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Detailed Study of Elastic Constants and Surface Waves of Superlattices*

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Abstract

Elastic constants of cubic materials with respect to coordinate systems on superlattices and their surface waves are studied. An exact expression to calculate surface waves is derived for superlattices supposed for two kinds of layers to be rigidly stacked upon each other. The formulations are performed for bulk superlattices and superlattices on glass. The result of numerical calculations for two kinds of superlattices Cu/Al and Cu/Ag is compared with that obtained by use of the known effective elastic constants [M. Grimsditch, Phys. Rev. B. 31, 6818 (1985)]. The comparison clarifies the region in which the Grimsditch's expressions may be used.

Key words: elastic constants, surfacewave, superlattice

[I] Introduction

The elastic properties of metallic multilayers have attracted much attention.[1-5] In order to understand these elastic properties we need the elastic constants of such superlattices. The effective elastic constants for a periodically laminated medium of orthorhombic symmetry have been derived by Grimsditch.[6,7] His effective elastic constants are valid in the long-wavelength regime, i.e., they can be used for superlattices with a short period, where a period means the shortest unit of layers which consist of the constituents of periodically layered structures. The meaning of a "short period" does not seem to be clear, though the effective elastic constants are often used in literatures.[5,8,9]

Metallic multilayers are usually made by sputtering or evaporation.[5,8] Such multilayer films have a "pencil type texture, i.e., one in which the grains have a common orientation normal to the film but are randomly oriented in the plane of the film.[10] The subject of our study in the present paper is sputtered or evaporated multilayer film.

In the present work, first we discuss the elastic constants for each of alternating layers of constituents in periodically layered structure , which is general multilayer and in which the grains may or may not be randomly oriented in the plane parallel to each layer. We will consider only cubic materials as constituents of superlattice and [001], [110] and [111] planes as the planes of superlattices. The present elastic constants in these cases are given in a symmetry adopted form. From these general elastic constants, we can obtain the well known elastic constants in sputtered or evaporated multilayer.[10]

By use of those elastic constants, we will formulate the equations for propagating elastic waves in each layer. We can deal with elastic propagating waves in periodically layered structures by connecting the above waves with the proper boundary conditions in each boundary of layers. There are quasi-transverse and qausi-longitudinal elastic waves, each of which has forward and backward modes in the noted (x', y') plane of the coordinate system

* The revised edition of the present paper will be publised soon, where this paper is rewritten compactly. The present paper contains some valuable descriptions and details passed over in the revised edition.

(x', y', z') defined for superlattice. This means that the propagating waves of interest are treated in terms of 4×4 matrices.

Among those elastic waves are involved the waves satisfying the condition of stress-free [11-12] on either terminal plane of the treated multilayer film, where bulk superlattice and superlattice developed on substrate are considered. These waves are the surface elastic waves which are known as the Rayleigh wave and the Sezawa waves, where the Sezawa waves have larger velocities than the Rayleigh wave. We restrict our discussion to the Rayleigh wave, though the Sezawa waves can be obtained from our derivation. Mathematically, the dispersion equation for a surface wave is equivalent to the condition that the determinant of a 4×4 matrix is zero.

We can regard multilayer as medium with the effective elastic constants which are determined by use of the Grimsditch' formulae.[5,6,8] The surface elastic wave can be found through the much easier calculation for the virtual medium than the direct and complicated calculation for superlattice, which is actually made in the present paper. The numerical calculations are performed for Cu／Al and Cu／Ag superlattices in the present work. One of our main purposes is to clarify the restriction of the approximate treatment based on the Grimsditch's expressions by comparison of the result obtained from the virtual medium model with that from the exact derivation. Another main purpose is just the exact derivation of the surface elastic wave in superlattice.

[II] Film geometric elastic constants

We have two kinds of coordinate systems; one is the crystallographic system ($x_1 = x$, $x_2 = y$, $x_3 = z$) and another is the film geometric system ($x_1' = x'$, $x_2' = y'$, $x_3' = z'$).[10] The axis z' is normal to the surface of the film and x' and y' are the two axes with arbitrary orientations in the film surface. The transformation from the coordinate system (x, y, z) to the one (x', y', z') is given by

$$x_i' = A_{ij}x_j \,, \tag{2.1}$$

where A_{ij} is the rotation matrix. Here and hereafter the usual convention regarding summation on repeated subscripts is used.[12,13]

The primary elastic modulus tensor λ_{ijkl} is related to the film geometric elastic modulus tensor λ_{pqrs}' by the following tensor transformation equation:[12,13]

$$\lambda_{pqrs}' = A_{pi}A_{qj}A_{rk}A_{sl}\lambda_{ijkl} \tag{2.2}$$

The tensor λ_{ijkl} has the symmetric properties:[13]

$$\lambda_{ijkl} = \lambda_{jikl} = \lambda_{ijlk} = \lambda_{klij} \tag{2.3}$$

The transformed tensor λ_{pqrs}' also has the same symmetric properties.
We have only three independent non-zero terms for the primary elastic tensor in the cubic system:[13]

$$\lambda_{xxxx} = \lambda_{yyyy} = \lambda_{zzzz} \equiv C_{11}\,, \quad \lambda_{xxyy} = \lambda_{yyzz} = \lambda_{xxzz} \equiv C_{12}\,, \quad \lambda_{yzyz} = \lambda_{zxzx} = \lambda_{xyxy} \equiv C_{44}\,. \tag{2.4}$$

Substituting the relations (2.3) and (2.4) in Eq. (2.2) yields the following expression:

$$\lambda_{pqrs}' = A_{pqrs}C_{11} + (\delta_{pq}\delta_{rs} - A_{pqrs})C_{12} + (\delta_{pr}\delta_{qs} + \delta_{ps}\delta_{qr} - 2A_{pqrs})C_{44}\,, \tag{2.5}$$

where δ_{pq} denotes the kronecker delta-symbol and the coefficient A_{pqrs} means

$$A_{pqrs} = A_{pi}A_{qi}A_{ri}A_{si}\,. \tag{2.6}$$

We will rewrite the expression (2. 5) in the following forms for our practical purposes:

$$\begin{aligned}\lambda_{pqrs}' &= C_{11}+(\delta_{pq}\delta_{rs}-1)C_{12}+(\delta_{pr}\delta_{qs}+\delta_{ps}\delta_{qr}-2)C_{44}+(A_{pqrs}-1)\varepsilon \\ &= C_{12}+(\delta_{pq}\delta_{rs}-1)C_{12}+(\delta_{pr}\delta_{qs}+\delta_{ps}\delta_{qr})C_{44}+A_{pqrs}\varepsilon \\ &= C_{44}+\delta_{pq}\delta_{rs}C_{12}+(\delta_{pr}\delta_{qs}+\delta_{ps}\delta_{qr}-1)C_{44}+A_{pqrs}\varepsilon \\ &= \delta_{pq}\delta_{rs}C_{12}+(\delta_{pr}\delta_{qs}+\delta_{ps}\delta_{qr})C_{44}+A_{pqrs}\varepsilon\end{aligned}, \qquad (2.7)$$

where $\varepsilon = C_{11}-C_{12}-2C_{44}$. The obtained results are summarized in Table I. Here we notice that the elastic tensor λ_{pqrs}' or C_{ij}' is independent of coordinates if $C_{11}-C_{12}-2C_{44}=0$. It is well known that the condition $C_{11}-C_{12}=2C_{44}$ holds for isotropic media.[12, 13]

In what follows, the expressions of tensors λ_{pqrs}' (or C_{ij}') (2. 5) or (2. 7) are given for three transformed coordinate systems (a), (b) and (c), where each z' axis is normal to the [001], [110] and [111] planes of the cubic coordinate system, respectively.

Table I Tensor C_{ij}' in the superlattice fixed coordinate (x', y', z')

i \ j	1(x'x')	2(y'y')	3(z'z')	4(y'z')	5(z'x')	6(x'y')
1(x'x')	$C_{11}+(A_{x'x'x'x'}-1)\varepsilon$	$C_{12}+A_{x'x'y'y'}\varepsilon$	$C_{12}+A_{x'x'z'z'}\varepsilon$	$A_{x'x'y'z'}\varepsilon$	$A_{x'x'z'x'}\varepsilon$	$A_{x'x'x'y'}\varepsilon$
2(y'y')		$C_{11}+(A_{y'y'y'y'}-1)\varepsilon$	$C_{12}+A_{y'y'z'z'}\varepsilon$	$A_{y'y'y'z'}\varepsilon$	$A_{y'y'z'x'}\varepsilon$	$A_{y'y'x'y'}\varepsilon$
3(z'z')			$C_{11}+(A_{z'z'z'z'}-1)\varepsilon$	$A_{z'z'y'z'}\varepsilon$	$A_{z'z'z'x'}\varepsilon$	$A_{z'z'x'y'}\varepsilon$
4(y'z')				$C_{44}+A_{y'z'y'z'}\varepsilon$	$A_{y'z'z'x'}\varepsilon$	$A_{y'z'x'y'}\varepsilon$
5(z'x')					$C_{44}+A_{z'x'z'x'}\varepsilon$	$A_{z'x'x'y'}\varepsilon$
6(x'y')						$C_{44}+A_{x'y'x'y'}\varepsilon$

$\varepsilon = C_{11} - C_{12} - 2C_{44}$

(a) The film coordinate system which arises from rotating the z axis of the original coordinate system by an arbitrary angle θ.

Here, the rotation matrix A is expressed as

$$A = \begin{pmatrix} \cos\theta & \sin\theta & 0 \\ -\sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix} \qquad (2.8)$$

Calculating the coefficients A_{pqrs} in Table I by substituting (2. 8) in the expression (2. 6), we obtain the elastic tensor shown in Table II in the present case (a).

