

MECHANISM OF FORMATION OF SPACE-CHARGE POLARIZATION IN DIELECTRICS

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A general mechanism of space-charge relaxation in dielectrics, whose separate manifestations were studied in [5–7], is investigated. A strict solution of a system of the nonlinear Fokker–Planck and Poisson equations has been derived in the form of a Fourier series; a recurrent relation is suggested for the oscillation modes which allows the mechanism of space-charge relaxation to be considered as an interaction of modes generated in crystals in an external electric field. Very cumbersome calculations do not allow us to estimate the opportunity of technical applications of the solution obtained within the framework of one paper.

1. RELAXATION MODES OF THE SPACE-CHARGE POLARIZATION

The space-charge polarization is a governing factor of the dielectric properties. It is a common mechanism of charge relaxation in thin films of microcircuit elements; the space-charge formation results in an unstable operation of MIS structures and their breakdown.

The space-charge relaxation in crystals has been investigated on the microlevel only in uniform weak electric fields [1, 2]. We were forced to use a phenomenological model which describes charge transfer by a system of the Fokker–Planck and Poisson equations [3, 4]. Its analytical solution was obtained in [4] in the first and in [5] in the second approximations of mathematical perturbation theory. We now write down these equations in dimensionless variables $\xi = \frac{x}{a}$ and $\tau = \frac{Dt}{a^2}$ [4]:

$$\begin{cases} \frac{\partial \rho}{\partial \tau} = \frac{\partial^2 \rho}{\partial \xi^2} - \theta \rho - \gamma \frac{\partial(z\rho)}{\partial \xi}, \\ \frac{\partial z}{\partial \xi} = \psi \rho, \\ \left. \frac{\partial \rho}{\partial \xi} \right|_{\xi=0, l/a} = \gamma(n_0 + \rho)z \Big|_{\xi=0, l/a}, \\ \rho(\xi, 0) = 0, \quad \int_0^{l/a} z d\xi = \frac{l}{a} \frac{E(\tau)}{E_0}. \end{cases} \quad (1)$$

Here the space-charge distribution is characterized by $\rho = n - n_0$, where n_0 is the equilibrium concentration of mobile carriers having charge q , $z = \frac{E}{E_0}$ is the dimensionless electric field strength, E_0 is the uniform electric field strength, a is

the lattice constant, D is the diffusion coefficient, $\psi = \frac{aq}{\epsilon_0 \epsilon_\infty E_0}$, $\gamma = \frac{\mu a E_0}{D}$, $\theta = \psi \gamma n_0$, l is the thickness of the dielectric, and μ is the mobility of charge carriers.

Far from the breakdown $\gamma < 1$; therefore, it is expedient to use series

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$$\rho = \sum_{n=1}^{+\infty} \gamma^n \rho_n, \quad z = \sum_{n=0}^{+\infty} \gamma^n z_n. \quad (2)$$

It is obvious that

$$\int_0^{l/a} z_n d\xi = 0. \quad (3)$$

Substituting Eq. (2) into Eq. (1) and equating terms with identical γ powers, we obtain

$$\begin{cases} \frac{\partial \rho_n}{\partial \tau} = \frac{\partial^2 \rho_n}{\partial \xi^2} - \theta \rho_n - z_0 \frac{\partial \rho_{n-1}}{\partial \xi} - \sum_{m=1}^{n-2} \frac{\partial}{\partial \xi} (\rho_m z_{n-m-1}), \\ \frac{\partial z_n}{\partial \xi} = \psi \rho_n, \\ \left[\frac{\partial \rho_n}{\partial \xi} - n_0 z_{n-1} - z_0 \rho_{n-1} - \sum_{m=1}^{n-2} (\rho_m z_{n-m-1}) \right]_{\xi=0, l/a} = 0, \\ \rho_n(\xi, 0) = 0, \quad \int_0^{l/a} z_n d\xi = 0. \end{cases} \quad (4)$$

We seek a solution of system (4) as a series in orthogonal functions $\Psi_m = \cos\left(\frac{\pi m a}{l} \xi\right)$ with norm $\|\Psi_m\|^2 = \frac{l}{2a}$:

$$\rho_n = \sum_{k=1}^{+\infty} A_n(k, \tau) \cos\left(\frac{\pi k a}{l} \xi\right). \quad (5)$$

