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PROPAGATION OF SHEAR WAVES IN PIEZOELECTRIC "SUPERLATTICE–SUBSTRATE" STRUCTURES

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The results of a computer simulation of the dispersion relations for the propagation of shear waves in piezoelectric "superlattice–substrate" structures are analyzed. The superlattice consists of a finite number of layers and is made up of materials with 6mm symmetry. The dispersion relations are obtained using a formulation for periodic hamiltonian systems. This approach makes it possible to account for the anisotropy, the piezoelectric interaction of the mechanical and electric fields, and an arbitrary number of layers in the superlattice. Numerical results are presented for CdS–ZnO layers. Selective spatial localization of acoustic modes is demonstrated for different spectral regions. The effects of the ordering of the superlattice layers, of their number, and of the boundary conditions on the dispersion spectra and on the form of the shear wave motion are examined.

Multilayer crystalline structures – superlattices created by high-precision thin film technologies – can be used in various branches of science and technology, so there is a need for detailed modelling and study of the physical and mechanical properties of these heterostructures. Of the many papers on the acoustic properties of infinite and semi-infinite superlattices, we note those dealing with volume and surface waves in piezoelectric CdS–ZnO systems [1–7] in which dispersion relations are constructed and analyzed by various mathematical approaches, specifically, transfer matrices [1, 2], Green functions [3, 4], and the periodic hamiltonian system formalism [5–7]. This last approach is also used to describe the propagation of acoustic waves in piezoelectric superlattices made up of a finite number of layers. Purely elastic, nonpiezoelectric "superlattice–substrate" structures have been examined in [8] and [9]. In this paper we present the results of a computer simulation of the dispersion relations for the propagation of shear waves in "superlattice–substrate" structures. These structures are modelled by periodic systems of layers on a homogeneous piezoelectric half space.

In a cartesian coordinate system $x_1x_2x_3$, let a superlattice occupy the region $0 \le x_2 \le H$ with the $x_2 = H$ plane bordering a vacuum and the $x_2 = 0$ plane forming an ideal contact with the piezoelectric half-space $x_2 < 0$. The physical and mechanical properties of the superlattice and the half space are described by the material relations for the *6mm* hexagonal class with a sixth order symmetry axis along the x_3 axis. Here the material characteristics of the superlattice (elastic modulus c_{44}, piezoelectric modulus e_{15}, dielectric permittivity ε_{11}, and density ρ) along the x_2 axis are periodic functions with period h:

$$\rho(x_2) = \rho(x_2 + h), \quad c_{44}(x_2) = c_{44}(x_2 + h),$$

$$e_{15}(x_2) = e_{15}(x_2 + h), \quad \varepsilon_{11}(x_2) = \varepsilon_{11}(x_2 + h),$$

which take finite values over the period.

It has been shown [5] that the general solution of the electroelasticity equations for shear waves in the direction where the properties are constant within the superlattice can be written in the form

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$$\left\{ D_2(x_1, x_2, t),\ \sigma_{23}(x_1, x_2, t),\ \varphi(x_1, x_2, t),\ u_3(x_1, x_2, t)\right\} =$$

$$= \left\{q_1(x_2),\ q_2(x_2),\ p_1(x_2),\ p_2(x_2)\right\}\exp(ikx_1 - i\omega t), \tag{1}$$

where D_2, σ_{23}, φ, and u_3 are, respectively, the normal component of the electric displacement vector, the component of the stress tensor, the electric potential, and the component of the (spatial) displacement vector. k is the wave vector and ω is the angular frequency.

In this case, to determine the column vectors $\vec{q} = \mathrm{col}[q_1, q_2]$ and $\vec{p} = \mathrm{col}[p_1, p_2]$, we obtain an h-periodic hamiltonian system of linear differential equations

$$\frac{d}{dx}\begin{bmatrix}\vec{q}\\ \vec{p}\end{bmatrix} = A\begin{bmatrix}\vec{q}\\ \vec{p}\end{bmatrix};\quad A(x_2) = \begin{bmatrix}0 & Q(x_2)\\ -P(x_2) & 0\end{bmatrix} \tag{2}$$

with the hamiltonian function $H(x_2, \vec{q}, \vec{p}) = \vec{q}^{\,*}P(x_2)\vec{q} + \vec{p}^{\,*}Q(x_2)\vec{p}$. Here $Q(x_2)$ and $P(x_2)$ are symmetric matrices of the form

$$Q(x_2) = \begin{bmatrix}-\varepsilon_{11}(x_2)k^2 & e_{15}(x_2)k^2\\ e_{15}(x_2)k^2 & c_{44}(x_2)k^2 - \rho(x_2)\omega^2\end{bmatrix};$$

$$P(x_2) = \begin{bmatrix}c_{44}(x_2)d(x_2) & -e_{15}(x_2)d(x_2)\\ -e_{15}(x_2)d(x_2) & 1/\bar{c}_{44}(x_2)\end{bmatrix};$$

$$\bar{c}_{44} = c_{44} + (e_{15})^2/\varepsilon_{11},\quad d = 1/(\varepsilon_{11}\bar{c}_{44}).$$