(b) The coordinate system which arises from rotating by an arbitrary angle θ the z'' of the transformed coordinate system (x'', y'', z''), where x'', y'' and z'' axes are directed toward (0, 0, 1), ($1/\sqrt{2}$, $-1/\sqrt{2}$, 0) and ($1/\sqrt{2}$, $1/\sqrt{2}$, 0) in the original coordinate system(x, y, z). In the present case, the rotation matrix A is given as

Table II Tensor C_{ij}' in the coordinate system (a)

$i \backslash j$	1(x'x')	2(y'y')	3(z'z')	4(y'z')	5(z'x')	6(x'y')
1(x'x')	$C_{11}-\frac{1-\cos 4\theta}{4}\varepsilon$	$C_{12}+\frac{1-\cos 4\theta}{4}\varepsilon$	C_{12}	0	0	$-\frac{\sin 4\theta}{4}\varepsilon$
2(y'y')		$C_{11}-\frac{1-\cos 4\theta}{4}\varepsilon$	C_{12}	0	0	$\frac{\sin 4\theta}{4}\varepsilon$
3(z'z')			C_{11}	0	0	0
4(y'z')				C_{44}	0	0
5(z'x')					C_{44}	0
6(x'y')						$C_{44}+\frac{1-\cos 4\theta}{4}\varepsilon$

$$\varepsilon = C_{11} - C_{12} - 2C_{44}$$

$$A = \begin{pmatrix} \cos\theta & \sin\theta & 0 \\ -\sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 0 & 0 & 1 \\ 1/\sqrt{2} & -1/\sqrt{2} & 0 \\ 1/\sqrt{2} & 1/\sqrt{2} & 0 \end{pmatrix} \tag{2.9}$$

By use of the above rotation matrix, the elastic tensor is calculated as in Table III.

(c) The coordinate system (x', y', z'), which is obtained from transforming the original axes whose unit vectors are (1, 0, 0), (0, 1, 0) and (0, 0, 1) first to the ones which have unit vectors ($1/\sqrt{6}$, $1/\sqrt{6}$, $-2/\sqrt{6}$), ($-1/\sqrt{2}$, $1/\sqrt{2}$, 0) and ($1/\sqrt{3}$, $1/\sqrt{3}$, $1/\sqrt{3}$), followed by rotating the new z axis directed toward ($1/\sqrt{3}$, $1/\sqrt{3}$, $1/\sqrt{3}$) by an angle θ. The present rotation matrix is

$$A = \begin{pmatrix} \cos\theta & \sin\theta & 0 \\ -\sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1/\sqrt{6} & 1/\sqrt{6} & -2/\sqrt{6} \\ -1/\sqrt{2} & 1/\sqrt{2} & 0 \\ 1/\sqrt{3} & 1/\sqrt{3} & 1/\sqrt{3} \end{pmatrix} \tag{2.10}$$

The elastic tensor results in Table IV in this case. Here we notice the relation $C_{11}'-C_{12}' = 2C_{66}'$, which means that cubic media are isotropic in [111] plane.

As described in Introduction, we treat evaporated or sputtered thin films in which numerous grains have a common orientation normal to the foil but are randomly oriented in the plane of the foil.[10] As planes of foils, [001], [110] and [111] planes are usually anticipated. The angular θ dependent parts of the elastic tensors in Table II, III and IV disappear under such a situation. The angular independent parts completely agree with those given in the literature.[5, 8, 10]

The present derivations of the elastic tensors are similar to that by Itoh [8], in which the rotations of the field are confused with the rotations of the coordinate system.[14] Furthermore, in addition to some misprints, the Itoh's expressions do not have the symmetry adopted forms as the present expressions: from his expressions, we can not easily detect the elastic tensors for evaporated or sputtered thin films, i.e., the angular independent parts of the elastic tensors as described above.

Table Ⅲ Tensor C_{ij}' in the coordinate system (b)

$i \backslash j$	1(x'x')	2(y'y')	3(z'z')	4(y'z')	5(z'x')	6(x'y')
1(x'x')	$C_{11}+\frac{3C4+4C2-7}{16}\varepsilon$	$C_{12}+\frac{3(1-C4)}{16}\varepsilon$	$C_{12}+\frac{1-C2}{4}\varepsilon$	0	0	$-\frac{3S4+2S2}{16}\varepsilon$
2(y'y')		$C_{11}+\frac{3C4-4C2-7}{16}\varepsilon$	$C_{12}+\frac{1+C2}{4}\varepsilon$	0	0	$\frac{3S4-2S2}{16}\varepsilon$
3(z'z')			$C_{11}-\frac{1}{2}\varepsilon$	0	0	$\frac{S2}{4}\varepsilon$
4(y'z')				$C_{44}+\frac{1+C2}{4}\varepsilon$	$\frac{S2}{4}\varepsilon$	0
5(z'x')					$C_{44}+\frac{1-C2}{4}\varepsilon$	0
6(x'y')						$C_{44}+\frac{3(1-C4)}{16}\varepsilon$

$C2=\cos 2\theta \quad S2=\sin 2\theta \quad C4=\cos 4\theta \quad S4=\sin 4\theta \quad \varepsilon = C_{11}-C_{12}-2C_{44}$

[Ⅲ] Elastic waves in media constituting superlattices

In the previous section, we have discussed the transformation of the elastic tensors of cubic materials with respect to the coordinate system. By use of the obtained results we can deal with propagating waves in a bulk elastic medium in an arbitrary coordinate system. Here we treat superlattices consisting of periodically alternating films, in each boundary of which a propagating wave undergoes reflection and refraction, that is, it splits in reflected and refracted waves. On the surface of a medium the refracted waves are lacking. There exist incident and reflected waves, which include quasi-transverse and quasi-longitudinal waves, and the mixtures of them yield surface modes known as Rayleigh wave and Sezawa waves for special frequencies. In the present section we formulate the equations giving surface waves in superlattices which consist of two kinds of evaporated or sputtered thin films.

The equation of motion for a material point in a medium i can be written in the form [11-13]

$$\rho^{(i)}\frac{\partial^2 u_r^{(i)}{}'}{\partial t^2}=\frac{\partial \sigma_{rs}^{(i)}{}'}{\partial x_s'}, \qquad r=1,\ 2,\ 3, \tag{3.1}$$

where $\rho^{(i)}$ denotes the density of the medium, $u_r^{(i)}{}'$ is the r-th component of the displacement of the medium at the point whose position vector has the s-th cartisian component x_s', and $\sigma_{rs}^{(i)}{}'$ is an element of the stress tensor. Superscript (i) and the symbol $'$ correspond to the medium i and the transformed coordinate system $(x_1', x_2', x_3') \equiv (x', y', z')$, respectively in the above equation. The stress tensor is specified by a generalized Hook's law [12] as

$$\sigma_{pq}^{(i)}{}' = \lambda_{pqrs}^{(i)}{}'\mu_{rs}, \qquad \mu_{rs}=\frac{1}{2}\left(\frac{\partial u_r^{(i)}{}'}{\partial x_s'}+\frac{\partial u_s^{(i)}{}'}{\partial x_r'}\right). \tag{3.2}$$

Here $\lambda_{pqrs}^{(i)}{}'$ is an element of the elastic constant tensor of the medium i in the transformed coordinate.

Table Ⅳ Tensor C_{ij}' in the coordinate system (c)

i \ j	1(x'x')	2(y'y')	3(z'z')	4(y'z')	5(z'x')	6(x'y')
1(x'x')	$C_{11}-\frac{1}{2}\varepsilon$	$C_{12}+\frac{1}{6}\varepsilon$	$C_{12}+\frac{1}{3}\varepsilon$	$\frac{\sin 3\theta}{3\sqrt{2}}\varepsilon$	$-\frac{\cos 3\theta}{3\sqrt{2}}\varepsilon$	0
2(y'y')		$C_{11}-\frac{1}{2}\varepsilon$	$C_{12}+\frac{1}{3}\varepsilon$	$-\frac{\sin 3\theta}{3\sqrt{2}}\varepsilon$	$\frac{\cos 3\theta}{3\sqrt{2}}\varepsilon$	0
3(z'z')			$C_{11}-\frac{2}{3}\varepsilon$	0	0	0
4(y'z')				$C_{44}+\frac{1}{3}\varepsilon$	0	$\frac{\cos 3\theta}{3\sqrt{2}}\varepsilon$
5(z'x')					$C_{44}+\frac{1}{3}\varepsilon$	$\frac{\sin 3\theta}{3\sqrt{2}}\varepsilon$
6(x'y')						$C_{44}+\frac{1}{6}\varepsilon$

$$\varepsilon = C_{11} - C_{12} - 2C_{44}$$

Substituting the elements of the elastic tensors in Tables Ⅱ, Ⅲ and Ⅳ in eq. (3.1) with (3.2) yields the equation of motion for the special case (a), (b) and (c) described in the previous section. We will write below the equation of motion for the medium i which is isotropic in the (x', y') plane, that is, which is assumed a layer of superlattice, in the case (c). Straightforward calculation gives the followings.

$$\rho^{(i)}\frac{\partial^2 u_x^{(i)\prime}}{\partial t^2} = \left(\overline{C_{11}^{(i)}}'\frac{\partial^2}{\partial x'^2}+\overline{C_{66}^{(i)}}'\frac{\partial^2}{\partial y'^2}+\overline{C_{44}^{(i)}}'\frac{\partial^2}{\partial z'^2}\right)u_x^{(i)\prime}+\left(\overline{C_{11}^{(i)}}'-\overline{C_{66}^{(i)}}'\right)\frac{\partial^2}{\partial x'\partial y'}u_y^{(i)\prime}$$
$$+\left(\overline{C_{13}^{(i)}}'+\overline{C_{44}^{(i)}}'\right)\frac{\partial^2}{\partial x'\partial z'}u_z^{(i)\prime} \qquad (3.3a)$$

$$\rho^{(i)}\frac{\partial^2 u_y^{(i)\prime}}{\partial t^2} = \left(\overline{C_{66}^{(i)}}'\frac{\partial^2}{\partial x'^2}+\overline{C_{11}^{(i)}}'\frac{\partial^2}{\partial y'^2}+\overline{C_{44}^{(i)}}'\frac{\partial^2}{\partial z'^2}\right)u_y^{(i)\prime}+\left(\overline{C_{11}^{(i)}}'-\overline{C_{66}^{(i)}}'\right)\frac{\partial^2}{\partial x'\partial y'}u_x^{(i)\prime}$$
$$+\left(\overline{C_{13}^{(i)}}'+\overline{C_{44}^{(i)}}'\right)\frac{\partial^2}{\partial y'\partial z'}u_z^{(i)\prime} \qquad (3.3b)$$

$$\rho^{(i)}\frac{\partial^2 u_z^{(i)\prime}}{\partial t^2} = \left(\overline{C_{44}^{(i)}}'\frac{\partial^2}{\partial x'^2}+\overline{C_{44}^{(i)}}'\frac{\partial^2}{\partial y'^2}+\overline{C_{33}^{(i)}}'\frac{\partial^2}{\partial z'^2}\right)u_z^{(i)\prime}+\left(\overline{C_{13}^{(i)}}'+\overline{C_{44}^{(i)}}'\right)\frac{\partial}{\partial z'}\left(\frac{\partial u_x^{(i)\prime}}{\partial x'}+\frac{\partial u_y^{(i)\prime}}{\partial y'}\right) \qquad (3.3c)$$

Here $\overline{C_{pq}^{(i)}}'$ denotes the angular independent parts of the elements of the tensor in Table Ⅳ; the averages of $\sin 3\theta$ and $\cos 3\theta$ are equal to zero. In the above calculation we have used the relation $\overline{C_{11}^{(i)}}' = \overline{C_{22}^{(i)}}'$, $\overline{C_{13}^{(i)}}' = \overline{C_{23}^{(i)}}'$, $\overline{C_{44}^{(i)}}' = \overline{C_{55}^{(i)}}'$, and $\overline{C_{11}^{(i)}}'-\overline{C_{66}^{(i)}}' = \overline{C_{12}^{(i)}}'+\overline{C_{66}^{(i)}}'$, the existence of which are obvious from Table Ⅳ.