According to the second equation of system (4),

$$z_n = \int \psi \rho_n d\xi + C(\tau); \quad (6)$$

otherwise,

$$z_n = \psi \sum_{k=1}^{+\infty} A_n(k, \tau) \left(\frac{l}{\pi k a}\right) \sin\left(\frac{\pi k a}{l} \xi\right) + C(\tau). \quad (7)$$

The term $C(\tau)$ in Eq. (7) is specified by the last equation of system (4):

$$C(\tau) = -\psi \sum_{k=1}^{+\infty} A_n(k, \tau) \left(\frac{2l}{\pi^2 k^2 a}\right) \sin^2\left(\frac{\pi k}{2}\right). \quad (8)$$

Thus we have

$$z_n = \psi \sum_{k=1}^{+\infty} A_n(k, \tau) \left(\frac{l}{\pi k a}\right) \left[\sin\left(\frac{\pi k a}{l} \xi\right) - \frac{2 \sin^2\left(\frac{\pi k}{2}\right)}{\pi k} \right]. \quad (9)$$

Let us designate

$$f_{n-1} = z_0 \rho_{n-1} + \sum_{m=1}^{n-2} \rho_m z_{n-m-1}. \quad (10)$$

In this case, the kinetic equation assumes the form

$$\frac{\partial \rho_n}{\partial \tau} = \frac{\partial^2 \rho_n}{\partial \xi^2} - \theta \rho_n - \frac{\partial f_{n-1}}{\partial \xi}. \quad (11)$$

Let us write down the boundary and initial conditions:

$$\left. \frac{\partial \rho_n}{\partial \xi} \right|_{\xi=0, l/a} = (n_0 z_{n-1} + f_{n-1})|_{\xi=0, l/a}, \quad \rho_n(\xi, 0) = 0 \quad (12)$$

and the relaxation mode amplitudes $A_n(k, \tau)$:

$$A_n(k, \tau) = \frac{2a^{l/a}}{l} \int_0^{l/a} \rho_n \cos\left(\frac{\pi k a}{l} \xi\right) d\xi. \quad (13)$$

Multiplication of Eqs. (11) and (12) by $\Psi_j = \cos\left(\frac{\pi j a}{l} \xi\right)$ yields

$$\Psi_j \frac{\partial \rho_n}{\partial \tau} = \Psi_j \frac{\partial^2 \rho_n}{\partial \xi^2} - \theta \Psi_j \rho_n - \Psi_j \frac{\partial f_{n-1}}{\partial \xi}, \quad (14)$$

$$\left. \Psi_j \frac{\partial \rho_n}{\partial \xi} \right|_{\xi=0, l/a} = \Psi_j (n_0 z_{n-1} + f_{n-1})|_{\xi=0, l/a}. \quad (15)$$

Integration of Eq. (14) over ξ from 0 to l/a yields

$$\int_0^{l/a} \Psi_j \frac{\partial \rho_n}{\partial \tau} d\xi = \int_0^{l/a} \Psi_j \frac{\partial^2 \rho_n}{\partial \xi^2} d\xi - \int_0^{l/a} \theta \Psi_j \rho_n d\xi - \int_0^{l/a} \Psi_j \frac{\partial f_{n-1}}{\partial \xi} d\xi. \quad (16)$$

We now transform the integral on the left side of Eq. (16) changing the order of integration over ξ and differentiation with respect to τ . From Eq. (13) it follows that

$$\frac{\partial}{\partial \tau} \int_0^{l/a} \Psi_j \rho_n d\xi = \frac{l}{2a} \frac{\partial A_n(j, \tau)}{\partial \tau}. \quad (17)$$

We now take by parts the first integral on the right side of Eq. (16) taking into account that $\frac{\partial^2 \Psi_j}{\partial \xi^2} = -\frac{\pi^2 j^2 a^2}{l^2} \Psi_j$:

$$\int_0^{l/a} \Psi_j \frac{\partial^2 \rho_n}{\partial \xi^2} d\xi = \Psi_j \left. \frac{\partial \rho_n}{\partial \xi} \right|_0^{l/a} - \rho_n \left. \frac{\partial \Psi_j}{\partial \xi} \right|_0^{l/a} - \frac{\pi^2 j^2 a^2}{l^2} A_n(j, \tau) \frac{l}{2a}. \quad (18)$$