The general solution of the system in the nth periodicity interval $(n-1)h \le x_2 \le nh$ is written the form [5–7]

$$\begin{bmatrix}\vec{q}(x_2 + nh - h)\\ \vec{p}(x_2 + nh - h)\end{bmatrix} = \sum_{l=1}^{4} K_l\,\chi_l^n\,U(x_2)\vec{Y}_l$$

$$(0 \le x_2 \le h;\ n = 1, 2, \ldots, N, N+1). \tag{3}$$

Here K_l are unknown coefficients, $U(x_2)$ is the matricant of the system of Eqs. (2), i.e., the fundamental matrix satisfying the condition $U(0) = E$, where E is the unit 4×4 matrix, χ_l and $\vec{Y}_l = \mathrm{col}[Y_l^{(1)}, Y_l^{(2)}, Y_l^{(3)}, Y_l^{(4)}]$ are the eigenvalues and corresponding eigenvectors of the monodromy matrix $U(h)$. According to the Lyapunov–Poincare theorem [10], the characteristic equation of the monodromy matrix has mutually inverse roots and when the substitution $\chi + \chi^{-1} = 2b$ is used, reduces to the equations

$$\chi^2 - 2b\chi + 1 = 0;\quad 2b_j = a_1/2 - (-1)^j\left[a_1^2/4 - 2a_2 + 2\right]^{1/2}\quad (j = 1, 2).$$

The coefficients a_1 and a_2 are expressed in terms of the elements of the matrix $U(h)$. In the most general case of arbitrary periodicity along the x_2 direction, the matricant $U(x_2)$ is constructed by numerical methods or through representing it in the form of converging matrix series. For superlattices whose properties are described by piecewise continuous functions, the matricant can be written in an analytic form [5, 6].

The following representations hold [11] for the components of the resolvent vector in the uniform piezoelectric half-space $x_2 < 0$:

$$u_3(x_1, x_2, t) = A_s\exp(ikx_1 + \alpha_s x_2 - i\omega t);$$

$$\varphi(x_1, x_2, t) = A_s e_{15,s}\varepsilon_{11,s}^{-1}\exp(ikx_1 + \alpha_s x_2 - i\omega t) + B_s\exp(ikx_1 + kx_2 - i\omega t);$$

$$\sigma_{23}(x_1, x_2, t) = A_s \alpha_s \bar{c}_{44.s} \exp(ikx_1 + \alpha_s x_2 - i\omega t) + B_s e_{15.s} k \exp(ikx_1 - i\omega t);$$

$$D_2(x_1, x_2, t) = -B_s k \varepsilon_{11.s} \exp(ikx_1 + kx_2 - i\omega t), \tag{4}$$

where A_s and B_s are arbitrary amplitudes; ρ_s, $c_{44.\,s}$, $e_{15.\,s}$, and $\varepsilon_{11.\,s}$ are parameters characterizing the half-space $x_2 < 0$; $\alpha_s = (k^2 - \rho_s \omega^2/\bar{c}_{44.\,s})^{1/2}$ (α_s is understood to be the branch of this function which satisfies the radiation condition for $x_2 \to -\infty$, i.e., when $k^2 > \rho_s \omega^2/\bar{c}_{44.\,s}$); and $\bar{c}_{44.\,s} = c_{44.\,s} + (e_{15.\,s})^2/\varepsilon_{11.\,s}$.

The ideal contact conditions are satisfied at the interface $x_2 = 0$:

$$D_2(x_1, -0, t) = D_2(x_1, +0, t), \quad \varphi(x_1, -0, t) = \varphi(x_1, +0, t),$$

$$\sigma_{23}(x_1, -0, t) = \sigma_{23}(x_1, +0, t), \quad u_3(x_1, -0, t) = u_3(x_1, +0, t).$$