The above mentioned relation $\overline{C_{11}^{(i)}}'-\overline{C_{12}^{(i)}}'-2\overline{C_{66}^{(i)}}' = 0$ ensures that the medium i is isotropic in the (x', y') plane. Actually, substituting

$$u_\alpha^{(i)\prime} = U_\alpha^{(i)}\exp\{\mathrm{i}(q_{x'}^{(i)}x' + q_{y'}^{(i)}y' - \omega t)\}\ (\mathrm{i}^2 = -1)$$

into (3. 3a), (3. 3b) and (3. 3c) ($\alpha = x'$, y' and z'), which are the displacements in the case assumed the elastic waves propagating in the (x', y') plane, yields the following solutions.

$$\rho^{(i)}\omega^2 = \overline{C_{11}^{(i)}}'[\mathbf{q}^{(i)}]^2; \quad U_x^{(i)}: U_y^{(i)} = q_{x'}^{(i)}: q_{y'}^{(i)}, \quad U_{z'}^{(i)} = 0$$

$$\rho^{(i)}\omega^2 = \overline{C_{66}^{(i)}}'[\mathbf{q}^{(i)}]^2; \quad U_x^{(i)}: U_y^{(i)} = q_{y'}^{(i)}: -q_{x'}^{(i)}, \quad U_{z'}^{(i)} = 0$$

$$\rho^{(i)}\omega^2 = \overline{C_{44}^{(i)}}'[\mathbf{q}^{(i)}]^2; \quad U_x^{(i)} = U_y^{(i)} = 0, \quad U_{z'}^{(i)} \neq 0$$

Here the notation $\mathbf{q}^{(i)} = (q_{x'}^{(i)},\ q_{y'}^{(i)},\ 0)$ is used for a wave vector and ω and t mean the frequency of the wave and time, respectively. Thus, we can confirm that there exist one longitudinal wave and two transverse waves for each frequency in the plane of the foil, which holds only for isotropic media.

As described above, the medium i with the tensor elements $\overline{C_{pq}^{(i)}}'$ is isotropic in the (x', y') plane. Considering this fact, we will be able to restrict the elastic waves to those propagating in the (x', z') plane. For the wave with the wave vector $\mathbf{q}^{(i)} = (q_{x'}^{(i)},\ 0,\ q_{z'}^{(i)})$ and frequency $\omega^{(i)}$, its displacement in the point (x', y', z') and time t is expressed in the form

$$u_\alpha^{(i)\prime} = U_\alpha^{(i)}\exp\{\mathrm{i}(q_{x'}^{(i)}x' + q_{z'}^{(i)}z' - \omega t)\} \quad (\alpha = x',\ y',\ z') \tag{3. 4}$$

Substitution of (3. 4) for (3. 3a) and (3. 3c) gives

$$\rho^{(i)}\omega^{(i)2}U_x^{(i)} = \left(\overline{C_{11}^{(i)}}' q_{x'}^{(i)2} + \overline{C_{44}^{(i)}}' q_{z'}^{(i)2}\right)U_x^{(i)} + \left(\overline{C_{13}^{(i)}}' + \overline{C_{44}^{(i)}}'\right)q_{x'}^{(i)}q_{z'}^{(i)}U_z^{(i)} \tag{3. 5a}$$

$$\rho^{(i)}\omega^{(i)2}U_z^{(i)} = \left(\overline{C_{44}^{(i)}}' q_{x'}^{(i)2} + \overline{C_{33}^{(i)}}' q_{z'}^{(i)2}\right)U_z^{(i)} + \left(\overline{C_{13}^{(i)}}' + \overline{C_{44}^{(i)}}'\right)q_{x'}^{(i)}q_{z'}^{(i)}U_x^{(i)} \tag{3. 5b}$$

Similarly, substituting (3. 4) in (3. 3b) yields

$$\rho^{(i)}\omega^{(i)2}U_y^{(i)} = \left(\overline{C_{66}^{(i)}}' q_{x'}^{(i)2} + \overline{C_{44}^{(i)}}' q_{z'}^{(i)2}\right)U_y^{(i)} \tag{3. 6}$$

The surface plane is assumed to be stress-free,[11-13] which means

$$\sigma_{zz}^{(i)\prime} = \sigma_{zx}^{(i)\prime} = \sigma_{zy}^{(i)\prime} = 0 \tag{3. 7}$$

We have incident and reflected waves on the surface. In order that the boundary condition may be satisfied for all x' and t, the reflected wave must have the same $q_{x'}$ and ω as the incident wave. This is generalized as below. In the present case, we have boundaries depending on z' axis, on each of which two surfaces of media contacts and incident, reflected and refracted waves appear. The boundary conditions depend only on z' axis and they do not depend on x', y' and t. Hence dependence of solution on x', y' and t remains the same in all space and time, i.e. ω, $q_{x'}$ and $q_{y'}$ (=0 in our case) for reflected and refracted waves are the same as in the incident wave.[15]

The solutions obtained from (3. 6) represent an incident transverse wave with wave vector $(q_{x'}^{(i)},\ 0,\ q_{z'}^{(i)})$ and a reflected transverse wave with wave vector $(q_{x'}^{(i)},\ 0,\ -q_{z'}^{(i)})$ in the vicinity of the surface of the medium. We can confirm that the present set of incident and reflected waves satisfy the boundary condition (3. 7) at the surface. Thus, this transverse wave reflected completely and can not make mixtures as described at the beginning of the present section. As a surface mode, this transverse wave is known to cause the Love wave. But the Love wave is out of our subject of investigation. Hence we do not deal with eq.(3. 6).

We can obtain quasi-transverse and quasi-longitudinal elastic waves from solving eqs. (3. 5a) and (3. 5b). As described already, the frequency $\omega^{(i)}$ and the x'-th component of the wave vector $q_{x'}^{(i)}$ of these waves do not depend on the medium i in the superlattices, where boundaries exist only on z' axis. Hereafter we will remove this superscript from these quantities. In order to simplify the treatment, we adopt the following notations:

$$Q_i = q_{z'}^{(i)}/q_{x'} \tag{3. 8}$$

$$U_i = U_z^{(i)}/U_x^{(i)} \tag{3. 9}$$

$$\xi_i^2 = \rho^{(i)}\omega^2/(\overline{C_{44}^{(i)}}{}'q_{x'}^2) \tag{3. 10}$$

By use of the above notations, eqs. (3. 5a) and (3. 5b) are rewritten as

$$U_i = -\frac{\overline{C_{44}^{(i)}}{}'Q_i^2+\overline{C_{11}^{(i)}}{}'-\overline{C_{44}^{(i)}}{}'\xi_i^2}{(\overline{C_{13}^{(i)}}{}'+\overline{C_{44}^{(i)}}{}')Q_i} = -\frac{(\overline{C_{13}^{(i)}}{}'+\overline{C_{44}^{(i)}}{}')Q_i}{\overline{C_{33}^{(i)}}{}'Q_i^2+\overline{C_{44}^{(i)}}{}'-\overline{C_{44}^{(i)}}{}'\xi_i^2} \tag{3. 11}$$

From the above equations, we have

$$(Q_i^2)^2+\{A_i-(1+B_i)\xi_i^2\}(Q_i^2)+(1-\xi_i^2)(C_i-B_i\xi_i^2) = 0 \tag{3. 12}$$

where A_i, B_i, and C_i denotes the followings.

$$A_i = \frac{\overline{C_{11}^{(i)}}{}'}{\overline{C_{44}^{(i)}}{}'}-\frac{\overline{C_{13}^{(i)}}{}'}{\overline{C_{33}^{(i)}}{}'}\left(2+\frac{\overline{C_{13}^{(i)}}{}'}{\overline{C_{44}^{(i)}}{}'}\right), \quad B_i = \frac{\overline{C_{44}^{(i)}}{}'}{\overline{C_{33}^{(i)}}{}'}, \quad C_i = \frac{\overline{C_{11}^{(i)}}{}'}{\overline{C_{33}^{(i)}}{}'} \tag{3. 13}$$

The equation (3. 12) is a quadratic equation with respect to (Q_i^2) and has two solutions for given ω and $q_{x'}$. We will represent these two solutions as Q_{i1}^2 and Q_{i2}^2 ($|Q_{i1}^2| \geq |Q_{i2}^2|$). The expression (3. 11) gives two values U_{i1} and U_{i2} for U_i corresponding to these Q_{i1}^2 and Q_{i2}^2. For a given Q_i^2 we have two waves. One represents the wave vector for a forward wave and the other is a backward wave. We can summarize the elastic waves derived from eqs. (3. 5a) and (3. 5b) as follows.

$$a_i(1,\ 0,\ U_{i1})\exp(\mathrm{i}q_{x'}Q_{i1}z')f(\omega,\ t) \tag{3. 14a}$$

$$b_i(1,\ 0,\ -U_{i1})\exp(-\mathrm{i}q_{x'}Q_{i1}z')f(\omega,\ t) \tag{3. 14b}$$

$$c_i(1,\ 0,\ U_{i2})\exp(\mathrm{i}q_{x'}Q_{i2}z')f(\omega,\ t) \tag{3. 14c}$$

$$d_i(1,\ 0,\ -U_{i2})\exp(-\mathrm{i}q_{x'}Q_{i2}z')f(\omega,\ t) \tag{3. 14d}$$

Here, a_i, b_i, c_i and d_i indicate the x'-th components of the amplitudes for the corresponding elastic waves and $f(\omega,\ t)$ is written as

$$f(\omega,\ t) = \exp\{\mathrm{i}(q_{x'}x'-\omega t)\} \tag{3. 15}$$

Now we notice that a propagating wave is characterized by a variable set ($\pm U_{ij}$, $\pm Q_{ij}$) with $j=1$ or 2. Forward waves are characterized by (U_{i1}, Q_{i1}) and (U_{i2}, Q_{i2}) and backward waves by ($-U_{i1}$, $-Q_{i1}$) and ($-U_{i2}$, $-Q_{i2}$). They are in opposite sign relationship to each other.