Since $\frac{\partial \Psi_j}{\partial \xi} \Big|_0^{l/a} = 0$, boundary conditions (12) change their form

$$\int_0^{l/a} \Psi_j \frac{\partial^2 \rho_n}{\partial \xi^2} d\xi = \Psi_j (n_0 z_{n-1} + f_{n-1}) \Big|_{\xi=l/a} - \Psi_j (n_0 z_{n-1} + f_{n-1}) \Big|_{\xi=0} - \frac{\pi^2 j^2 a^2}{l^2} A_n(j, \tau). \quad (19)$$

We note that

$$\Psi_j n_0 z_{n-1} \Big|_{\xi=l/a} = -\frac{2l \psi n_0}{\pi^2 a} \cos(\pi j) \sum_{k=1}^{+\infty} A_{n-1}(k, \tau) \frac{\sin^2\left(\frac{\pi k}{2}\right)}{k^2}, \quad (20)$$

$$\Psi_j n_0 z_{n-1} \Big|_{\xi=0} = -\frac{2l \psi n_0}{\pi^2 a} \sum_{k=1}^{+\infty} A_{n-1}(k, \tau) \frac{\sin^2\left(\frac{\pi k}{2}\right)}{k^2}. \quad (21)$$

Taking by parts the last integral in Eq. (16), we derive the following equation for the relaxation mode amplitudes $A_n(j, \tau)$:

$$\frac{\partial A_n(j, \tau)}{\partial \tau} = -\left(\theta + \frac{\pi^2 j^2 a^2}{l^2}\right) A_n(j, \tau) + F(\tau). \quad (22)$$

Here we have introduced the function

$$F(\tau) = \frac{8\psi n_0}{\pi^2} \sin^2\left(\frac{\pi j}{2}\right) \sum_{k=1}^{+\infty} A_{n-1}(k, \tau) \frac{\sin^2\left(\frac{\pi k}{2}\right)}{k^2} + \frac{2a^{l/a}}{l} \int_0^{l/a} f_{n-1}(\xi, \tau) \frac{\partial \Psi_j}{\partial \xi} d\xi. \quad (23)$$

A solution of differential equation (23) with initial condition $A_n(j, 0) = 0$ is

$$A_n(j, \tau) = \int_0^\tau \exp\left[\left(\theta + \frac{\pi^2 j^2 a^2}{l^2}\right)(t' - \tau)\right] F(t') dt'. \quad (24)$$

Combining Eqs. (23) and (24), we find the recursion relation for $A_n(j, \tau)$:

$$A_n(j, \tau) = \int_0^\tau \exp\left[\left(\theta + \frac{\pi^2 j^2 a^2}{l^2}\right)(t' - \tau)\right] \left\{ \frac{8n_0 \psi}{\pi^2} \sin^2\left(\frac{\pi j}{2}\right) \times \sum_{k=1}^{+\infty} A_{n-1}(k, \tau) \frac{\sin^2\left(\frac{\pi k}{2}\right)}{k^2} + \frac{2a^{l/a}}{l} \int_0^{l/a} f_{n-1}(\xi, t') \frac{\partial \Psi_j}{\partial \xi} d\xi \right\} dt'. \quad (25)$$

Because of cumbersome calculations, the integral over the spatial variable ξ in Eq. (25) is calculated in the Appendix. We obtain

$$\begin{aligned}
& \int_0^{l/a} f_{n-1}(\xi, t') \frac{\partial \Psi_j}{\partial \xi} d\xi = -\frac{\pi j a}{l} \left\{ z_0(t') \sum_{p=1}^{+\infty} A_{n-1}(p, t') \frac{2lj}{\pi a} \frac{\sin^2\left(\frac{\pi(j+p)}{2}\right)}{j^2 - p^2} \right. \\
& + \psi \sum_{m=1}^{n-2} \sum_{p,s=1}^{+\infty} A_m(p, t') A_{n-m-1}(s, t') \frac{l}{\pi s a} \left\{ \frac{l}{4a} [\delta(p+s-j) + \delta(p+j-s) \right. \\
& \left. \left. - \delta(s+j-p)] - \frac{2 \sin^2\left(\frac{\pi s}{2}\right)}{\pi s} \frac{l}{\pi a} \frac{2j}{j^2 - p^2} \sin^2\left[\frac{\pi(j+p)}{2}\right] \right\} \right\}. \quad (26)
\end{aligned}$$

