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Effects of dislocations on electron channeling

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Abstract
The phenomenon of electron channeling in a crystal affected by dislocations is considered. Earlier we had considered the quantum aspects of the positron channeling in a crystal bent by dislocations where the effects of longitudinal motion of the particle were also considered along with the transverse motion. In this paper, the effective potential for the electron case is found for the two regions of dislocation-affected channel. There is considerable shift in the potential minima due to dislocations. The frequency and the corresponding spectrum of the channeling radiation due to electrons channeling through the perfect channel and the two regions of dislocation-affected channels are calculated. The spectral distribution of radiation intensity changes with the parameters of dislocation. The continuity of wavefunctions and their derivatives is used at the three boundaries and the reflection and transmission coefficients are found using these boundary conditions in the same way as in the positron case.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

Emission of channeling radiation by relativistic e^+ and e^- are of great importance in atomic physics and accelerator-based research and was a matter of discussion from the very beginning. But the observation of this radiation appeared to be precluded since the oscillatory frequencies of the channeled particles are low, the corresponding energies being of the order of a few eV only. However, the realization that relativistic effects will shift the photon energy into the keV or even MeV region for MeV and GeV positrons and electrons, respectively, was a turning point. The radiation was reported for the first time back in 1979. Thereafter, channeling radiation has been investigated and reviewed by several authors [1–12].

One of the main applications of ion channeling is defects studies. The effects of defects on charged particle propagation were an area of research for a long time with some experiments to explore their application [5]. The classical description of the dislocation effects on the channeling of positrons in the planar and axial cases [6] gave an idea of the effects on the energy loss mechanism. A quantum mechanical treatment of the effects of dislocation on dechanneling was given later [7].

Previously we have developed a quantum mechanical model for the effects of dislocations on positron channeling [13], considering both transverse and longitudinal motion of particles. Here, we consider the effects of dislocations on planar channeling of electrons. Both the transverse and longitudinal motion of the particles are considered. The change in energy spectrum and the spectral distribution of intensity of the emitted radiation due to dislocations are investigated for the first time.

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2. Effects of dislocations on electron channeling

Just like in the previous case [13], we consider a typical channel at some distance from the dislocation core, outside the dechanneling cylinder [7]. The model is shown in figure 1. The whole channel is divided into four regions. The dislocation-affected parts of the channel are regions II and III. Here ρ_0 corresponds to the radial coordinate of the channel center as measured from the origin and φ_0 is the corresponding angular coordinate.

The Schrödinger equation for planar channeling for a particle of mass m moving in region I (perfect channel) can be written as

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial z^2}\right)\Psi^{\mathrm{I}}(x,z)+U(x)\Psi^{\mathrm{I}}(x,z)=E^{\mathrm{I}}\Psi^{\mathrm{I}}(x,z). \tag{1}$$

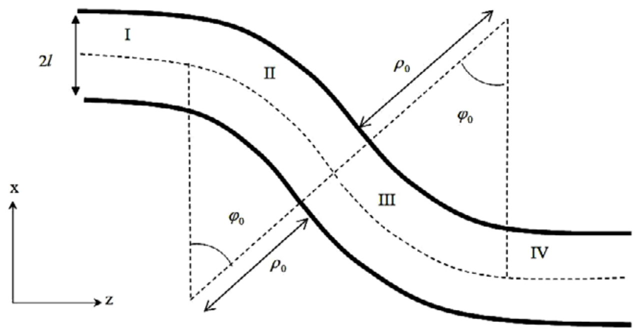

Figure 1. The model.

For an electron

$$U(x) = -\frac{V_0}{x + a_T} \tag{2}$$

where

$$V_0 = 2\pi Z_1 Z_2 e^2 N d_p C a_T^2 \tag{3}$$

where C is the Lindhard's constant ($=\sqrt{3}$), a_T is the Thomas–Fermi screening distance:

$$a_T = \frac{0.8853 a_0}{Z_1^{2/3} + Z_2^{2/3}} \tag{4}$$

a_0 is the Bohr radius, Z_1 and Z_2 are the atomic numbers of the incident ion and target atoms, respectively, Nd_p is the planar density of atoms, N being the bulk density of atoms in the crystal and d_p the interplanar spacing.