We will roughly estimate variable sets (U_{ij}, Q_{ij}) before going ahead. From Table IV we have

$$\overline{C_{11}^{(i)}}' - \overline{C_{33}^{(i)}}' = \varepsilon/6 \text{ and } \overline{C_{11}^{(i)}}' - \overline{C_{13}^{(i)}}' - 2\overline{C_{44}^{(i)}}' = -\varepsilon/6 .$$

These suggests that we can approximately have the relations $\overline{C_{11}^{(i)}}' \approx \overline{C_{33}^{(i)}}'$ and $\overline{C_{11}^{(i)}}' - \overline{C_{13}^{(i)}}' - 2\overline{C_{44}^{(i)}}' \approx 0$. Substituting these relations in (3. 13) gives $A_i = 2$ and $C_i = 1$. Then the quadratic equation have two solutions

$$Q_{i1}^2 = \xi_i^2 - 1 , \quad Q_{i2}^2 = \left(\frac{\overline{C_{44}^{(i)}}'}{\overline{C_{33}^{(i)}}'} \right) \xi_i^2 - 1$$

which correspond to the transverse and longitudinal waves in an isotropic medium. Substitution of the above into (3. 11) gives the corresponding solutions as

$$U_{i1} = -1/Q_{i1} , \quad U_{i2} = Q_{i2} \qquad (3.16)$$

The relation (3. 16) can be used as a rough estimation of elastic waves and a verification of the obtained results for the present purpose. Glass, which is treated in the next section as a substrate on which superlattices grow, is just a isotropic material corresponding to the present case.

[IV] Elastic waves and surface waves in superlattices

As in literature,[11-12] we take specimens in the half-space $z' < 0$, with the surface as the plane $z' = 0$. The specimens consists of alternating layers of thickness d_1 of constituent 1 and thickness d_2 of constituent 2. These specimens are referred to as periodically layered structures or superlattices, where one spatial period is $D = d_1 + d_2$.

The l -th constituent 1 from the surface is located at $-(l-1)D \geq z' \geq -(l-1)D - d_1$. The solution of the wave equation in this region is written as follows by reference to (3. 14a) − (3. 14d).[16]

$$\begin{aligned} u_x^{(1)}{}'/f(\omega,\ t) = &\\ &a_{1l}^{+}\exp\{iq_{x'}Q_{11}[z'+(l-1)D]\} + b_{1l}^{+}\exp\{-iq_{x'}Q_{11}[z'+(l-1)D]\}\\ &+c_{1l}^{+}\exp\{iq_{x'}Q_{12}[z'+(l-1)D]\} + d_{1l}^{+}\exp\{-iq_{x'}Q_{12}[z'+(l-1)D]\}\\ = &\ a_{1l}^{-}\exp\{iq_{x'}Q_{11}[z'+(l-1)D+d_1]\} + b_{1l}^{-}\exp\{-iq_{x'}Q_{11}[z'+(l-1)D+d_1]\}\\ &+c_{1l}^{-}\exp\{iq_{x'}Q_{12}[z'+(l-1)D+d_1]\} + d_{1l}^{-}\exp\{-iq_{x'}Q_{12}[z'+(l-1)D+d_1]\} \end{aligned} \qquad (4.1a)$$

$$\begin{aligned} u_z^{(1)}{}'/f(\omega,\ t) = &\\ &a_{1l}^{+}U_{11}\exp\{iq_{x'}Q_{11}[z'+(l-1)D]\} - b_{1l}^{+}U_{11}\exp\{-iq_{x'}Q_{11}[z'+(l-1)D]\}\\ &+c_{1l}^{+}U_{12}\exp\{iq_{x'}Q_{12}[z'+(l-1)D]\} - d_{1l}^{+}U_{12}\exp\{-iq_{x'}Q_{12}[z'+(l-1)D]\}\\ = &\ a_{1l}^{-}U_{11}\exp\{iq_{x'}Q_{11}[z'+(l-1)D+d_1]\} - b_{1l}^{-}U_{11}\exp\{-iq_{x'}Q_{11}[z'+(l-1)D+d_1]\}\\ &+c_{1l}^{-}U_{12}\exp\{iq_{x'}Q_{12}[z'+(l-1)D+d_1]\} - d_{1l}^{-}U_{12}\exp\{-iq_{x'}Q_{12}[z'+(l-1)D+d_1]\} \end{aligned} \qquad (4.1b)$$

Here the amplitudes a_{1l}^{+}, b_{1l}^{+}, c_{1l}^{+} and d_{1l}^{+} are related to the waves with the phases referred to the upper end of the layer, and the amplitudes a_{1l}^{-}, b_{1l}^{-}, c_{1l}^{-} and d_{1l}^{-} are related to those referred to the lower end of the layer.

In the l -th layer of the second medium, which is located in the region $-(l-1)D-d_1 \geq z' \geq -lD$, the components of the displacement are

$$
\begin{aligned}
&u_x^{(2)\prime}/f(\omega,\ t) = \\
&\qquad a_{2l}^{+}\exp\{iq_{x'}Q_{21}[z'+(l-1)D+d_1]\} + b_{2l}^{+}\exp\{-iq_{x'}Q_{21}[z'+(l-1)D+d_1]\} \\
&\qquad +c_{2l}^{+}\exp\{iq_{x'}Q_{22}[z'+(l-1)D+d_1]\} + d_{2l}^{+}\exp\{-iq_{x'}Q_{22}[z'+(l-1)D+d_1]\} \\
&\quad = a_{2l}^{-}\exp\{iq_{x'}Q_{21}[z'+lD]\} + b_{2l}^{-}\exp\{-iq_{x'}Q_{21}[z'+lD]\} \\
&\qquad +c_{2l}^{-}\exp\{iq_{x'}Q_{22}[z'+lD]\} + d_{2l}^{-}\exp\{-iq_{x'}Q_{22}[z'+lD]\}
\end{aligned}
\tag{4. 2a}
$$

and

$$
\begin{aligned}
&u_z^{(2)\prime}/f(\omega,\ t) = \\
&\qquad a_{2l}^{+}U_{21}\exp\{iq_{x'}Q_{21}[z'+(l-1)D+d_1]\} - b_{2l}^{+}U_{21}\exp\{-iq_{x'}Q_{21}[z'+(l-1)D+d_1]\} \\
&\qquad +c_{2l}^{+}U_{22}\exp\{iq_{x'}Q_{22}[z'+(l-1)D+d_1]\} - d_{2l}^{+}U_{22}\exp\{-iq_{x'}Q_{22}[z'+(l-1)D+d_1]\}\ . \\
&\quad = a_{2l}^{-}U_{21}\exp\{iq_{x'}Q_{21}[z'+lD]\} - b_{2l}^{-}U_{21}\exp\{-iq_{x'}Q_{21}[z'+lD]\} \\
&\qquad +c_{2l}^{-}U_{22}\exp\{iq_{x'}Q_{22}[z'+lD]\} - d_{2l}^{-}U_{22}\exp\{-iq_{x'}Q_{22}[z'+lD]\}
\end{aligned}
\tag{4. 2b}
$$

The meaning of the amplitudes a_{2l}^{+}, … and a_{2l}^{-}, … is identical to that in medium 1.

Two expressions for the displacement (4. 1a) or (4. 1b) must be the same at the end of layer. It holds also to (4. 2a) or (4. 2b). Thus, the amplitudes are related by

$$
|u_{i,l}^{-}\rangle = P_i|u_{i,l}^{+}\rangle\ , \tag{4. 3}
$$

where we have denoted

$$
|u_{i,l}^{\pm}\rangle = \begin{pmatrix} a_{il}^{\pm} \\ b_{il}^{\pm} \\ c_{il}^{\pm} \\ d_{il}^{\pm} \end{pmatrix} \tag{4. 4}
$$

and P_i is the matrix expressed as

$$
P_i = \begin{pmatrix} F_{i1} & \hat{o} \\ \hat{o} & F_{i2} \end{pmatrix} \tag{4. 5}
$$

with

$$
F_{ij} = \begin{pmatrix} f_{ij} & 0 \\ 0 & f_{ij}^{-1} \end{pmatrix},\quad \hat{o} = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}, \tag{4. 6}
$$

where f_{ij} is given by

$$
f_{ij} = \exp(-iq_{x'}Q_{ij}d_i)\ . \tag{4. 7}
$$

The displacement $(u_x^{(i)\prime},\ 0,\ u_z^{(i)\prime})$ by the elastic waves must be continuous at the boundary $z' = -(l-1)D-d_1$, i.e., $u_x^{(1)\prime} = u_x^{(2)\prime}$ and $u_z^{(1)\prime} = u_z^{(2)\prime}$:

$$a_{1l}^{-}+b_{1l}^{-}+c_{1l}^{-}+d_{1l}^{-} = a_{2l}^{+}+b_{2l}^{+}+c_{2l}^{+}+d_{2l}^{+} \tag{4.8}$$

and

$$U_{11}(a_{1l}^{-}-b_{1l}^{-})+U_{12}(c_{1l}^{-}-d_{1l}^{-}) = U_{21}(a_{2l}^{+}-b_{2l}^{+})+U_{22}(c_{2l}^{+}-d_{2l}^{+}) \ . \tag{4.9}$$