Designating j by k and k by p in Eqs. (25) and (26) and substituting Eq. (26) into Eq. (25), we derive the recursion relation for the relaxation mode amplitude in the n th order of the perturbation theory:

$$\begin{aligned}
A_n(k, \tau) &= \int_0^\tau \exp\left[\left(\theta + \frac{\pi^2 k^2 a^2}{l^2}\right)(t' - \tau)\right] \left\{ \frac{8n_0 \psi}{\pi^2} \sin^2\left(\frac{\pi k}{2}\right) \right. \\
& \times \sum_{p=1}^{+\infty} A_{n-1}(p, t') \frac{\sin^2\left(\frac{\pi p}{2}\right)}{p^2} - \frac{4ak^2}{l} z_0 \sum_{p=1}^{+\infty} A_{n-1}(p, t') \frac{\sin^2\left(\frac{\pi(k+p)}{2}\right)}{k^2 - p^2} \\
& \left. - \psi \frac{2ak}{l} \sum_{m=1}^{n-2} \sum_{p,s=1}^{+\infty} A_m(p, t') A_{n-m-1}(s, t') \left\{ \frac{l}{4as} [\delta(p+s-k) + \delta(p+k-s) - \delta(s+k-p)] \right. \right. \\
& \left. \left. - \frac{4lk}{\pi^2 s^2 a} \sin^2\left(\frac{\pi s}{2}\right) \frac{\sin^2\left[\frac{\pi(k+p)}{2}\right]}{k^2 - p^2} \right\} \right\} dt'. \quad (27)
\end{aligned}$$

Here $\delta(p+s-k)$, $\delta(p+k-s)$, and $\delta(s+k-p)$ are Kronecker's delta symbols. It should be emphasized that $n \geq 2$ in Eq. (27).

The relaxation mode amplitudes in the first order of the perturbation theory for $n=1$ are calculated using Eqs. (23) and (24):

$$A_1(k, \tau) = -\frac{4a}{l} n_0 \sin^2\left(\frac{\pi k}{2}\right) \int_0^\tau z_0(t') \exp\left[\left(\theta + \frac{\pi^2 k^2 a^2}{l^2}\right)(t' - \tau)\right] dt'. \quad (28)$$

For an ac electric field, $z_0(t') = \exp(i\omega_1 t')$, and formula (28) assumes the form

$$A_1(k, \tau) = -\frac{4a}{l} n_0 \sin^2\left(\frac{\pi k}{2}\right) \frac{\exp(i\omega_1 \tau) - \exp\left[-\left(\theta + \frac{\pi^2 k^2 a^2}{l^2}\right)\tau\right]}{\theta + \frac{\pi^2 k^2 a^2}{l^2} + i\omega_1}, \quad (29)$$

where $\omega_1 = \frac{\omega a^2}{D}$ is the dimensionless frequency of the external electric field.

2. MECHANISM OF SPACE-CHARGE FORMATION

In the first-order approximation of the perturbation theory, the space charge accumulation in dielectrics and semiconductors can be considered as an excitation in an external electric field of relaxation modes with the amplitude $A_1(k, \tau)$, wavelength $\lambda_k = \frac{2l}{k}$, and relaxation time τ_k [4]:

$$\frac{1}{\tau_k} = \frac{1}{\tau_M} + \frac{1}{\tau_{Dk}}. \quad (30)$$

Here τ_M is the Maxwell relaxation time:

$$\tau_M = \frac{\epsilon_0 \epsilon_\infty}{\mu n_0 q} \quad (31)$$

and τ_{Dk} is the diffusion relaxation time of the k th mode:

$$\tau_{Dk} = \frac{l^2}{\pi^2 D k^2} \quad (32)$$

With increase in k , the relaxation time τ_k and the wavelength λ_k of the relaxation modes decrease. The relaxation time for the k th mode, according to Eq. (30), is determined by the formula

$$\tau_k = \frac{\tau_M \tau_D}{\tau_D + k^2 \tau_M}, \quad (33)$$

where τ_D is the diffusion relaxation time for the mode with $k = 1$.

