SURFACE ACOUSTIC SOLITONS – QUANTUM THEORETICAL APPROACH

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Since surface acoustic waves propagate along the solid surface concentrating their energy within about one wavelength from the surface, the lattice anharmonicity is enhanced especially in high frequency region. This anharmonicity will be balanced with the dispersive effects due to the intrinsic or extrinsic origins and consequently we can expect the formation of surface acoustic solitons of the envelope type $\lceil 1 \rceil$.

Even in low frequency region, if there exist some surface structures which confine the acoustic waves in the vicinity of the surface, for example thin film deposited on the substrate supporting the Love waves, the lattice anharmonicity might be also enhanced. As a consequence, we can anticipate the generation of surface acoustic solitons due to the balance between the anharmonicity and the dispersion characteristic to such surface structure. In this paper, we show that the Love waves can support the KdV type acoustic soliton approximately.

Consider a semi-infinite elastic medium (A), on which is deposited a thin film (B) with thickness d. It has the stress-free plane boundary perpendicular to the x_3 -axis. The displacement fields in each medium can be obtained from the equation of elasticity theory and should satisfy the necessary boundary conditions at the surface and the interface. As we need no explicit expressions of the wave functions for phonons to develop further, we only assume the existence of a complete orthogonal set of eigensolutions $\{u_i^{J\vec{k}}(\vec{r})\}$ satisfying the elasticity equation, where J is a set of quantum numbers, \vec{k} is the wave vector parallel to the surface, *i* denotes the space components and $\vec{r} = (x_1, x_2, x_3)$.

We then define the phonons in this system by expanding the displacement fields $u_i(\tilde{r}, t)$ in terms of the eigensolutions $\{u_i^{J\vec{k}}(\tilde{r})\}$ as

$$u_{i}(\tilde{r}, t) = \sum_{J, \vec{k}} (2\rho\omega_{k}^{J})^{-1/2} [\tilde{a}_{\vec{k}}^{J}(t) u_{i}^{J\vec{k}}(\tilde{r}) + \text{H.C.}], \qquad (1)$$

where the expansion coefficient $a_{\vec{t}}^{J}(t)$ and its hermitian conjugate $a_{\vec{t}}^{J^{+}}(t)$ are the

annihilation and creation operators of the J-mode phonon, respectively, obeying the standard commutation relation of the Bose type. Among these eigenmodes, there must exist a Love-wave mode which is confined in a thin film and we refer to it as Love-mode phonon (L-mode, J = L).

The electron field operator $\chi(\tilde{r}, t)$ can be generally written as

$$\chi(\vec{r}, t) \sum_{\vec{q}, \sigma} \tilde{b}_{\vec{q}\sigma}(t) \psi_{\sigma}(\vec{r}), \qquad (2)$$

where σ is a quantum number specifying the electronic states in the layered structure; other notations are conventional. We need no explicit forms for the electronic wave function on $\psi_{\sigma}(\vec{r})$.

Substituting Eq. (1) into the elastic energy up to cubic in the deformation tensor and adding the relevant electron-phonon interaction with use of Eq. (2), we obtain

$$\begin{split} H &= H_{0} + H_{\text{ph-ph}} + H_{e\text{-ph}}, \\ H_{0} &= \sum_{J,\vec{k}} \omega_{k}^{J} \tilde{a}_{\vec{k}}^{J^{+}} \tilde{a}_{\vec{k}}^{J} + \sum_{\vec{q}\sigma} \varepsilon_{q\sigma} \tilde{b}_{\vec{q}}^{+} \tilde{b}_{\vec{q}\sigma}, \\ H_{\text{ph-ph}} &= 2\rho \sum (2\rho\omega_{k}^{J} \omega_{k'}^{J'} \omega_{\vec{k}+\vec{k'}}^{J'})^{1/2} \Phi_{\vec{k},\vec{k'},-\vec{k}-\vec{k'}}^{JJ'J''} \tilde{A}_{\vec{k}}^{J'} \tilde{A}_{\vec{k'}}^{J'} \tilde{A}_{-\vec{k}-\vec{k'}}^{J''}, \\ H_{e\text{-ph}} &= \sum_{\vec{k},\vec{q},\sigma\sigma'} (2\rho\omega_{k}^{J})^{1/2} \theta_{\sigma\sigma'}(\vec{k}) \tilde{b}_{\vec{q}+\vec{k}\sigma'}^{+} \tilde{b}_{\vec{k}} \tilde{A}_{\vec{k}}^{J} \tilde{A}_{\vec{k}}^{J'} \end{array}$$
(3)

where $\tilde{A}_{\vec{k}}^{J} \equiv (2\rho\omega_{k}^{J})^{-1/2}(\tilde{a}_{\vec{k}}^{J} + \tilde{a}_{-\vec{k}}^{J^{+}}).$