We have the same stress components $\sigma_{zz}^{(i)\prime}$ and $\sigma_{zx}^{(i)\prime}$ at the boundary, where $\sigma_{zz}^{(i)\prime} = \overline{C_{13}^{(i)}}{}^{\prime}\dfrac{\partial u_x^{(i)\prime}}{\partial x^{\prime}}+\overline{C_{33}^{(i)}}{}^{\prime}\dfrac{\partial u_z^{(i)\prime}}{\partial z^{\prime}}$ and $\sigma_{zx}^{(i)\prime} = \overline{C_{44}^{(i)}}{}^{\prime}\left(\dfrac{\partial u_x^{(i)\prime}}{\partial z^{\prime}}+\dfrac{\partial u_z^{(i)\prime}}{\partial x^{\prime}}\right)$. Thus we have

$$\begin{aligned}&\overline{C_{13}^{(1)}}{}^{\prime}(a_{1l}^{-}+b_{1l}^{-}+c_{1l}^{-}+d_{1l}^{-})+\overline{C_{33}^{(1)}}{}^{\prime}[Q_{11}U_{11}(a_{1l}^{-}+b_{1l}^{-})+Q_{12}U_{12}(c_{1l}^{-}+d_{1l}^{-})]\\ &= \overline{C_{13}^{(2)}}{}^{\prime}(a_{2l}^{+}+b_{2l}^{+}+c_{2l}^{+}+d_{2l}^{+})+\overline{C_{33}^{(2)}}{}^{\prime}[Q_{21}U_{21}(a_{2l}^{+}+b_{2l}^{+})+Q_{22}U_{22}(c_{2l}^{+}+d_{2l}^{+})]\end{aligned} \tag{4.10}$$

and

$$\begin{aligned}&\overline{C_{44}^{(1)}}{}^{\prime}[(Q_{11}+U_{11})(a_{1l}^{-}-b_{1l}^{-})+(Q_{12}+U_{12})(c_{1l}^{-}-d_{1l}^{-})]\\ &= \overline{C_{44}^{(2)}}{}^{\prime}[(Q_{21}+U_{21})(a_{2l}^{+}-b_{2l}^{+})+(Q_{22}+U_{22})(c_{2l}^{+}-d_{2l}^{+})]\end{aligned} \tag{4.11}$$

The boundary conditions (4. 8)−(4. 11) are summarized as

$$T_1U|u_{1,l}^{-}\rangle = T_2U|u_{2,l}^{+}\rangle \ , \tag{4.12}$$

Where the matrix T_i (i =1 or 2) is written as

$$T_i = \begin{pmatrix} T_{11}^{(i)} & T_{12}^{(i)} \\ T_{21}^{(i)} & T_{22}^{(i)} \end{pmatrix} \tag{4.13}$$

with

$$T_{1k}^{(i)} = \begin{pmatrix} 1 & 0 \\ 0 & U_{ik} \end{pmatrix} \tag{4.14}$$

and

$$T_{2k}^{(i)} = \begin{pmatrix} \overline{C_{13}^{(i)}}{}^{\prime}+\overline{C_{33}^{(i)}}{}^{\prime}Q_{ik}U_{ik} & 0 \\ 0 & \overline{C_{44}^{(i)}}{}^{\prime}(Q_{ik}+U_{ik}) \end{pmatrix} \tag{4.15}$$

and the matrix U means

$$U = \begin{pmatrix} U_0 & \hat{0} \\ \hat{0} & U_0 \end{pmatrix} \tag{4.16}$$

with

$$U_0 = \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}. \tag{4.17}$$

Similarly at the boundary $z' = -lD$ we have

$$T_2 U|u_{2,l}^-\rangle = T_1 U|u_{1,l+1}\rangle \tag{4.18}$$

From the expressions (4. 12) and (4. 18) with (4. 13), the amplitudes in the l-th layer and $l+1$-th layer are related by the following representations.

$$|u_{1,l+1}^+\rangle = T_{12}^{-1}P_2T_{12}P_1|u_{1,l}^+\rangle\ , \tag{4.19}$$

$$|u_{2,l}^+\rangle = T_{12}P_1|u_{1,l}^+\rangle\ . \tag{4.20}$$

Here the matrix T_{12} denotes

$$T_{12} = U^{-1}T_2^{-1}T_1U \tag{4.21}$$

and X^{-1} means the inverse matrix of the matrix X.

Let us assume that the thickness of the superlattice is $LN\cdot D$. The amplitudes of the elastic waves on the surface at $z' = 0$ are represented by $|u_{1,1}^+\rangle$, while those on the opposite side surface, i.e., the surface at $z' = -LN\cdot D$, are characterized by $|u_{2,LN}^-\rangle$. The relationship between these two kinds of the amplitudes of elastic waves are given by

$$|u_{2,LN}^-\rangle = T|u_{1,1}^+\rangle \tag{4.22}$$

where

$$T = P_2T_{12}P_1[T_{12}^{-1}P_2T_{12}P_1]^{LN-1} \tag{4.23}$$

As described in the previous section, the stress components $\sigma_{zz}^{(i)\prime}$ and $\sigma_{zx}^{(i)\prime}$ must be zero on the surface. This condition at $z' = 0$ corresponds to

$$A_1U|u_{1,1}^+\rangle = 0\ , \tag{4.24}$$

while the condition at $z' = -LN\cdot D$ gives

$$A_2U|u_{2,LN}^-\rangle = 0\ , \tag{4.25}$$

where the matrix A_j ($j = 1$ or 2) is expressed as

$$A_j = (T_{21}^{(j)}\quad T_{22}^{(j)})\ . \tag{4.26}$$

Here the definition for matrices (4. 15) and (4. 16) is used. By use of (4. 22), the above boundary conditions (4. 24) and (4. 25) are summarized as

$$B|u_{1,1}^+\rangle = 0 \tag{4.27}$$

with the 4×4 matrix B defined by

$$B = \begin{pmatrix} A_1 U \\ A_2 UT \end{pmatrix}. \tag{4. 28}$$

In order that the equation (4. 27) has a non-trivial solution, the determinant of the matrix B must be zero:

$$\det B = 0 \tag{4. 29}$$

The elastic wave satisfying the above solubility condition (4.29) is the desired surface wave. This equation is a dispersion equation.

The surface wave obtained from the condition (4. 29) is the one for a bulk superlattice. In practice, however, superlattices are formed on the substrate such as glass. So we will derive the condition to obtain the surface wave for a superlattice on a substrate.

Let us assume that the substrate is located in the region $-LN\cdot D \geq z' \geq -(LN+LS)\cdot D$. The above derivations and relations for the constituents 1 and 2 of the superlattice remain unchanged for the substrate. The boundary condition at $z' = -LN\cdot D$ is expressed as

$$T_2 U|u_{2,LN}^-\rangle = T_s U|u_s^+\rangle , \tag{4. 30}$$

where T_s denotes the matrix obtained from putting s , which is the script meaning substrate, instead of i in (4. 13)－(4. 15), where Q_{sk} and U_{sk} (k =1 or 2) are calculated by use of the elastic constants of the substrate, and $|u_s^+\rangle$ is the amplitude of the elastic waves on the surface of substrate contacting with the superlattice. We will write the amplitude at the other end of substrate as $|u_s^-\rangle$. Then we have a similar relation as (4. 3):

$$|u_s^-\rangle = P_s|u_s^+\rangle \tag{4. 31}$$

Here $|u_s^{\pm}\rangle$ is obviously expressed as

$$|u_s^{\pm}\rangle = \begin{pmatrix} a_s^{\pm} \\ b_s^{\pm} \\ c_s^{\pm} \\ d_s^{\pm} \end{pmatrix}, \tag{4. 32}$$

and P_s is the matrix corresponding to replacing i by s in eqs. (4. 5) and (4. 6) with

$$f_{sj} = \exp(-\mathrm{i}q_x Q_{sj}\cdot LS\cdot D) . \tag{4. 33}$$

Substituting (4. 22) in (4. 30) yields

$$|u_s^+\rangle = T_{2s} T|u_{1,1}^+\rangle \tag{4. 34}$$

where the matrix T_{2s} means

$$T_{2s} = U^{-1}T_s^{-1}T_2 U . \tag{4. 35}$$

When the substrate is sufficiently thick, we have no backward wave for the surface wave [17] in this medium. This means that a_s^+ and c_s^+ are zero in (4. 32). The present condition is expressed as

$$S_1 | u_{1,1}^+ \rangle = 0 \tag{4. 36}$$

with

$$S_1 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix} T_{2s} T . \tag{4. 37}$$

The boundary condition (4. 24) and (4. 36) are summarized as

$$B_{s1} | u_{1,1}^+ \rangle = 0 , \tag{4. 38}$$

where the 4×4 matrix B_{s1} is given by

$$B_{s1} = \begin{pmatrix} A_1 U \\ S_1 \end{pmatrix} \tag{4. 39}$$

Thus we have the following dispersion equation determining the surface wave in the superlattice on thick substrate:

$$\det\ B_{s1} = 0 . \tag{4. 40}$$

We must consider the boundary condition on the surface of substrate, i.e., at $z' = -(lN+LS)D$, in the case where substrate is thin. It is apparent from the analogy to (4. 24)and (4. 25) that we have the boundary condition

$$A_s U | u_s^- \rangle = 0 \tag{4. 41}$$

with the 2×4 matrix

$$A_s = (T_{21}^{(s)} \quad T_{22}^{(s)}) . \tag{4. 42}$$

The boundary condition(4. 24) and (4. 41) together with (4. 31) and (4. 34) gives the following dispersion equation for the surface wave.

$$\det \begin{pmatrix} A_1 U \\ A_s U P_s T_{2s} T \end{pmatrix} = 0 \tag{4. 43}$$

[V] Results and discussions

We have derived the dispersion equations (4. 29), . (4. 40) and (4. 43), each of which corresponds to the surface wave of a bulk superlattice, a superlattice on a thick substrate and a superlattice on a substrate of arbitrary thickness, respectively. Solving these dispersion equations determines the numerical values ξ_i defined by (3. 10) for a given ω and $q_{x'}$. Now we will define

$$\nu_T^{(i)} \equiv \left[C_{44}^{(i)} / \rho^{(i)} \right]^{1/2} , \tag{5. 1}$$

Table V Numerical values of elastic constants $\overline{C_{pq}^{(i)}}$, which are isotropic in (x', y') plane[a], density $\rho^{(i)}$ [b] and transverse wave density $\nu_T^{(i)}$ for media i.

i	$\overline{C}_{11}^{(i)}/10^9$Pa	$\overline{C}_{33}^{(i)}/10^9$Pa	$\overline{C}_{13}^{(i)}/10^9$Pa	$\overline{C}_{44}^{(i)}/10^9$Pa	$\rho^{(i)}/10^3$Kgm^{-3}	$\nu_T^{(i)}/10^3$mS^{-1}
Cu	22.09	23.82	8.74	4.08	8.96	2.13
Al	11.40	11.57	5.97	2.47	2.70	3.02
Ag	15.16	16.15	7.23	2.49	10.50	1.54
Glass[c]	7.85	7.85	1.61	3.12	2.20	3.77

[a] **Calculated from Table of Landolt Börnstein**

[b] **Obatained from Dictionary of Physics and Chemistry (In Japanese, 4th ed., Iwanami, 1987)**

[c] **Used datum for quartz glass in Physical constants (In Japanese, New ed., Asakura, 1978) p.25.**

which is anticipated to be the velocity of the transverse wave in the medium i. When (5. 1) is substituted in (3. 10), we obtain

$$\xi_i = \omega/(\nu_T^{(i)} q_{x'}) = \nu_S/\nu_T^{(i)} . \tag{5. 2}$$

Here $\nu_S(=\omega/q_{x'})$ is the velocity of the surface wave on a superlattice. It is clear from (5. 2) that ξ_1, ξ_2 and ξ_S are not independent. This means that we can choose one, for instance ξ_1, as a standard variable.