If the Maxwell relaxation time for the first mode $\tau_M \gg \tau_D$, then $\tau_k \approx \tau_{Dk}$ and the space-charge relaxation is determined by diffusion of defects. For $\tau_M \ll \tau_D$, there exists the serial number of the relaxation mode k_1 for which $\tau_D \approx \tau_M k^2$ and $\tau_M \approx \tau_{Dk}$. Then for $k \ll k_1$, the relaxation time of the mode will be equal to the Maxwell one: $\tau_k \approx \tau_M$, and Eq. (33) must be used to calculate the relaxation time for $k \approx k_1$. For relaxation modes with $k \gg k_1$, $\tau_k \approx \tau_{Dk}$. For example, for the Ih ice at $T = 260$ K and sample thickness $l \approx 10^{-3}$ m, this is the case when the charged defect concentration is $n_0 \geq 10^{15} \text{ m}^{-3}$. If relaxation times for the Maxwell and diffusion mechanisms are of the same orders $\tau_M \approx \tau_D$, the serial number of the mode will be k_2 . In this case, $\tau_M \gg \tau_{Dk_2} = \frac{\tau_D}{k_2^2}$ and $\tau_k \approx \tau_{Dk_2}$. For $k < k_2$, Eq. (33) must be used.

Thus, for the relaxation modes with short wavelengths λ_k , the space-charge relaxation time is equal to τ_{Dk} , and the relaxation mechanism is diffusion one. The modes with long wavelengths λ_k give the main contribution to the polarization; therefore, the monorelaxation process is observed in the second case with the Maxwell relaxation time, and the diffusion mechanism can be realized only for a very small concentration of the charged defects.

For crystalline dielectrics, the minimum wavelength of the relaxation mode is $2a$; therefore, the serial number of the corresponding mode k cannot exceed $k_{\max} = l/a$. As a rule, this restriction can be ignored in calculations, because the

relaxation mode amplitudes are inversely proportional to the squared serial number of modes and quickly decrease with increasing serial number.

The suggested mechanism of space-charge accumulation and relaxation allows us to interpret very simply recurrent relation (27) for the relaxation mode amplitudes in the n th order of the perturbation theory. Thus, the first term in the integrand of this formula describes the linear interaction of the odd k th mode with other odd modes, including the self-action, thereby resulting in an increase in the mode amplitude. The second term in the integrand of recurrent formula (27) for the amplitude $A_n(k, \tau)$ describes the nonlinear interaction of the external ac electric field with the relaxation modes, and this interaction is linear in a dc electric field $z_0 = 1$. For odd k , the contribution to the amplitude $A_n(k, \tau)$ comes from the interaction of the electric field with the even relaxation modes, whereas for even k , the contribution comes from the interaction with odd relaxation modes, and the self-action is excluded. The third term of integrand (27) characterizes the nonlinear interaction between two relaxation modes, and terms with Kronecker's delta symbols describe generation $[\delta(p+s-k)]$ and destruction $[\delta(p+k-s)$ and $\delta(p-s-k)]$ of the k th relaxation modes.

To elucidate a role of the nonlinear interactions in the space-charge relaxation, analytical expressions for the relaxation mode amplitudes were calculated in [6] for the first three harmonics. According to the results of these calculations, only odd relaxation modes are generated at the main frequency ω in all perturbation orders in the approximation of linear interaction. The nonlinear interactions result in generation of frequency harmonics. The second term in recursion relation (27), describing the nonlinear interaction of modes in an external electric field, describes generation of frequency harmonics $n\omega$, whereas the nonlinear interactions of modes described by the third term of the recursion relation generate $(n-1)\omega$ frequency harmonics in the n th order of the perturbation theory. Odd relaxation modes are excited for odd n , and even modes are excited for even n . The odd relaxation modes excited at even frequencies and the even modes at odd frequencies decay the faster, the greater the serial mode number k , that is, the shorter the wavelength λ_k .

This suggests that the physical mechanism of space-charge formation in dielectrics and semiconductors consists in generation of relaxation modes in an external electric field. In the initial stage, short-wavelength modes with small relaxation times and amplitudes are generated; as a result, small-scale inhomogeneities arise in the space-charge distribution whose relaxation is described by the diffusion mechanism. For time intervals comparable to the relaxation time of the main mode with $k = 1$, long-wavelength modes are excited. Exactly these modes form the space charge on macroscopic scales in the sample. It seems likely that spontaneous generation of relaxation modes in the absence of external electric field is also possible. Due to the nonlinear interaction character, in the case of spontaneous symmetry breaking this can lead to the phase transition of the dielectric into the ferroelectric or metastable electret state.

The dimensional effects of interlayer polarization in crystals with hydrogen bonds we calculated in [7] can serve as an illustration of the above-described space-charge relaxation mechanism.