After separation of variables, the total wavefunction for region I becomes

$$\Psi^I(x, z) = X_n^I(x - x_0) Z^I(z) \tag{5}$$

where x_0 is the initial amplitude of the channeled electron. Considering the effects of transverse states, the above equation can be written as

$$\Psi^I(x, z) = A_0 X_0^I e^{ik_0 z} + \sum_{n=0} B_n X_n^I e^{-ik_n z}. \tag{6}$$

Now consider the two regions in the channel which are affected by dislocation. These curved regions are due to the centrifugal force proportional to $\frac{\mu^2}{\rho^2}$, where $\mu^2 = l(l+1)$ with l as the orbital angular momentum quantum number and ρ is the radius of curvature of the channel.

The Schrödinger equation for region II in terms of the polar coordinates ρ and φ is

$$-\frac{\hbar^2}{2m}\left[\frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial}{\partial\rho}\right) + \frac{1}{\rho^2}\frac{\partial^2}{\partial\varphi^2}\right]\Psi^{II}(\rho,\varphi) - \frac{V_0}{(\rho-\rho_0)+a_T}\Psi^{II}(\rho,\varphi) = E^{II}\Psi^{II}(\rho,\varphi). \tag{7}$$

Separating variables gives azimuthal and radial equations as

$$F''^{II}(\varphi) = -\mu^2 F^{II}(\varphi) \tag{8}$$

$$R''^{II}(\rho) + \frac{2m}{\hbar^2}\left[E^{II} + \frac{V_0}{(\rho-\rho_0)+a_T} - \frac{\hbar^2}{2m}\frac{\mu^2}{\rho^2}\right]R^{II}(\rho) = 0. \tag{9}$$

From the radial equation, the effective potential for region II can be written as

$$V_{eff}(\rho) = -\frac{V_0}{(\rho-\rho_0)+a_T} + \frac{\hbar^2}{2m}\frac{\mu^2}{\rho^2}. \tag{10}$$

Keeping $\xi = \rho - \rho_0$ and simplifying the above equation, we get the effective potential in the form given by the equation

$$V_{eff}(\xi) = \frac{\hbar}{2m}\left\{\frac{\lambda_1'^3}{\lambda_1^2\rho_0^4 a_T^3[2\xi + \frac{\lambda_1'}{\lambda_1}]} - \frac{\lambda_1'^2}{\lambda_1\rho_0^4 a_T^3} + \frac{\lambda_1''}{\rho_0^4 a_T^3}\right\} \tag{11}$$

where

$$\lambda_1 = -2a^4\rho_0^4 + 3\mu^2 a_T^3 \tag{12}$$

$$\lambda_1' = -a^4\rho_0^4 a_T + \mu^2 a_T^3 \rho_0 \tag{13}$$

$$\lambda_1'' = -2a^4\rho_0^4 a_T^2 + \mu^2 a_T^3 \rho_0^2. \tag{14}$$

From equation (11) we can see a shift in the minimum of the potential, which is due to the shift is the equilibrium axis due to dislocation. The wavefunction of region II can be written as

$$\Psi^{II}(\rho,\varphi) = \sum_{m=0} R_m^{II}[C_m e^{i\mu\varphi} + D_m e^{-i\mu\varphi}]. \tag{15}$$

Similarly, proceeding to region III, the Schrödinger equation can be written as

$$-\frac{\hbar^2}{2m}\left[\frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial}{\partial\rho}\right) + \frac{1}{\rho^2}\frac{\partial^2}{\partial\varphi^2}\right]\Psi^{III}(\rho,\varphi) - \frac{V_0}{(\rho-\rho_0)+a_T}\Psi^{III}(\rho,\varphi) = E^{III}\Psi^{III}(\rho,\varphi). \tag{16}$$

Separating variables gives azimuthal and radial equations as

$$F''^{III}(\varphi) = -\mu^2 F^{III}(\varphi) \tag{17}$$

$$R''^{III}(\rho) + \frac{2m}{\hbar^2}\left[E^{III} + \frac{V_0}{(\rho-\rho_0)+a_T} + \frac{\hbar^2}{2m}\frac{\mu^2}{\rho^2}\right]R^{III}(\rho) = 0. \tag{18}$$