We shall assume that the following boundary conditions are satisfied at the surface $x_2 = H$:

$$\sigma_{23}(x_1, H, t) = 0, \quad \varphi(x_1, H, t) = 0 \tag{5}$$

for a metallized surface that is free of mechanical loads or

$$\sigma_{23}(x_1, H, t) = 0, \quad D_2(x_1, H - 0, t) = D_2(x_1, H + 0, t),$$

$$\varphi(x_1, H - 0, t) = \varphi(x_1, H + 0, t) \tag{6}$$

for a free unmetallized surface. Here the potential and the component of the electric displacement in the vacuum (for $x_2 > H$) are given by [11]

$$\varphi(x_1, x_2, t) = B_0 \exp(ikx_1 - k(x_2 - H) - i\omega t);$$

$$D_2(x_1, x_2, t) = k B_0 \exp(ikx_1 - k(x_2 - H) - i\omega t). \tag{7}$$

Substituting solutions (3), (4), and (7) in the corresponding boundary conditions at the surfaces $x_2 = 0$ and $x_2 = H$, we obtain dispersion relations for determining the phase velocities of the waves. In the case of an unmetallized surface at $x_2 = H$, the propagation of shear modes is described by the equation

$$\det S = 0, \tag{8}$$

where the nonzero elements of the seventh order matrix S are given by

$$S_{ij} = Y_j^{(i)} \ (i, j = 1, \ldots, 4); \quad S_{16} = -\varepsilon_{11.s} k, \quad S_{25} = \bar{c}_{44.s} \alpha_s,$$

$$S_{26} = e_{15.s} k, \quad S_{35} = e_{15.s}/\varepsilon_{11.s}, \quad S_{36} = S_{45} = S_{77} = 1,$$

$$S_{57} = \varepsilon_0 k, \quad \alpha_s = \left(k^2 - \rho_s \omega^2 / \bar{c}_{44.s}\right)^{1/2},$$

$$S_{mn} = \chi_n^N \sum_{j=1}^{4} U_{(m-4)j}(H - Nh) Y_n^{(j)} \ (m = 5, 6, 7, \ n = 1, \ldots, 4).$$

Here $U_{ij}(x_2)$ are the elements of the matricant $U(x_2)$; ε_0 is the dielectric permittivity of the vacuum; and $Nh \le H \le Nh + h$.

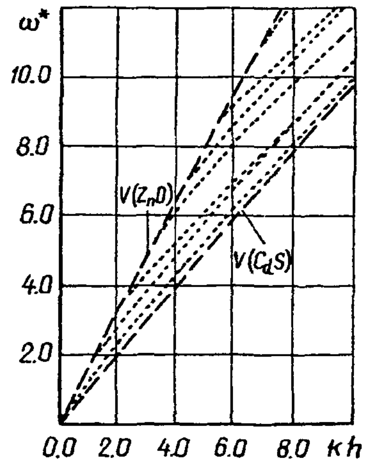

Fig. 1

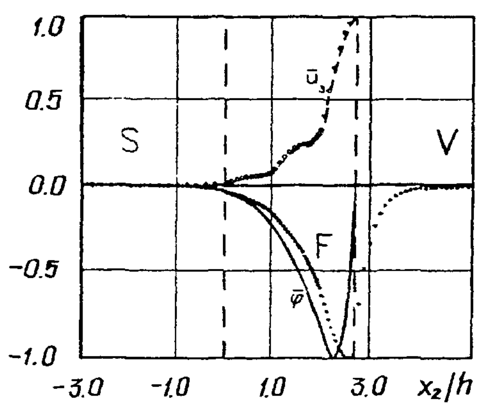

Fig. 2

If the surface $x_2 = H$ is metallized, then the propagation of shear waves is described by the equation

$$\det \bar{S} = 0, \tag{9}$$

where the elements of the matrix $\bar{S}_{6\times6}$ are given by

$$\bar{S}_{ij} = S_{ij}, \quad \bar{S}_{mj} = S_{(m+1)j} \quad \left(i = \overline{1, 4}, \ \ m = 5, 6, \ \ j = \overline{1, 6}\right).$$

In the following we present the dispersion modes and corresponding displacements and potentials for shear waves in a finite CdS–ZnO superlattice deposited on a ZnO half-space.

Figure 1 shows the modes for this system when the superlattice is bounded on both sides by a softer layer of CdS. In this case, the dispersion curves are similar to the curves for Love waves and exist only within the sector formed by the straight lines corresponding to volume waves in CdS and ZnO layers. The axes correspond to the dimensionless angular frequency $\omega^* = \omega(\rho_0/c_0)^{1/2}$ and wave number $k^* = kh$. Here it was assumed that $\rho_0 = 3\cdot10^3$ kg/m^3 and $c_0 = 10^{10}$ Pa, while the free surface was unmetallized, so that Eq. (8) could be used, and the superlattice consists of 3 layers of CdS and 2 layers of ZnO ($H = Nh + h_1$, $h = h_1 + h_2$, $N = 2$, $h_1 = h_{CdS} = 0.7h$, $h_2 = h_{ZnO} = 0.3h$).