By using the Hamiltonian (3), the equation for the J-mode phonons can be obtained as follows: For the L-mode phonon we have

$$\begin{split} \tilde{A}_{\vec{k}}^{L} &= -\omega_{k}^{L^{2}} \tilde{A}_{\vec{k}}^{L} - 6 \sum_{\vec{k}'} (2\rho\omega_{k}^{L} \,\omega_{k'}^{L} \,\omega_{\vec{k}-\vec{k}'}^{L})^{1/2} \Phi_{-\vec{k},\vec{k}',\vec{k}-\vec{k}'}^{LLL} \tilde{A}_{\vec{k}'}^{L} \tilde{A}_{\vec{k}-\vec{k}'}^{L} \tilde{A}_{\vec{k}-\vec{k}'}^{L} \\ &- 12 \sum_{\substack{J(=L)\\ \vec{k}'}} (2\rho\omega_{k}^{L} \,\omega_{k'}^{J} \,\omega_{\vec{k}-\vec{k}'}^{J})^{1/2} \Phi_{-\vec{k},\vec{k}',\vec{k}-\vec{k}'}^{LLJ} \tilde{A}_{\vec{k}'}^{L} \tilde{A}_{\vec{k}-\vec{k}'}^{J} \\ &- 6 \sum_{\substack{J,J'(=L)\\ \vec{k}'}} (2\rho\omega_{k}^{L} \,\omega_{k'}^{J} \,\omega_{\vec{k}-\vec{k}'}^{J})^{1/2} \Phi_{-\vec{k},\vec{k}',\vec{k}-\vec{k}'}^{LJJ'} \tilde{A}_{\vec{k}'}^{J} \tilde{A}_{\vec{k}-\vec{k}'}^{J} \\ &- (2\omega_{k}^{L}/\rho)^{1/2} \sum_{\vec{q}\sigma\sigma'} \theta_{\sigma\sigma'}^{J} (\vec{k}) \tilde{b}_{\vec{q}-\vec{k}\sigma'}^{+} \tilde{b}_{\vec{q}\sigma}^{J}. \end{split}$$
(4)

For the electrons and the other modes of phonons, referred to as bulk phonons, we can easily derive similar equations which are not explicitly given here. To eliminate the electron and the bulk-phonon variables in Eq. (4), we solve the equations for these variables assuming that the effect of the anharmonic interaction upon the bulk-phonon states and also the effect of the electron-phonon interaction upon the electronic states can be considered as a perturbation. Then

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we take the expectation value of the equation with respect to the stationary states of the electrons and bulk phonons.

Following the working hypothesis presented before [1], we assume that the *L*-mode surface acoustic soliton is a macroscopic entity of Love waves corresponding to a state in which a large number of *L*-mode phonons are excited and, consequently, the fluctuation of the occupation number of the phonons can be neglected. We can therefore derive the classical wave equation by taking the expectation value of the equation (4) in a coherent state of the *L*-mode phonons, $|\{\alpha_{\underline{L}}^{\underline{L}}\}\rangle$.

We can finally rewrite Eq. (4) as

$$\ddot{A}_{\vec{k}}^{L} + \omega_{k}^{L^{2}} A_{\vec{k}}^{L} + \sum_{\vec{k'}} F_{\vec{k},\vec{k'}} A_{\vec{k'}}^{L} A_{\vec{k}-\vec{k'}}^{L} + (18\Gamma_{\vec{k}}^{(a)} + \Gamma_{\vec{k}}^{(e)}) \dot{A}_{\vec{k}}^{L} = 0, \qquad (5)$$