From the radial equation, the effective potential for region III can be written as

$$V_{eff}(\rho) = -\frac{V_0}{(\rho-\rho_0)+a_T} - \frac{\hbar^2}{2m}\frac{\mu^2}{\rho^2} \tag{19}$$

which, upon simplification,

$$V_{eff}(\xi) = \frac{\hbar}{2m}\left\{\frac{\lambda_1'^3}{\lambda_2^2\rho_0^4 a_T^3[2\xi + \frac{\lambda_2'}{\lambda_2}]} - \frac{\lambda_2'^2}{\lambda_2\rho_0^4 a_T^3} + \frac{\lambda_2''}{\rho_0^4 a_T^3}\right\} \tag{20}$$

where

$$\lambda_2 = -2a^4\rho_0^4 - 3\mu^2 a_T^3 \tag{21}$$

$$\lambda_2' = -a^4\rho_0^4 a_T - \mu^2 a_T^3 \rho_0 \tag{22}$$

$$\lambda_2'' = -2a^4\rho_0^4 a_T^2 - \mu^2 a_T^3 \rho_0^2. \tag{23}$$

The above equation shows a shift in the potential minimum. Figure 2 shows the potential shift in this region. The wavefunction of region III can be written as

$$\Psi^{III}(\rho,\varphi) = \sum_{m=0} R_m^{III}[G_m e^{i\mu\varphi} + H_m e^{-i\mu\varphi}]. \tag{24}$$

Table 1. The change in energy (in eV) for various materials for electrons channeling along the (110) direction at different incident energies for a value of $\rho_0 = 0.5 \times 10^{-7}$ m.

	50 MeV		20 MeV		10 MeV	
	Straight channel	Dislocation-affected channel	Straight channel	Dislocation-affected channel	Straight channel	Dislocation-affected channel
Si	2.83×10^{-3}	2.861×10^{-3}	0.93×10^{-3}	0.942×10^{-3}	0.476×10^{-3}	0.481×10^{-3}
Cu	3.257×10^{-3}	3.293×10^{-3}	1.3×10^{-3}	1.31×10^{-3}	0.651×10^{-3}	0.658×10^{-3}

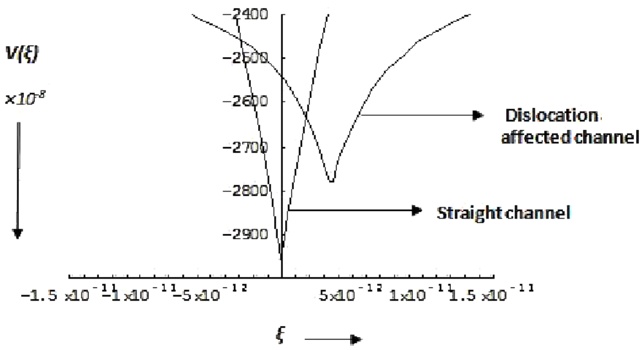

Figure 2. The shift in potential due to dislocations.

The fourth region is the perfect channel. There will be only a transmitted wave in this region and the wavefunction is written as

$$\Psi^{\mathrm{IV}}(x, z) = X_n^{\mathrm{IV}} I_n \mathrm{e}^{\mathrm{i}k_n z}. \tag{25}$$

Now we proceed to find the reflection and transmission coefficients. The boundary conditions across the three boundaries are given by

$$\Psi^{\mathrm{I}}|_{z=0} = \Psi^{\mathrm{II}}|_{\varphi=0} \quad \text{and} \quad \left.\frac{\partial \Psi^{\mathrm{I}}}{\partial z}\right|_{z=0} = \frac{1}{\rho_0}\left.\frac{\partial \Psi^{\mathrm{II}}}{\partial \varphi}\right|_{\varphi=0} \tag{26}$$

$$\Psi^{\mathrm{II}}|_{\varphi=\varphi_0} = \Psi^{\mathrm{III}}|_{\varphi=0} \quad \text{and} \quad \left.\frac{\partial \Psi^{\mathrm{II}}}{\partial \varphi}\right|_{\varphi=\varphi_0} = \left.\frac{\partial \Psi^{\mathrm{III}}}{\partial \varphi}\right|_{\varphi=0} \tag{27}$$

$$\Psi^{\mathrm{III}}|_{\varphi=\varphi_0} = \Psi^{\mathrm{IV}}|_{z=t} \quad \text{and} \quad \frac{1}{\rho_0}\left.\frac{\partial \Psi^{\mathrm{III}}}{\partial \varphi}\right|_{\varphi=\varphi_0} = \left.\frac{\partial \Psi^{\mathrm{IV}}}{\partial z}\right|_{z=t}. \tag{28}$$