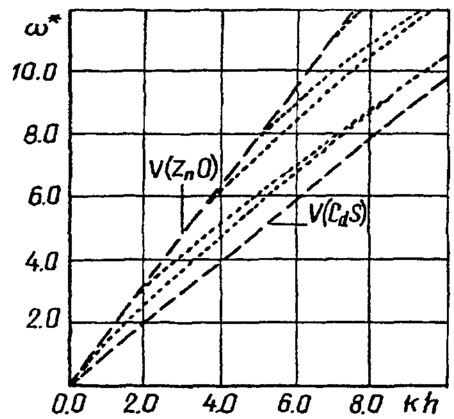

Fig. 3

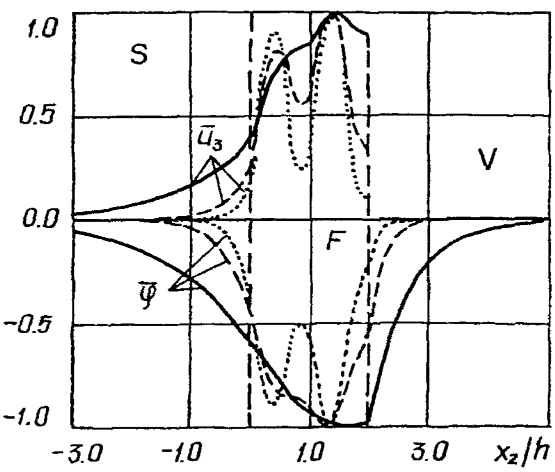

Fig. 4

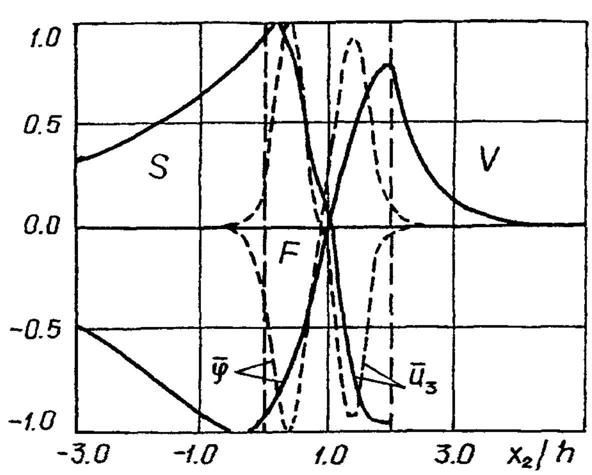

Fig. 5

These calculations show that as N increases, part of the curves (1-st, 4-th, 7-th, ...) varies extremely slowly and approaches the surface modes for a half-infinite superlattice [5–7]. As Fig. 2 shows, even for very small N in the fundamental mode the motion is localized near the free surface and the wave essentially does not penetrate into the structure. The other branches in Fig. 1 correspond to bulk motion inside the superlattice; their number increases with N and as $N \to \infty$ they form the transmission band for volume waves in an infinite superlattice.

Calculations based on Eq. (9) showed that metallizing the $x_2 = H$ surface only leads to a slight reduction in the phase velocities in the modes (on this scale the corresponding dispersion relations are essentially the same as those shown in Fig. 1), but there is a significant difference in the profiles of the amplitudes. As a comparison, Fig. 2 shows typical distributions of the amplitudes of the mechanical displacement and electrical potential in the vacuum (V), superlattice (F), and half-space (S) calculated for unmetallized (plot points indicated by circles) and metallized (dashed and solid curves) surfaces $x_2 = H$ in the fundamental mode.

Figure 3 shows the dispersion curves for the case when a more "rigid" ZnO layer adjoins the unmetallized surface ($H = Nh$, $N = 2$, $h_1 = h_{ZnO} = 0.3h$, $h_2 = h_{CdS} = 0.7h$). The motion takes place in the bulk for all modes in a way similar to that shown in Fig. 4 for the fundamental mode. The smooth, dashed, and dot-dashed curves correspond to ω^* equal to 2, 5, and 8.

Figure 5 shows the results for the second mode, with ω^* equal to 3 and 10 (smooth and dot-dashed curves). It is interesting to note that for this mode the displacement and potential have maxima near the boundary between the superlattice and the uniform piezoelectric half-space, or even in the half-space, as happens with the potential for $\omega^* = 3$.

In conclusion, we note that comparing the dispersion spectrum of systems similar to those examined above with infinite and semi-infinite superlattices makes it possible to indicate regions in the frequency and wave number for which the motion these systems will either take place within the volume (wave energy spread over the entire thickness of the superlattice and half-space) or at the surface (energy localized within a few upper layers of the superlattice and the wave does not penetrate into the half-space). The properties of the upper and lower layers of the superlattice and half-space, the relative thickness of the layers within the superlattice, and planar defects such as local failure of periodicity, can have a significant effect on the dispersion characteristics.

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