CONCLUSIONS

1. Based on the solution of the system of the Fokker–Planck and Poisson equations, the phenomenological model of charge transfer in dielectrics has been constructed. The strict solution of the system of the nonlinear Fokker–Planck and Poisson equations was derived as a Fourier series in the relaxation modes whose amplitudes in the n th approximation are expressed through the amplitudes of the preceding approximation and hence through the amplitude of the first approximation according to the recursion formulas.

2. The mechanism of space-charge polarization formation in dielectrics was suggested, consisting in the excitation of the relaxation modes in an external electric field and subsequent interaction of these modes; the relaxation times were calculated, and it was established that modes with long wavelengths make the main contribution to the space-charge polarization.

3. From the suggested mechanism of the kinetics of space-charge polarization in dielectrics, the dimensional effects unambiguously follow considered in [7] for crystals with hydrogen bonds and the Maxwell relaxation.

APPENDIX

Since $\Psi_j = \cos\left(\frac{\pi ja}{l} \xi\right)$, then $\frac{\partial \Psi_j}{\partial \xi} = -\frac{\pi ja}{l} \sin\left(\frac{\pi ja}{l} \xi\right)$, and taking into account that $f_{n-1} = z_0 \rho_{n-1} + \sum_{m=1}^{n-2} \rho_m z_{n-m-1}$,

we obtain

$$\int_0^{l/a} f_{n-1} \frac{\partial \Psi_j}{\partial \xi} d\xi = -\frac{\pi ja}{l} \left[\int_0^{l/a} z_0 \rho_{n-1}(\xi, t') \sin\left(\frac{\pi ja}{l} \xi\right) d\xi + \sum_{m=1}^{n-2} \int_0^{l/a} \rho_m(\xi, t') z_{n-m-1}(\xi, t') \sin\left(\frac{\pi ja}{l} \xi\right) d\xi \right]. \quad (A 1)$$

Having substituted into Eq. (A 1) distributions of space charges ρ_m and ρ_{n-1} :

$$\rho_m = \sum_{p=1}^{+\infty} A_m(p, t') \cos\left(\frac{\pi pa}{l} \xi\right), \quad (A 2)$$

$$\rho_{n-1} = \sum_{p=1}^{+\infty} A_{n-1}(p, t') \cos\left(\frac{\pi pa}{l} \xi\right) \quad (A 3)$$

and $z_{n-m-1}(\xi, t')$ written as

$$z_{n-m-1}(\xi, t') = \psi \sum_{s=1}^{+\infty} A_{n-m-1}(s, t') \frac{l}{\pi sa} \left[\sin\left(\frac{\pi sa}{l} \xi\right) - \frac{2 \sin^2\left(\frac{\pi s}{2}\right)}{\pi s} \right], \quad (A 4)$$

we find

$$\begin{aligned} \int_0^{l/a} f_{n-1} \frac{\partial \Psi_j}{\partial \xi} d\xi = & -\frac{\pi ja}{l} \sum_{p=1}^{+\infty} A_{n-1}(p, t') \int_0^{l/a} \cos\left(\frac{\pi pa}{l} \xi\right) \sin\left(\frac{\pi ja}{l} \xi\right) d\xi \\ & + \psi \sum_{m=1}^{+\infty} \sum_{p,s=1}^{+\infty} A_m(p, t') A_{n-m-1}(s, t') \frac{l}{\pi sa} \left[\int_0^{l/a} \cos\left(\frac{\pi pa}{l} \xi\right) \sin\left(\frac{\pi sa}{l} \xi\right) \sin\left(\frac{\pi ja}{l} \xi\right) d\xi \right. \\ & \left. - \frac{2 \sin^2\left(\frac{\pi s}{2}\right)}{\pi s} \int_0^{l/a} \cos\left(\frac{\pi pa}{l} \xi\right) \sin\left(\frac{\pi ja}{l} \xi\right) d\xi \right]. \quad (A 5) \end{aligned}$$

The integral $\int_0^{l/a} \cos\left(\frac{\pi pa}{l} \xi\right) \sin\left(\frac{\pi ja}{l} \xi\right) d\xi$ in Eq. (A 5) can be expressed as $\int_0^{l/a} \cos(Ax) \sin(Bx) dx$, where

