$

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If it is considered that the total energy flowing into area A per unit time must be equal to the energy flowing out per unit time, then it can be expressed that:

$$
I_i \text{ A} \cos \theta_i = I_r \text{ A} \cos \theta_r + I_t \text{ A} \cos \theta_t \qquad [10]
$$

or simply

$$
R + T = 1 \tag{11}
$$

The Fresnel coefficients in terms of their parallel and perpendicular components are given by:

$$
R_{\perp,\parallel} = \left(\frac{E_{or}}{E_{oi}}\right)_{\perp,\parallel}^2
$$
 [12]

$$
T_{\perp, \parallel} = \left(\frac{n_t \cos \theta_t}{n_i \cos \theta_t}\right) t_{\perp, \parallel}^2 \tag{13}
$$

In summary the expressions for reflectance and transmittance are described by (Born & Wolf 1999), considering again that $\theta_t = \theta_i = 0$ Equation [12 and 13] are therefore expressed as:

$$
T_{\perp\parallel} = \left(\frac{2}{n+1}\right) A_{\perp\parallel} \tag{14}
$$

$$
R_{\perp\parallel} = \left(\frac{n-1}{n+1}\right) A_{\perp\parallel} \tag{15}
$$

Where:

 $n = n_2/n_1$ and represents the refractive indices is considered unitary.

Equation [14 and 15], represent the transmitted and reflected rays at an interface with two refractive indices. From these, the analysis is developed to determine an expression representing an anti-reflection film.

Despite advances, challenges remain to improve the reliability and performance of ARCs in the real world, requiring continued research and development in this field (Khan *et al*., 2017).

Methodology

For our study, a wave travelling in the air with a rate of $n_1 = 1$ index on an anti-reflection (AR) film with thickness d and refractive index n_2 desconocgone. However, because of the characteristics considered in the RA, the wave first reflects (r_1) and is subsequently transmitted (t_1) . The transmitted wave is reflected (r_2) at the surface of a solar cell with refractive index $n_3 = 3.5$, this in turn is reflected again (r'_1) on the inside of the RA. The light travelling inside the RA travels a distance of L. Eventually, the wave is transmitted (t'_1) to travel in the air, as shown in figure 3.

Box 3

Figure 3

Diagram of the incident wave on an AR of a solar cell

Source: Own elaboration

Considering that the incidence is normal $\theta_i = 0$ and taking as a basis the equations [14, 15], the reflection and transmission coefficients are given by:

$$
r_1 = \frac{n_1 - n_2}{n_1 + n_2} \tag{16}
$$

$$
t_1 = \frac{2n_1}{n_1 + n_2} \tag{17}
$$

$$
r_2 = \frac{n_2 - n_3}{n_2 + n_3} \tag{18}
$$

$$
r_1' = \frac{n_2 - n_1}{n_2 + n_1} \tag{19}
$$

$$
t_1' = \frac{2n_2}{n_1 + n_2} \tag{20}
$$

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If the amplitude of the wave is unitary and the phase is 0, then Figure 3 can be expressed by a wave travelling a certain distance L and acquiring a phase e^{niL} for all positive integer n, which is incremented each time it is internally reflected in the RA. Therefore, the reflected wave would be the sum of all reflected and transmitted waves as seen in figure 4. And it is represented by the equation [21].

$$
r = r_1 + t_1 r_2 t_1' e^{2iL} + t_1 r_2^2 r_1' t_1' e^{4iL} + t_1 r_2^3 r_1'^2 t_1' e^{6iL} + \dots + \qquad [21]
$$

Figure 4

Reflected and transmitted waves in a RA

Source: *own elaboration*

Whereas $t_1 r_2 t_1' e^{2iL}$ es a common factor of the equation [21], it can be expressed as:

$$
r = r_1 + t_1 r_2 t_1' e^{2iL} \left(1 + r_2 r_1' e^{2iL} + r_2^2 r_1'^2 e^{4iL} + r_2^3 r_1'^3 e^{6iL} + \dots \right)
$$
\n
$$
\left[22 \right]
$$