In the present calculation we will assume that the wavelength of the surface wave λ_S, which is associated with $q_{x'}$ by $q_{x'} = 2\pi/\lambda_S$, is $LD \cdot D$:

$$\lambda_S = LD \cdot D . \tag{5. 3}$$

We have assumed that the thickness of the superlattice is $LN \cdot D$ and that of substrate $LS \cdot D$. It is confirmed

Table VIa Relative surface waves velocities in bulk Cu/Al superlattices ($LN/LD = 1.0$)

LD	Cu:Al=1:3	Cu:Al=1:2	Cu:Al=1:1	Cu:Al=2:1	Cu:Al=3:1	
2	1. 04337	1. 00656	0. 96825	0. 94650	0. 93688	Pure Cu
6	1. 07963	1. 03895	0. 98072	0. 94424	0. 93206	0. 91602
12	1. 08022	1. 04053	0. 98304	0. 94638	0. 93397	
18	1. 08016	1. 04073	0. 98359	0. 94701	0. 93456	Pure Al
30	1. 08010	1. 04082	0. 98389	0. 94737	0. 93489	1. 27602
54	1. 08007	1. 04086	0. 98401	0. 94752	0. 93503	
90	1. 08007	1. 04087	0. 98405	0. 94756	0. 93507	
270	1. 08006	1. 04087	0. 98407	0. 94759	0. 93509	
∞	1. 08006	1. 04087	0. 98407	0. 94759	0. 93509	

Table VIb Relative surface wave velocities in Cu/Al superlattices on glass ($LN/LD = 1.0$)

LD	Cu:Al=1:3	Cu:Al=1:2	Cu:Al=1:1	Cu:Al=2:1	Cu:Al=3:1	
2	1.06543	1.02806	0.99504	0.98464	0.98256	**Pure Cu**
6	1.13861	1.09719	1.04014	1.00991	0.99602	0.98266
12	1.14751	1.10727	1.04948	1.01298	1.00068	
18	1.14961	1.10958	1.05166	1.01456	1.00189	Pure Al
30	1.15109	1.11114	1.05307	1.01558	1.00267	1.35045
54	1.15202	1.11207	1.05386	1.01614	1.00310	
90	1.15248	1.11252	1.05422	1.01639	1.00328	
270	1.15293	1.11296	1.05456	1.01661	1.00345	
∞	1.15316	1.11317	1.05473	1.01672	1.00353	

∞: Calculated for the virtual medium with the effective elastic constants determined by use of Grimsditch's expressions

that this wavelength λ_S is just equal to that of incident wave λ_i used in the experiment to detect surface waves.[8] The numerical calculation by use of (4.40) and (4.43) shows that we can obtain almost same results for $LS/LD \geq 3.5$. This means that if the thickness of the substrate is about more than three times the wavelength of the surface wave, it may be taken as infinite.

Here we will calculate the surface waves for Cu/Al and Cu/Ag superlattices. The used elastic constants $\overline{C_{pq}'}$, which are isotropic with respect to (x', y') plane, are given in Table V. We will take the thickness of Cu to be equal to d_1 and that of Al or Ag to d_2. The calculations are performed for both bulk superlattice and

Table VIIa Relative surface wave velocities in bulk Cu/Al superlattices ($LN/LD = 1.5$)

LD	Cu:Al=1:3	Cu:Al=1:2	Cu:Al=1:1	Cu:Al=2:1	Cu:Al=3:1	
2	1.05963	1.02250	0.98685	0.96801	0.96099	**Pure Cu**
6	1.10921	1.06751	1.00825	0.97120	0.95874	0.94169
12	1.11084	1.06982	1.01056	0.97285	0.96010	
18	1.11094	1.07011	1.01102	0.97330	0.96050	**Pure Al**
30	1.11097	1.07023	1.01127	0.97356	0.96073	1.31428
54	1.11097	1.07028	1.01137	0.97366	0.96083	
90	1.11097	1.07029	1.01139	0.97369	0.96086	
270	1.11098	1.07030	1.01140	0.97371	0.96087	
∞	1.11098	1.07030	1.01141	0.97371	0.96087	∞: Grimsditch

Table Ⅶb Relative surface wave velocities in Cu/Al superlattices on glass ($LN/LD = 1.5$)

LD	Cu:Al=1:3	Cu:Al=1:2	Cu:Al=1:1	Cu:Al=2:1	Cu:Al=3:1	
2	1.06316	1.02616	0.99305	0.98184	0.97915	Pure Cu
6	1.13119	1.09002	1.03343	1.00028	0.98989	0.97754
12	1.13910	1.09888	1.04144	1.00558	0.99371	
18	1.14094	1.10088	1.04327	1.00688	0.99469	Pure Al
30	1.14223	1.10223	1.04445	1.00771	0.99532	1.34300
54	1.14304	1.10303	1.04511	1.00816	0.99567	
90	1.14344	1.10341	1.04541	1.00836	0.99582	
270	1.14383	1.10378	1.04570	1.00855	0.99595	
∞	1.14403	1.10396	1.04583	1.00863	0.99601	∞: Grimsditch

superlattice on a substrate, as which we adopt quartz glass.

In order to investigate the width effect of superlattice, we calculate the dispersion equation (4.29) and (4.40) in the cases $LN/LD = 1.0$, 1.5 and 2.0 for Cu/Al, that is, the calculations are attempted for the superlattices of the same width as the wavelength of the surface wave λ_S, 1.5 and 2.0 times the width of the wavelength λ_S. The

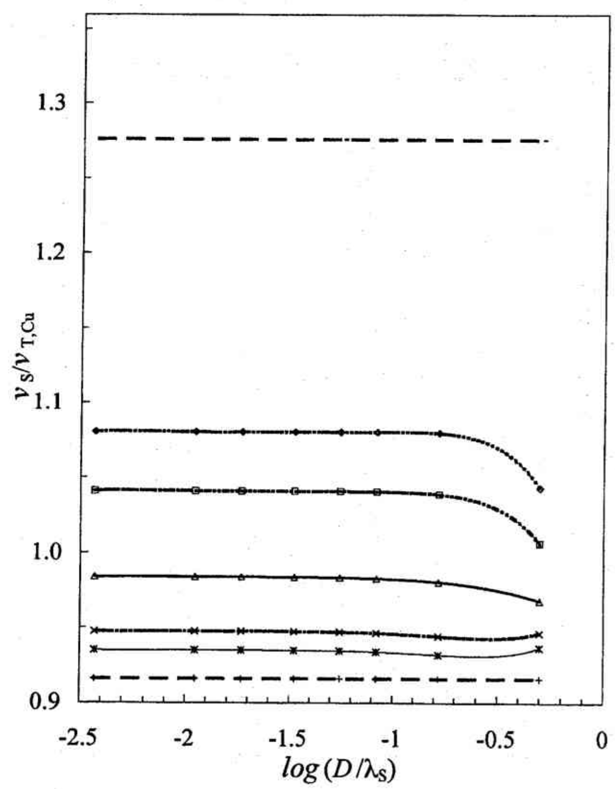

Fig. 1 Relative surface wave velocities $\nu_S/\nu_{T,Cu}$ in bulk Cu/Al superlattices of λ_S thick. The lower dashed line denotes the velocity of pure Cu ($d_2 = 0$) and the upper dashed line means the velocity of pure Al ($d_1 = 0$). Curves, successively from the top to the bottom, indicate the relative velocities in the superlattices of constitution ratio $d_1 : d_2 = 1:3, 1:2, 1:1, 2:1$ and $3:1$.

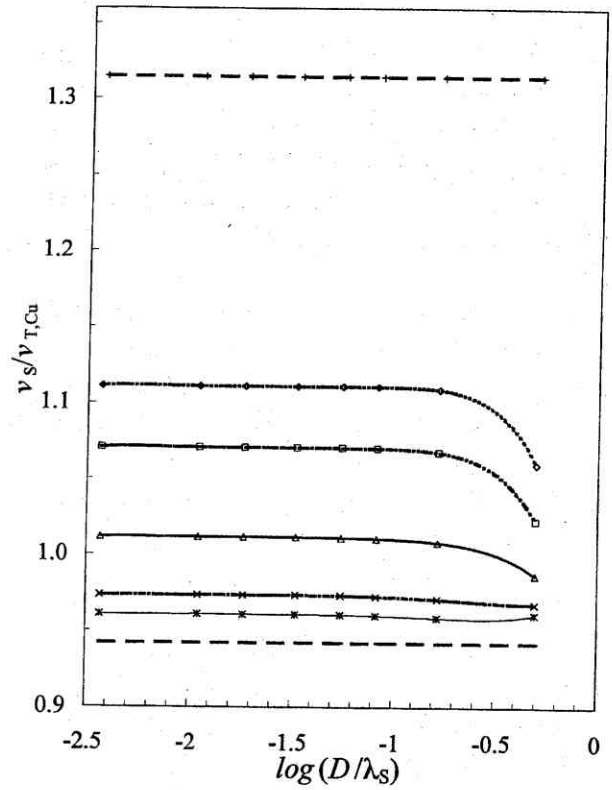

Fig. 2 Relative surface wave velocities $\nu_S/\nu_{T,Cu}$ in bulk Cu/Al superlattices of 1.5 λ_S thick. The meaning of lines and curves is the same as in Fig. 1.

results are given in Fig. 1−Fig. 6: Fig. 1−Fig. 3 are that for the bulk superlattices and Fig. 4−Fig. 6 for the superlattices on glass substrate. In each figure, the surface wave velocities ν_S relative to the velocity $\nu_{T,Cu}$, which is the velocity of the transverse wave of Cu and calculated from (5. 1), are plotted for the various periods $D = d_1+d_2$ of the superlattices with d_1/D = 1/4, 1/3, 1/2, 2/3, 3/4 together with pure Cu (d_2 = 0) and Al (d_1 = 0). We can understand the followings from these figures.