$A = \frac{\pi pa}{l}$ and $B = \frac{\pi ja}{l}$; then

$$\int_0^{l/a} \cos(Ax) \sin(Bx) dx = - \left[\frac{\cos(B-A)x}{2(B-A)} + \frac{\cos(A+B)x}{2(A+B)} \right]_0^{l/a};$$

otherwise,

$$\int_0^{l/a} \cos\left(\frac{\pi p a}{l} \xi\right) \sin\left(\frac{\pi j a}{l} \xi\right) d\xi = \frac{l}{\pi a} \left[\frac{\sin^2 \frac{\pi(j-p)}{2}}{j-p} + \frac{\sin^2 \frac{\pi(j+p)}{2}}{j+p} \right]. \quad (A 6)$$

Let us take into account that if j and p are even or odd numbers, $j-p$ and $j+p$ will be even, and Eq. (A.6) will be equal to zero. If one of these numbers is even and another odd, $j-p$ and $j+p$ will be odd numbers, and

$$\sin^2 \frac{\pi(j-p)}{2} = \sin^2 \frac{\pi(j+p)}{2} = 1 \quad \text{and} \quad \frac{1}{j-p} + \frac{1}{j+p} = \frac{2j}{j^2 - p^2}. \quad (A 7)$$

Thus, integral (A 6) can be written as follows:

$$\int_0^{l/a} \cos\left(\frac{\pi p a}{l} \xi\right) \sin\left(\frac{\pi j a}{l} \xi\right) d\xi = \frac{l}{\pi a} \frac{2j}{j^2 - p^2} \sin^2 \frac{\pi(j+p)}{2}. \quad (A 8)$$

Formula (A 8) automatically takes into account that one of the numbers is even and another odd, and consequently, $j \neq p$.

The second integral in Eq. (A 5) is expressed as

$$\int_0^{l/a} \cos(Ax) \sin(Bx) \sin Cx dx,$$

where

$$A = \frac{\pi p a}{l}, \quad B = \frac{\pi j a}{l}, \quad C = \frac{\pi s a}{l};$$

then we easily derive

$$\int_0^{l/a} \cos(Ax) \sin(Bx) \sin Cx dx = \frac{1}{4} \left[\frac{\sin(A+C-B)x}{A+C-B} + \frac{\sin(A+B-C)x}{A+B-C} - \frac{\sin(A+B+C)x}{A+B+C} - \frac{\sin(B+C-A)x}{B+C-A} \right]_0^{l/a} = 0.$$

If the denominators on the right side of the equation are equal to zero, the integral is expressed through Kronecker's delta symbols:

$$\int_0^{l/a} \cos(Ax) \sin(Bx) \sin Cx dx = \frac{l}{4a} [\delta(A+C-B) + \delta(A+B-C)]$$

$$-\delta(A+B+C)-\delta(B+C-A)], \quad (\text{A } 9)$$

and Eq. (A 9) is reduced to the form

$$\int_0^{l/a} \cos\left(\frac{\pi p a}{l} \xi\right) \sin\left(\frac{\pi s a}{l} \xi\right) \sin\left(\frac{\pi j a}{l} \xi\right) d\xi = \frac{l}{4a} [\delta(p+s-j) + \delta(p+j-s) - \delta(j+s-p)], \quad (\text{A } 10)$$

where it has been taken into account that $\delta(p+j+s)=0$ for $j \geq 1$, $p \geq 1$, and $s \geq 1$.

As a result, the final expression for the integral assumes the form

$$\begin{aligned} \int_0^{l/a} f_{n-1}(\xi, t') \frac{\partial \Psi_j}{\partial \xi} d\xi = & -\frac{\pi j a}{l} \left\{ z_0(t') \sum_{p=1}^{+\infty} A_{n-1}(p, t') \frac{2j}{\pi a} \frac{2 \sin^2\left(\frac{\pi(j+p)}{2}\right)}{j^2 - p^2} \right. \\ & + \psi \sum_{m=1}^{n-2} \sum_{p,s=1}^{+\infty} A_m(p, t') A_{n-m-1}(s, t') \frac{l}{\pi s a} \left\{ \frac{l}{4a} [\delta(p+s-j) + \delta(p+j-s) \right. \\ & \left. \left. - \delta(s+j-p)] - \frac{2 \sin^2\left(\frac{\pi s}{2}\right)}{\pi s} \frac{l}{\pi a} \frac{2j}{j^2 - p^2} \sin^2\left[\frac{\pi(j+p)}{2}\right] \right\} \right\}. \end{aligned} \quad (\text{A } 11)$$

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