In a simplified expression the equation is represented by:

$$
r = r_1 + t_1 r_2 t_1' e^{2iL} \sum_{m=0}^{\infty} (r_2 r_1' e^{2iL})^m
$$
 [23]

According to the properties of summation, $\sum_{m=0}^{\infty} (x)^m = \frac{1}{1-x^2}$ $1-x$ we can represent the equation as

$$
r = r_1 + \frac{t_1 r_2 t_1' e^{2iL}}{1 - r_2 r_1' e^{2iL}} \tag{24}
$$

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Equation [24] represents the total reflection of the incident, reflected and transmitted wave within an anti-reflection film. It is desirable that the reflection equation does not contain transmission parameters. For this purpose, the product of $t_1 * t_1'$ y $r_1 * r_1$, therefore,

$$
t_1 t_1' = \frac{4n_1 n_2}{(n_1 + n_2)^2} \tag{25}
$$

and

$$
r_1 * r_1 = \left(\frac{n_1 - n_2}{n_1 + n_2}\right)^2 \tag{26}
$$

$$
r_1^2 = \frac{n_1^2 - 2n_1n_2 + n_2^2}{(n_1 + n_2)^2} \tag{27}
$$

The relationship $t_1 t_1' + r_1^2$ es,

$$
t_1 t_1' + r_1^2 = \left(\frac{4n_1 n_2}{(n_1 + n_2)^2} + \frac{n_1^2 - 2n_1 n_2 + n_2^2}{(n_1 + n_2)^2}\right)
$$
 [28]

$$
t_1 t_1' + r_1^2 = \left(\frac{4n_1 n_2 + n_1^2 - 2n_1 n_2 + n_2^2}{(n_1 + n_2)^2}\right)
$$
 [29]

$$
t_1 t_1' + r_1^2 = \frac{n_1^2 + 2n_1 n_2 + n_2^2}{(n_1 + n_2)^2}
$$
 [30]

$$
t_1 t_1' + r_1^2 = 1 \tag{31}
$$

$$
t_1 t_1' = 1 - r_1^2 \tag{32}
$$

According to equation [16 and 19] it can be related that $r'_1 = -r_1$, Therefore, substituting equation [32] into [24], it is obtained that:

$$
r = r_1 + \frac{(1 - r_1^2)r_2 e^{2il}}{1 + r_2 r_1 e^{2il}}
$$
 [33]

$$
r = \frac{r_1 + r_2 r_1^2 e^{2iL} + r_2 e^{2iL} - r_1^2 r_2 e^{2iL}}{1 + r_2 r_1 e^{2iL}}
$$
 [34]

$$
r = \frac{r_1 + r_2 e^{2iL}}{1 + r_2 r_1 e^{2iL}}
$$
 [35]

The argument e^{2iL} is a complex number and is related to Euler's identity $e^{ix} = \cos x +$ *isen x*. Therefore, the complex conjugate of the equation [35] is:

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$$
R = rr^* = \frac{r_1 + r_2 e^{2iL}}{1 + r_2 r_1 e^{2iL}} * \frac{r_1 + r_2 e^{-2iL}}{1 + r_2 r_1 e^{-2iL}} \quad [36]
$$

$$
R = \frac{r_1^2 + r_2^2 + r_1 r_2 e^{-2iL} + r_1 r_2 e^{2iL}}{1 + r_1^2 r_2^2 + r_1 r_2 e^{-2iL} + r_1 r_2 e^{2iL}}
$$
 [38]

Factoring $r_1 r_2$ you get:

$$
R = \frac{r_1^2 + r_2^2 + r_1 r_2 (e^{2iL} + e^{-2iL})}{1 + r_1^2 r_2^2 + r_1 r_2 (e^{2iL} + e^{-2iL})}
$$
 [39]

$$
(e^{2iL} + e^{-2iL}) = \cos 2L + 2i \operatorname{sen} L + \cos 2L - 2i \operatorname{sen} L
$$
 [40]

Reducing terms:

$$
(e^{2iL} + e^{-2iL}) = 2 \cos 2L
$$
 [41]

Rewriting equation 39, we have:

$$
R = \frac{r_1^2 + r_2^2 + 2r_1r_2\cos 2L}{1 + r_1^2r_2^2 + 2r_1r_2\cos 2L}
$$
 [42]

Equation [42] represents the reflectance of a thin film in terms of the reflection of the first and second interface as shown in figure 5.