The width effect of the superlattice with respect to the wavelength λ_S becomes small as the width increases. It will be expected to be negligibly small for $LD/LD \geq 3$; actually we have confirmed this fact on the basis of the calculation for several superlattices including Cu/Al and Cu/Ag. The comparison of Figs. 1−3 with Figs. 3−6 shows that the width effect of the surface waves for bulk superlattices is much larger than the one for substrated superlattices.

For the small period D we have almost constant surface wave velocity ν_S ; the velocity change is negligible for $D/\lambda_S < 10^{-1.5} \cong 0.032$ and it is slight for $10^{-1.5} < D/\lambda_S < 10^{-1} = 0.1$. But this velocity change becomes non-negligible for large period $D(D/\lambda_S > 0.1)$. The velocity change is large for superlattices on the substrate than bulk superlattices, while the ways of the velocity change differ from each other according to the constitution ratio d_1/D of superlattice.

We summarize the surface waves for the bulk superlattice and the substrated superlattice comprised of Cu and Ag as in Figs. 7 and 8, where the width of the superlattice are taken as 1.5 times the wavelength (LN/LD = 1.5). Here we can see similar properties mentioned with respect to the period D for superlattice Cu/Al. In the present case, the velocities of the surface waves corresponding to different constituent superlattices become divergent with increasing period, while those in the case Cu/Al converge.

As described above, we can expect a constant velocity for the superlattice with the small period. This means that such superlattice has its own elastic constants. As such elastic constants, the effective elastic constants derived by Grimsditch[6] are well known. These effective elastic constants

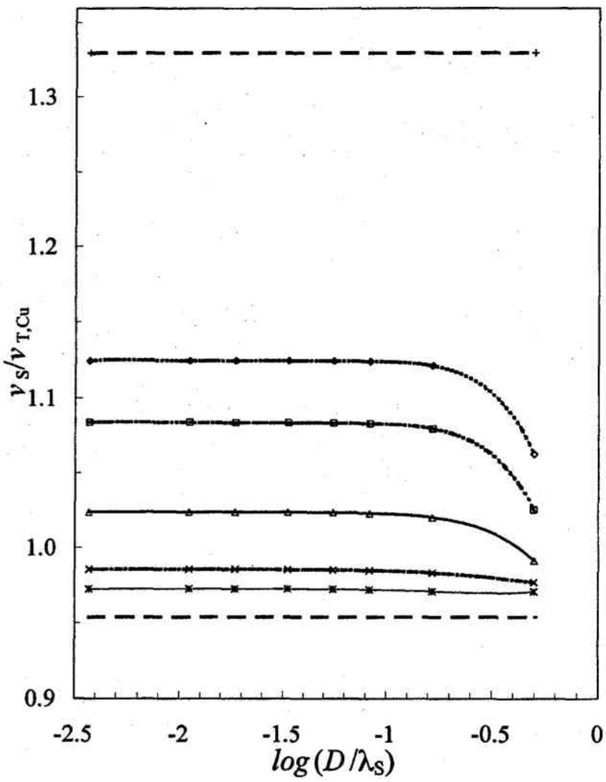

Fig. 3 Relative surface wave velocities $\nu_S/\nu_{T,Cu}$ in bulk Cu/Al superlattices of 2.0 λ_S thick. The meaning of lines and curves is the same as in Fig. 1.

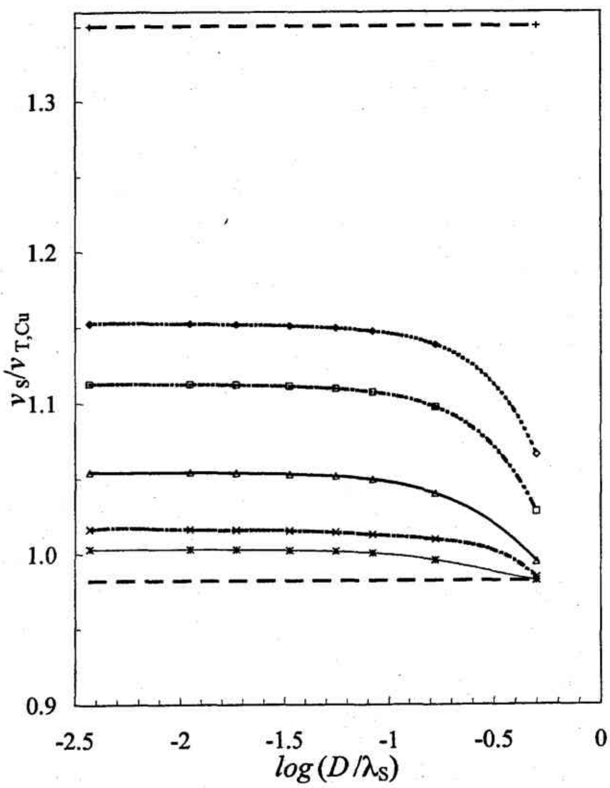

Fig. 4 Relative surface wave velocities $\nu_S/\nu_{T,Cu}$ in Cu/Al superlattices of λ_S thick, which are on glass substrate. The meaning of lines and curves is the same as in Fig. 1.

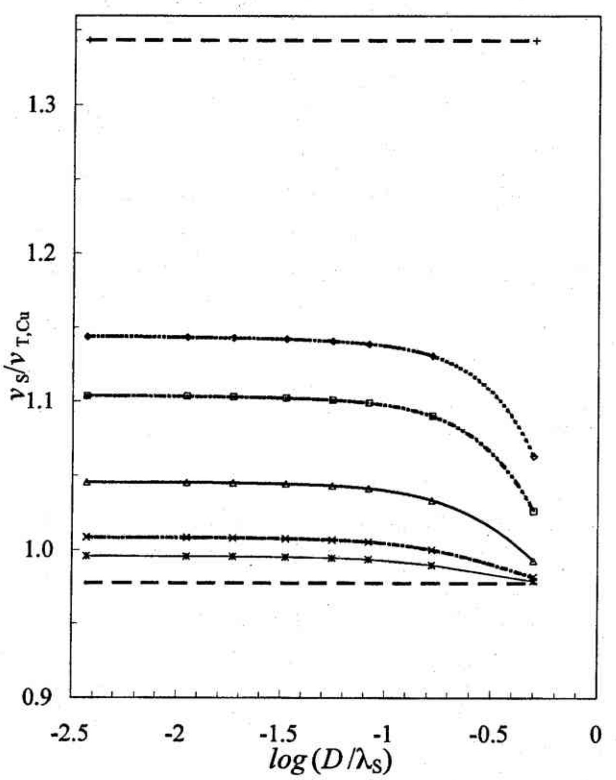

Fig. 5 Relative surface wave velocities $\nu_S/\nu_{T,Cu}$ in Cu／Al superlattices of 1.5 λ_S thick, which are on glass substrate. The meaning of lines and curves is the same as in Fig. 1.

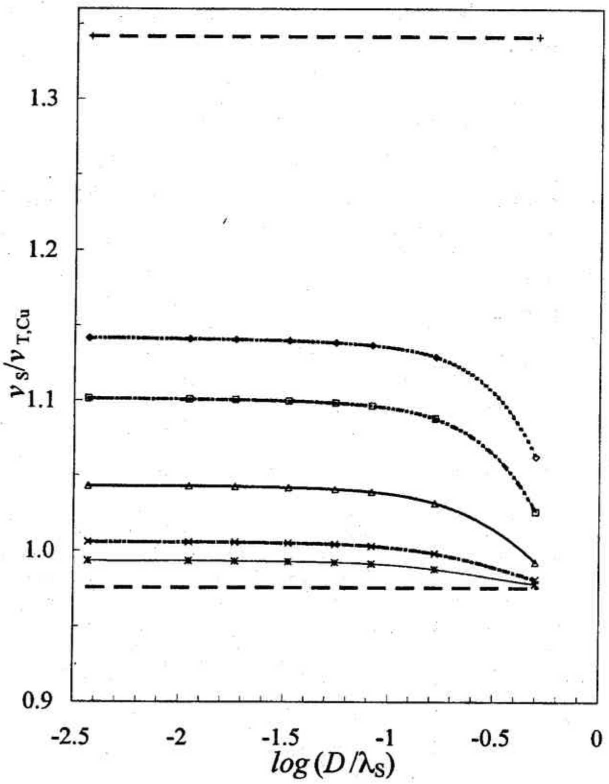

Fig. 6 Relative surface wave velocities $\nu_S/\nu_{T,Cu}$ in Cu／Al superlattices of 2.0 λ_S thick, which are on glass substrate. The meaning of lines and curves is the same as in Fig. 1.

$\overline{C_{33}'}$, $\overline{C_{44}'}$, $\overline{C_{13}'}$ and $\overline{C_{11}'}$ are given as follows in our case.

$$\frac{1}{\overline{C_{33}'}} = \frac{f_1}{C_{33}^{(1)\prime}} + \frac{f_2}{C_{33}^{(2)\prime}} \tag{5.4a}$$

$$\frac{1}{\overline{C_{44}'}} = \frac{f_1}{C_{44}^{(1)\prime}} + \frac{f_2}{C_{44}^{(2)\prime}} \tag{5.4b}$$

$$\frac{\overline{C_{13}'}}{\overline{C_{33}'}} = f_1\left(\frac{\overline{C_{13}^{(1)\prime}}}{\overline{C_{33}^{(1)\prime}}}\right) + f_2\left(\frac{\overline{C_{13}^{(2)\prime}}}{\overline{C_{33}^{(2)\prime}}}\right) \tag{5.4c}$$

$$\overline{C_{11}'} = f_1\overline{C_{11}^{(1)\prime}} + f_2\overline{C_{11}^{(2)\prime}} + f_1\left(\frac{\overline{C_{13}^{(1)\prime}}}{\overline{C_{33}^{(1)\prime}}}\right)(\overline{C_{13}'} - \overline{C_{13}^{(1)\prime}}) + f_2\left(\frac{\overline{C_{13}^{(2)\prime}}}{\overline{C_{33}^{(2)\prime}}}\right)(\overline{C_{13}'} - \overline{C_{13}^{(2)\prime}}) \tag{5.4d}$$

Here $f_1 = d_1/D$ and $f_2 = d_2/D$.