From the above boundary conditions, we get the reflection and transmission coefficients as

$$|R|^2 = \frac{(-\mu^2 + k^2\rho_0^2)^2 \sin^2(2\mu\varphi_0)}{4k^2\mu^2\rho_0^2\cos^2(2\mu\varphi_0) + (\mu^2 + k^2\rho_0^2)^2\sin^2(2\mu\varphi_0)} \tag{29}$$

$$|T|^2 = \frac{4k^2\mu^2\rho_0^2\mu^2}{4k^2\mu^2\rho_0^2\cos^2(2\mu\varphi_0) + (\mu^2 + k^2\rho_0^2)^2\sin^2(2\mu\varphi_0)}. \tag{30}$$

These give the dechanneling and channeling probabilities, respectively. The variation of these coefficients with the value of ρ_0 and incident energy E is given in equations (3) and (4).

The eigenspectrum of electron channeling is given by [14]

$$|E_n| = \frac{V_0^2}{2\hbar^2(n + \delta n)^2} \tag{31}$$

$$\delta n = 2a_{\mathrm{T}}/a_{\mathrm{TF}} \tag{32}$$

$$a_{\mathrm{T}} = \sqrt{a_{\mathrm{TF}}^2 + u^2} \tag{33}$$

where u^2 is the mean-square vibrational amplitude. The additional centrifugal force due to the dislocation changes the spectrum. This change in energy due to channeling of electrons in a dislocation-affected channel for various materials and various energies is given in table 1 and compared with that in a straight channel for a value of $\rho_0 = 0.5 \times 10^{-7}$ m.

3. Spectral distribution of radiation intensity

Now we consider the effect of dislocation on the spectral distribution of the radiation intensity. The probability of transition from an initial state (i) to a final state (f) of the electron per unit time is determined by the well-known formula [15]

$$W_{\mathrm{fi}} = \frac{4\pi^2 e^2}{\hbar V}\sum_{\vec{q}} |\vec{q}|^{-1} |\vec{\alpha}_{\mathrm{fi}} \cdot \vec{e}_k|^2 \delta(\omega_{\mathrm{fi}} - \omega) \tag{34}$$

where V is the volume of the system, and $\vec{q}$ and $\vec{e}_k$ are the wavevector and polarization vectors of a quantum of electromagnetic field:

$$\hbar\omega_{\mathrm{fi}} = E_{n\mathrm{i}} - E_{n\mathrm{f}}. \tag{35}$$

The matrix elements $\vec{\alpha}_{\mathrm{fi}}$ are given by

$$\vec{\alpha}_{\mathrm{fi}} = \delta_{\sigma_{\mathrm{iz}}\sigma_{\mathrm{fz}}} \delta_{p_{\mathrm{iy}}, p_{\mathrm{fy}} + \hbar q_y} \vec{D}_{\mathrm{fi}} \tag{36}$$

$$\vec{D}_{\mathrm{fi}} = -\mathrm{i}x_{\mathrm{fi}}(\Omega_{\mathrm{fi}}, 0, q_x\beta) \tag{37}$$

$$x_{\mathrm{fi}} = \int_{\infty}^{-\infty} x S_{n_{\mathrm{f}}E_{\mathrm{f}}}(x) S_{n_{\mathrm{i}}E_{\mathrm{i}}}(x)\,\mathrm{d}x \tag{38}$$

where s_{nE} are oscillatory wavefunctions which obey the Schrödinger equation given by

$$\left[-\frac{\hbar^2}{2E}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + U(x)\right] S_E(x) = E S_E(x). \tag{39}$$