Figure 5

Schematic of a single-layer reflectance

Source: *Own elaboration*

Calculation of the refractive index of the antireflective film

In order to calculate the refractive index of the film, it can be considered that $r_1 = r_2$, p Therefore, equating equations [16 and 18), we have that:

$$
\frac{n_1 - n_2}{n_1 + n_2} = \frac{n_2 - n_3}{n_2 + n_3} \tag{43}
$$

Carrying out operations:

$$
(n_1 - n_2)(n_2 + n_3) = (n_2 - n_3)(n_1 + n_2)
$$
 [44]

$$
n_1 n_2 + n_1 n_3 - n_2^2 - n_2 n_3 = n_1 n_2 + n_2^2 - n_1 n_3 - n_2 n_3
$$
 [45]

Reducing terms:

$$
n_1 n_3 - n_2^2 = n_2^2 - n_1 n_3 \tag{46}
$$

$$
2n_2^2 = 2n_1n_3 \to n_2^2 = n_1n_3 \tag{47}
$$

$$
n_2 = \sqrt{n_1 n_3} \tag{48}
$$

Thickness of anti-reflective film

Light travelling a certain distance within the RA which is given by:

$$
L = \frac{2\pi n_2}{\lambda_0} d \tag{49}
$$

Where:

 n_2 is the index of refraction of the RA.

 d is the thickness of the film.

 λ_0 the wavelength.

To calculate the thickness of the film, the distance travelled by the light is considered to be $L=\frac{\pi}{2}$ $\frac{\pi}{2}$, Therefore, the equation [49], can be rewritten as:

$$
\frac{\pi}{2} = \frac{2\pi n_2}{\lambda_0} d \tag{50}
$$

By subtracting d, we have:

$$
d = \frac{\lambda_0}{4n_2} \tag{51}
$$

Simulation of an anti-reflective film

For the anti-reflection film simulation, equations [16,18,42,48,49 and 51] were used.

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These expressions are part of a computational algorithm that allows the calculation of the refractive index of an AR from the refractive index of the air of 1 and of the silicon solar cell of 3.5. It also allows the calculation of the thickness of the AR and subsequently the reflected wave r_1 y r_2 . The data found are considered to find the reflectance described by equation [42].

Figure 6 shows the representative flowchart of the algorithm for calculating the reflectance of an incident wave of varying wavelength.

Flowchart of an AR layer

Source: *own elaboration*

Simulation of double anti-reflection film

For the simulation of double anti-reflection film, we have considered analysing the reflection coefficients in four media, one considering the air, two for the anti-reflection layer and the fourth for the solar cell. The analysis is similar to that described in the Methodology section. The expression of the reflectance for the double layer is given by:

$$
R = \frac{r_1^2 + r_2^2 + r_3^2 + r_1^2 r_2^2 r_3^2 + }{1 + r_2^2 r_3^2 + r_1^2 r_2^2 + r_1^2 r_3^2 +}
$$
\n
$$
+ 2r_1 r_2 (1 + r_3^2) \cos(2L_2) + 2r_2 r_3 (1 + r_1^2) \cos(2L_3)
$$
\n
$$
(52)
$$