where $A_{\vec{k}}^L \equiv \langle \{\alpha_{\vec{k}}^L\} | \tilde{A}_{\vec{k}}^L| \{\alpha_{\vec{k}}^L\} \rangle$, $F_{\vec{k},\vec{k'}} = 6(2\rho\omega_k^L\omega_{\vec{k'}}^L\omega_{\vec{k'}-\vec{k'}}^L)^{1/2}\Phi_{-\vec{k},\vec{k'},\vec{k}-\vec{k'}}^{LLL}$, $\Gamma_{\vec{k}}^{(n)}$ is the anharmonic attenuation rate of the *L*-mode phonons and $\Gamma_{\vec{k}}^{(c)}$ is the attenuation rate due to the electron-phonon interaction. The second term denotes the dispersive term, the third term denotes the nonlinear term and the last term denotes the attenuation due to the electrons and bulk thermal phonons. $\Gamma_{\vec{k}}^{(n)}$ is always positive implying that the *L*-mode phonons are attenuated by the anharmonic interaction with the bulk thermal phonons, while $\Gamma_{\vec{k}}^{(c)}$ changes its sign from positive to negative as the electron drift velocity exceeds the sound velocity by applying an external dc electric field. Therefore we assume hereafter that the condition $\Gamma_{\vec{k}}^{(e)} = -8\Gamma_{\vec{k}}^{(n)}$ holds.

The dispersion relation of the L-mode phonon in a thin isotropic film B with thickness d deposited on the semi-infinite cubic substrate A is given by

$$\omega_{k}^{L^{2}} = c_{t_{1}}^{A^{2}} k^{2} + 4 \left(c_{t_{2}}^{A^{2}} - c_{t_{1}}^{A^{2}} \right) \frac{k_{1}^{2} k_{2}^{2}}{k^{2}} - d^{2} \left(\frac{\rho^{B}}{\rho^{A}} \right)^{2} \frac{1}{c_{t_{1}}^{A^{2}}} \left[\left(c_{t_{1}}^{A^{2}} - c_{t}^{B^{2}} \right) k^{2} + 4 \left(c_{t_{2}}^{A^{2}} - c_{t_{1}}^{A^{2}} \right) \frac{k_{1}^{2} k_{2}^{2}}{k^{2}} \right]^{2} + \mathcal{O}\left(d^{4} \right), \quad (6)$$

where $c_{t_1}^A$ and $c_{t_2}^A$ denote the velocities of the fast and slow transverse waves in A, respectively.

For the anharmonic phonon-phonon vertex function $F_{\vec{k},\vec{k}'}$, we obtain k^4 -dependence from the crystal symmetry after integrating with respect to the angular variables. Then the one-dimensional version $(k_1=0, k_2=0)$ of Eq. (5) in the coordinate representation leads to

$$u_n - c^2 u_{xx} - M u_{xxxx} - N (u_x^2)_{xx} = 0, \quad (M, N > 0)$$
(7)

where $u(x, t) = \sum_{k_1} A_{k_1}(t) e^{ik_1 x}$. Making the variable transformation $\xi = x - ct$, $\tau = t$, we can show Eq. (7) is equivalent to the following nonlinear equation,

$$u_{z} + \alpha u_{z} u_{zz} + \beta u_{zzz} = 0, \qquad (8)$$

where $\alpha = N/c$ and $\beta = M/(2c)$. Differentiating Eq. (8) twice with respect to ξ , we have finally

$$w_{z} + 3\alpha w w_{z} + \beta w_{zzz} + \alpha v w_{zz} = 0, \qquad (9)$$

where $v_{\xi} = w$. This is the KdV-Burgers equation with variable dissipationcoefficient. The approximate solution of Eq. (9) can be obtained by treating the dissipation term as a small perturbation and by using the method of conserved quantities as

$$w(\xi,\tau) = 2\kappa^2(\tau)\operatorname{sech}^2\left[\kappa(\tau)(\xi - 4\kappa^2(\tau)\tau)\right]$$
(10)

with

$$\kappa(\tau) = \kappa(0) \left[\frac{5}{32\kappa(0)^3 \tau + 5} \right]^{1/3},$$
(11)

where $\kappa(0)$ is the soliton amplitude at $\tau=0$ and the values of parameters were taken as $\alpha=2\beta=2$. It should be noted that the amplitude (11) shows algebraic damping in time.

REFERENCE

[1] T. Sakuma and T. Miyazaki, Phys. Rev. B33 (1986) 1036.