Let us define a vector of polarization $\vec{e}_1$ in the plane having the wavevector $\vec{q}$ and the z axis and a vector $\vec{e}_2 \perp \vec{e}_1$ in the plane having the axes x and y. If φ and θ are the azimuth and polar angle of the wavevector $\vec{q}$

$$\vec{e}_1 = (\cos\theta\cos\varphi, \cos\theta\sin\varphi, -\sin\theta) \tag{40}$$

$$\vec{e}_2 = (-\sin\varphi, \cos\varphi, 0). \tag{41}$$

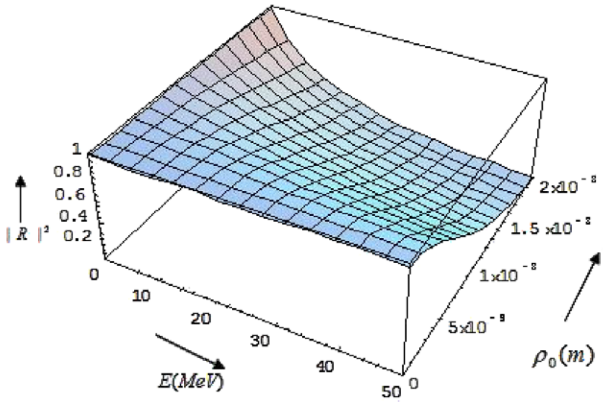

Figure 3. Variation of the reflection coefficient/dechanneling probability with ρ_0 and incident energy E of the electron.

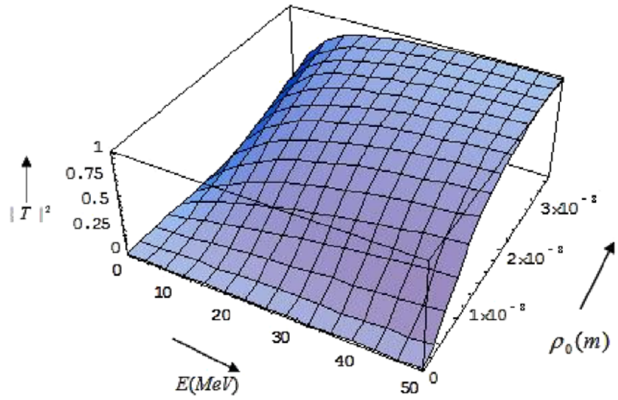

Figure 4. Variation of the transmission coefficient/channeling probability with ρ_0 and incident energy E of the electron.

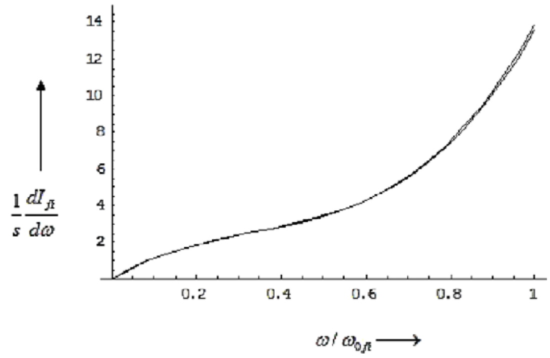

Figure 5. Spectral distribution of radiation intensity.

The summation in equation (34) is written in the integral form as

$$W_{\mathrm{fi}} = \frac{e^2}{2\pi\hbar}\int (|\vec{\alpha}_{\mathrm{fi}}\cdot\vec{e}_1|^2 + |\vec{\alpha}_{\mathrm{fi}}\cdot\vec{e}_2|^2)|\vec{q}|^{-1}|\delta(\omega_{\mathrm{fi}}-\omega)\,\mathrm{d}\vec{q}. \quad (42)$$