Now we suppose a bulk superlattice and a substrated superlattice with the above effective elastic constants $\overline{C_{11}'}$, $\overline{C_{33}'}$, $\overline{C_{13}'}$ and $\overline{C_{44}'}$. Here the substrated superlattice means the superlattice in contact with glass as substrate. The thickness of superlattice is considered to be $LN\cdot D$. Let us assume that the amplitudes of the displacements for elastic waves at $z' = 0$ and $-LN\cdot D$ are described by $|u_{e,LN}^{+}\rangle$ and $|u_{e,LN}^{-}\rangle$, respectively.

The amplitudes $|u_{e,LN}^{\pm}\rangle$ correspond to those obtained from replacing i and l in (4.4) by e and LN. Apparently from (4.4), these amplitudes are related by

$$|u_{e,LN}^{-}\rangle = P_e|u_{e,LN}^{+}\rangle\,, \tag{5.5}$$

where P_e is the matrix just obtained from the replacement of i by e in (4.5). Then the coefficient f_{ej} is expressed as

$$f_{ej} = \exp(-iq_x Q_{ej} \cdot LN \cdot D) \tag{5.6}$$

The variable Q_{ej} ($j = 1$ or 2) is calculated from (3.12) by use of the effective elastic constants as those in (3.11). Then the discussions and derivations in Section 4 hold for the present imaginary medium with the effective elastic constants given by (5.4). For instance, we can easily derive the dispersion equation of the surface wave for the bulk imaginary medium:

$$\det \begin{pmatrix} A_e U \\ A_e U P_e \end{pmatrix} = 0 \tag{5.7}$$

Table VIIIa Relative surface wave velocities in bulk Cu/Ag superlattices ($LN/LD = 1.5$)

LD	Cu:Ag=1:2	Cu:Ag=1:1	Cu:Ag=2:1	
2	0.75213	0.79633	0.84282	Pure Cu 0.94169
4	0.75080	0.79115	0.83509	
6	0.74971	0.78932	0.83334	
12	0.74890	0.78859	0.83306	
18	0.74876	0.78856	0.83316	Pure Ag 0.67996
30	0.74869	0.78857	0.83323	
54	0.74866	0.78858	0.83327	
90	0.74866	0.78858	0.83328	
136	0.74865	0.78858	0.83328	
270	0.74865	0.78858	0.83329	
∞	0.74865	0.78858	0.83329	∞: Grimsditch

Table VIIIb Relative surface wave velocities in Cu/Ag superlattices on glass ($LN/LD = 1.5$)

LD	Cu:Ag=1:2	Cu:Ag=1:1	Cu:Ag=2:1	
2	0.79533	0.84235	0.88837	Pure Cu 0.97753
4	0.78862	0.83084	0.87597	
6	0.78676	0.82818	0.87309	
12	0.78421	0.82543	0.87059	
18	0.78315	0.82434	0.86968	Pure Ag 0.70942
30	0.78224	0.82340	0.86889	
54	0.78163	0.82275	0.86833	
90	0.78132	0.82242	0.86804	
136	0.78116	0.82225	0.86790	
270	0.78101	0.82208	0.86775	
∞	0.78086	0.82192	0.86761	∞: Grimsditch

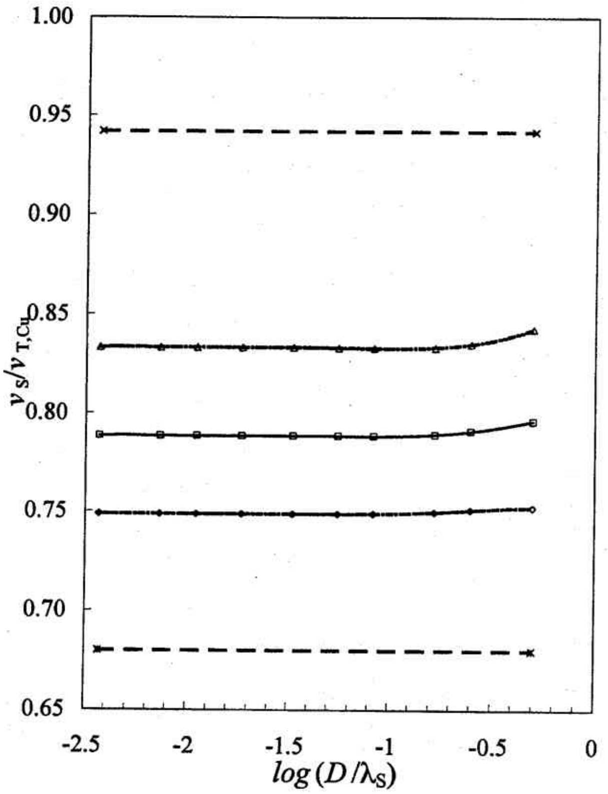

Fig. 7 Relative surface wave velocities $\nu_S/\nu_{T,Cu}$ in bulk Cu／Ag superlattices of 1.5 λ_S thick. The upper dashed line means the velocity of pure Cu metal ($d_2 = 0$) and the lower dashed is the one of pure Ag metal ($d_1 = 0$). Dotted, solid and dash-dotted curves show the velocities in the superlattices of constitution ratio $d_1 : d_2 = 2:1$, $1:1$, and $1:2$.

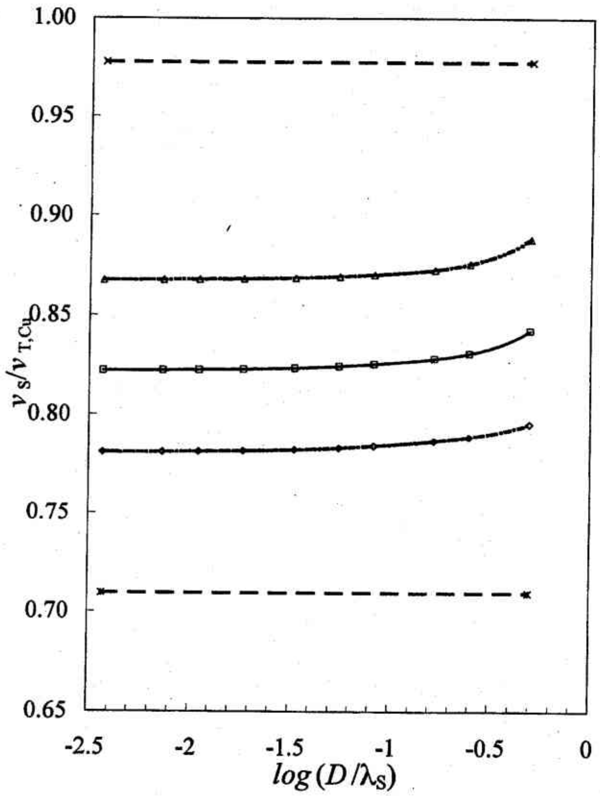

Fig. 8 Relative surface wave velocities $\nu_S/\nu_{T,Cu}$ in Cu／Ag superlattices of 1.5 λ_S thick, which are on glass substrate. The meaning of lines and curves is the same as in Fig. 7.

Here A_e is the matrix obtained from replacing j by e in (4. 26), where the matrix defined by (4. 15) appears and have to be calculated for the effective elastic constants. Thus we can calculate the velocity of the surface wave for the medium with the effective elastic constants according to the hitherto outlined way.

We will tabulate in Tables Ⅵ－Ⅷ the velocities ν_S of the surface waves derived from the calculation for the above imaginary media with effective elastic constants together with those already calculated for the superlattices. The latter data are the accurate numerical values corresponding to the plots in Figs. 1－8, except Figs 3 and 6. In these Tables, LD means the number of the period D contained in the superlattice of λ_S thick; LD layers consisting of Cu／Al or Cu／Ag exist in the sample of λ_S thick. The larger value of LD denotes the smaller period D ; $D = \lambda_S/LD$. As already described, the surface wave velocities ν_S in these Tables are taken relative to the standard velocity $\nu_{T,Cu}$, which is the velocity of the transverse wave in pure Cu metal.

The data in Tables Ⅵa and Ⅶa represent the relative velocities $\nu_S/\nu_{T,Cu}$ of the bulk superlattices and the bulk media with the effective elastic constants in the cases $LN/LD = 1.0$ and 1.5, where the ratios Cu : Al $(= d_1 : d_2)$ represent the ratios the thickness of Cu and Al constituents in one layer in the media. Similarly those in Tables Ⅵb and Ⅶb are the relative velocities for the same superlattices and imaginary media in contact with glass. In Tables Ⅷa and Ⅷb are given the results for the superlattices which are made up by the periodical superposition of Cu and Ag and the corresponding imaginary media with the effective elastic constants in the case $LN/LD = 1.5$. Here the meanings of a, b and Cu : Ag $(= d_1 : d_2)$ are the same as in Tables Ⅵ and Ⅶ.

It is apparent from these Tables our prediction of the existence of the effective elastic constants for the superlattices with the small period exceeds our expectation. The detailed investigations elucidate the followings.

The results calculated by use of the effective elastic constants derived from the expressions by Grimsditch are just those of the periodically layered structures in the limit of the zero period ($D \rightarrow 0$ or $LD \rightarrow \infty$). This is reasonable because Grimsditch has derived his expressions in such a limit.[6] The bulk superlattices with period below $\lambda_S/270$ are completely regarded as the media with the zero period. In bulk superlattices the treatment of them as the imaginary media with the effective elastic constants is valid in sufficient accuracy up to the period $D = \lambda_S/12$. However such a model fails, strictly speaking, even for the smallest calculated period $\lambda_S/270$ in the substrated superlattices or the superlattices directly contacting with glass. From these Tables we can confirm that the calculated values approach those obtained from the model as the period D becomes smaller. We must appreciate, of course, that, to a fairly good approximation even in this case, the present model can reproduce the calculated results derived from the exact treatment of the periodically layered structures, which needs really complicated calculations with respect to hundreds of matrices, while we only deal with few matrices in the model.

In conclusion, the model based on the Grimsditch's expression for the effective elastic constants gives a good approximate result for the surface wave of superlattice except that with a large period. The greatest merit of the calculation by use of the effective elastic constants is that it is much easier than the exact calculation. Grimsditch has derived his effective elastic constants which is valid only for excitation wavelengths longer than the modulation wavelengths.[6] However its applicable region has not been clear. In our paper a criterion for that has been presented.

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16) The essential notations developed here correspond to the extension of those given in §7. 1 of Reference 11.
17) The terms "forward wave and backward wave" have only relative meaning. According to the definition in §3, the present backward wave is rather forward wave. However, we now deal with the damping wave propagating toward -z' direction. So we prefer the present usage here.

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