 $2r_1r_3\cos(2(L_3+L_2))+2r_1r_2^2r_3\cos(2(L_3-L_2))$

+2 $r_1r_2(1+r_3^2)\cos(2L_2)+2r_2r_3(1+r_1^2)\cos(2L_3)$

 $2r_1r_3\cos(2(L_3+L_2))+2r_1r_2^2r_3\cos(2(L_3-L_2))$

Where

$$
r_1 = \frac{n_1 - n_2}{n_1 + n_2}
$$

$$
r_2 = \frac{n_2 - n_3}{n_2 + n_3}
$$

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$$
r_3 = \frac{n_3 - n_4}{n_3 + n_4}
$$

$$
L_2 = \frac{2\pi n_2}{\lambda_0} d_2
$$

 $L_3 = \frac{2\pi n_3}{\lambda_3}$ $rac{\lambda_{0}^{n}a_{3}}{\lambda_{0}}d_{3}$

 $L₂$

Refractive index:

$$
n_1
$$
 of the air.

 n_2 layer 1 of the RA.

 n_3 layer 2 of the RA.

 n_4 of the solar cell.

Phase acquired by the wave:

 L_2 layer 1 of the RA.

 L_3 layer 2 of the RA.

 λ_0 Lambda from 300 to 1200 nm.

RA thicknesses (nm).

 d_2 layer 1.

 d_3 layer 2.

Figure 7 shows a representative flow diagram for calculating the reflectance of an incident wave on an AR bilayer in the electromagnetic spectrum from 300 to 1200 nm.

Box 7 12 = 2*pi*n2*d2. /lambda; % The phase acquired by the wave in first AR

3 = 2*pi*n3*d3. /lambda; % The phase acquired by the wave in second AI
 $r2 = (n2-n3) / (n2+n3)$;
 $r2 = (n2-n3) / (n2+n3)$;

numerator = r1^2+r2^2+r3^2+(r1*r2*r Star ed by the wave in second AR Ţ Refractive index $n1 = 1$; % air
 $n2 = 1.35$; % layer 2
 $n3 = 2.48$; % layer 3
 $n4 = 3.5$; % solar cell R = 100*(numerador. / denominador); Thickness
d2 = 100: %n $d3 = 55; %$ R = 100*(numerador. / denominador); \perp lambda = 200:1:1200; % plot (lambda, R) normalized way End **Figure 7**

Matlab code of two ARC layers

Source: *Own elaboration*

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Results

Solving equation 21, from the expressions described in [16 - 20]. An expression [42] was obtained to represent the reflectance of a thin film. Also with the proposed algorithm it is possible to calculate the refractive index of the antireflective film so that the user can indicate the wavelength where the reflectance is desired to be zero as shown in figure 8. In particular a wavelength of 500 nm was indicated, that is why the reflectance is zero at that point.

Source: *Own elaboration*

For the simulation of an AR bilayer, the equation [52] is used, which represents the reflectance of an indecent wave over an electromagnetic spectrum from 300 to 1200 nm. In figure 9, zero reflectance was achieved in the range of 450 to 700 nm. Thus, it can be interpreted that for this range of the visible the thin film bilayer is anti-reflective.

Reflectance of an AR film bilayer

Source: *Own elaboration*

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Conclusions

With the results obtained, it is possible to show an algorithm capable of simulating an antireflection thin film. So the user can indicate the refractive index of the medium in which the wave propagates before hitting the AR and the semiconductor medium. With this data the algorithm calculates the refractive index and the thickness of the film so that there is zero reflectance corresponding to a wavelength.

In a similar way it was possible to develop an algorithm to simulate an AR film bilayer. Where the user enters the refractive indices of the media in which the wave propagates, as well as the range of the electromagnetic spectrum of interest. Resulting in zero reflectance in the visible spectrum.

Declarations

Conflict of interest

The authors declare that they have no conflicts of interest. They have no known competing financial interests or personal relationships that might have appeared to influence the article reported in this paper.

Authors' contribution

Canales-Pacheco, Benito: Contributed to the project idea, research method and technique.

Noriega-Loredo, Raymundo Sergio: Contributed to the development of diagrams and writing of the article.

Austría-González, León Felipe: Contributed to the analysis and writing of the article.

Reyes-Ramírez, Bartolome: Contributed to the development of the concept and writing of the article.

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Abbreviations

AR Anti-reflective

ARCs Anti-reflective Coating

SLAR Single layer anti-reflective coatings

CIGS Copper indium gallium selenide solar cell

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Background

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