Solving, we get the transmission probabilities as

$$\frac{\mathrm{d}W_{\mathrm{fi}}}{\mathrm{d}\Omega} = \frac{e^2 x_{\mathrm{fi}}^2 \Omega_{\mathrm{fi}}^3}{2\pi\hbar(1-\beta\cos\theta)^4} \times [(1-\beta\cos\theta)^2 - (1-\beta^2)\sin^2\theta\cos^2\varphi] \quad (43)$$

$$\frac{\mathrm{d}W_{\mathrm{fi}}}{\mathrm{d}\omega} = x_{\mathrm{fi}}^2\Omega_{\mathrm{fi}}^2\frac{e^2}{2\hbar\beta^3} \times \left[1+\beta^2 - 2(1+\beta)\frac{\omega}{\omega_{0\mathrm{fi}}} + 2(1+\beta)^2\left(\frac{\omega}{\omega_{0\mathrm{fi}}}\right)^2\right] \quad (44)$$

$$\frac{\mathrm{d}I_{\mathrm{fi}}}{\mathrm{d}\Omega} = \frac{e^2 x_{\mathrm{fi}}^2 \Omega_{\mathrm{fi}}^3}{2\pi(1-\beta\cos\theta)^5} \times [(1-\beta\cos\theta)^2 - (1-\beta^2)\sin^2\theta\cos^2\varphi] \quad (45)$$

$$\frac{\mathrm{d}I_{\mathrm{fi}}}{\mathrm{d}\omega} = e^2 x_{\mathrm{fi}}^2\Omega_{\mathrm{fi}}^2\frac{\omega}{2\beta^3} \times \left[1+\beta^2 - 2(1+\beta)\frac{\omega}{\omega_{0\mathrm{fi}}} + 2(1+\beta)^2\left(\frac{\omega}{\omega_{0\mathrm{fi}}}\right)^2\right] \quad (46)$$

where

$$\omega_{0\mathrm{fi}} \approx 2\Omega_{\mathrm{fi}}\gamma^2. \quad (47)$$

The spectral intensity of radiation of a channeled electron in the case of a straight and a dislocation-affected channel are plotted in figures 5 and 6 with

$$s = \frac{3e^2 x_{\mathrm{fi}}^2}{8\beta^3\gamma^2}. \quad (48)$$

It is found that the change in the effective potential and frequency of oscillations proportionally changes the spectral distribution of radiation intensity.

4. Results and discussions

The effects of centrifugal force developed due to the distortions in the channels have been discussed. The transverse potential in the perfect channel and the two regions of dislocation-affected channels are found. This centrifugal force causes a shift in the potential minima and is plotted in figure 2.

The curvature of the channel induces a shift in the equilibrium axis which changes the frequency in both the dislocation-affected channels. The effects of the change in frequency is reflected in the spectral distribution of radiation intensity. The energy change is calculated for various materials and various incident energies of the electrons and is given in table 1. A comparison with the straight channel values is also made here.

The continuity of wavefunctions and their derivatives is used at the three boundaries. The reflection and transmission coefficients are found using these boundary conditions which are the dechanneling and channeling probabilities, respectively. Figures 3 and 4 show the variation of these dechanneling and channeling probabilities respectively with ρ_0 and incident energy E of the electron. The spectral distribution of radiation intensity is calculated and compared with that of the straight channel and is plotted in figures 5 and 6.

5. Conclusions

We have developed a quantum mechanical model for the effects of dislocations on electron channeling. The shift in potential minima due to the dislocation in the channel is found. The corresponding change in energy is calculated and compared with that of the straight channel. We find a fractional change in

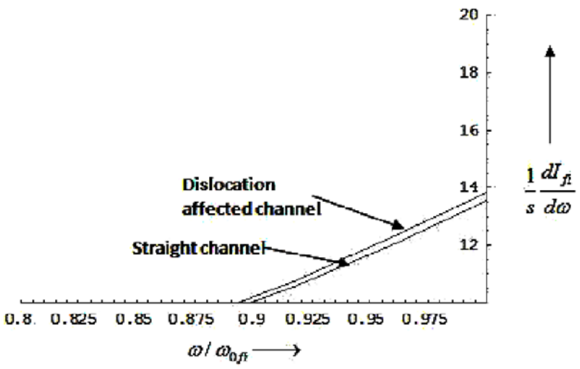

Figure 6. Spectral distribution of radiation intensity, showing clearly the fractional change due to the effects of dislocations.

the parameters due to effects of dislocations. The channeling and dechanneling probabilities are found using the boundary conditions across the boundaries. The spectral distribution of radiation intensity is calculated and compared with that of the straight channel.

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