Brief Reports

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Surface waves in a layered material

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Results of a numerical calculation of the velocities of surface waves in layered isotropic materials are presented. They do not explain the behavior of previous experimental results on Nb-Cu heterostructures. Mode crossings are found in certain cases between the Rayleigh wave and higher-order surface modes.

I. INTRODUCTION

In a recent publication[1] it was shown that a plot of Rayleigh wave velocity as a function of layer thickness in Nb-Cu heterostructures shows a distinct dip. The dip occurs in a region where the layer thickness d is much smaller than the wavelength λ of the phonons being probed and hence is unexpected. When treating the problem of long wavelength elastic waves in layered media ($d \ll \lambda$), one expects to be able to use an effective-modulus picture, in which the medium is treated as a homogeneous solid whose elastic properties are derived from those of the constituent media. In this limit, the elastic moduli are found to be independent of layer thickness.[2] It is to the validity of the effective-modulus model that we address ourselves here. We have calculated surface wave velocities in systems of up to 1000 layers and found that the effective-modulus model is indeed a good approximation in the region of $d \ll \lambda$. Furthermore, we have also solved for the velocity of higher-order surface waves (Sezawa waves) and found interesting mode-crossing behavior in certain cases. This behavior does not, however, explain the results of Ref. 1

II. BACKGROUND AND OUTLINE OF CALCULATION

Rayleigh waves in an isotropic medium propagate with a velocity v which can be calculated analytically from the implicit equation due to Stoneley[3]:

$$\left[2-\left(\frac{v}{v_t}\right)^2\right]^2 = 4\left[1-\left(\frac{v}{v_l}\right)^2\right]^{1/2}\left[1-\left(\frac{v}{v_t}\right)^2\right]^{1/2} , \quad (1)$$

or it can be approximated by the explicit equation[4]

$$v = v_t(0.87c_{11}+2c_{12})/(c_{11}+2c_{12}) , \quad (2)$$

where v_t and v_l are the velocities of the transverse and longitudinal bulk waves and c_{ij} are the elastic stiffness constants. When the medium is not isotropic there is no analytic expression for the velocity of the Rayleigh wave; instead it must be calculated numerically.[5]

The problem of calculating the speed of a Rayleigh wave propagating on the surface of a system of alternating layers with different elastic properties has applications to seismology, and much of the literature on the problem is in that field. The simplest treatment involves replacing the layered medium by a homogeneous one with elastic moduli given by an appropriate average of those of the constituent layers. This would seem a reasonable approximation to make in the case where the acoustic wavelength is long compared to the layer thickness.

The effective bulk elastic moduli for a thinly laminated medium have previoulsy been calculated,[2] and a comparison of the calculated surface wave velocity in such a system with that calculated for a six-layer system is given in Ref. 6. A comparison is also made in Ref. 7 in what appear to be relatively thick layers in the limit of an infinite number of layers—good agreement is claimed.

It is well known that for a single layer on a substrate in addition to the ordinary Rayleigh wave, higher-order (Sezawa) modes exist under certain conditions.[8] The number of these modes increases with the layer thickness. In our calculation we have also obtained the velocity of a few of these higher modes

TABLE I. Elastic moduli (10^{11} dyn/cm^2) and densities (g/cm^3) of copper and niobium compared with those chosen for media I and II.

	c_{11}	c_{12}	c_{44}	ρ
Nb	24.6	13.4	2.87	8.57
Medium I	23.69	14.31	4.69	8.57
Cu	16.9	12.2	7.53	8.92
Medium II	18.63	10.47	4.08	8.92

in systems of varying numbers of layers.

Our calculations were done for a system of n layers of two alternating isotropic solids (the complications arising from a generalization to nonisotropic media are considerable) on a substrate of the material with the larger transverse bulk wave velocity. This latter choice has as its object the separation of the modes originating in the layers from the continuum of modes that exist in the substrate with velocities greater than that of the bulk transverse wave.

The formulation of the problem is the same as that used in Refs. 6 and 7, i.e., a general solution for a wave propagating with a velocity v parallel to the free surface is written for each layer, the boundary conditions at each interface (viz., continuity of the displacement and equality of the appropriate stress tensor elements) and at the free surface are imposed, and the condition of a nondivergent solution in the substrate is demanded. This leads to $4(n+1)$ equations with $4(n+1)$ variables which only have a nontrivial solution for certain values of v. These values of v are the velocities of the Rayleigh wave and higher-order surface waves. Once the velocity has been determined, the system of equations can be solved to yield the amplitude of the wave as a function of distance from the surface.

Because in the Nb-Cu system which we wish to investigate neither Nb nor Cu is isotropic, we were obliged to invent fictitious isotropic materials in order to approximate them. Hence we chose c_{11} and c_{12} for each material so as to minimize

$$F=(c_{11}-c_{11}^*)^2+(c_{12}-c_{12}^*)^2+\left[\frac{c_{11}-c_{12}}{2}-c_{44}^*\right]^2 ,$$

where c_{ij}^* are the moduli of Cu or Nb. The stiffness constants and densities of the two media are given in Table I.

III. RESULTS

Our calculations were carried out on systems of 1, 2, 5, 6, 10, 11, 20, 21, 50, 51, 101, 150, 151, and 1000 layers. The calculations yield the velocity of the surface waves as a function of the dimensionless quantity kd where k is the magnitude of the phonon wave vector and d is the thickness of one layer. In order to compare with the results of Ref. 1 we have chosen a typical wave vector encountered in Brillouin scattering experiments ($k=1.79\times10^{-3}$ Å^{-1}) and evaluated the scale $\Lambda=2d=(2kd/1.79\times10^{-3})$, which is also shown in the figures.

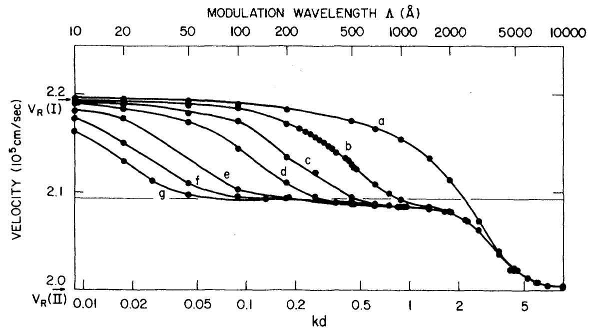

FIG. 1. Velocity of the lowest-order surface wave *vs* kd in laminated systems of odd numbers of layers on a substrate. Curves are: a-1 layer, b-5 layers, c-11 layers, d-21 layers, e-51 layers, f-101 layers, and g-151 layers.

Figures 1 and 2 show the variation of surface wave velocity as a function of kd for the systems listed above. The arrows on the vertical axes show the Rayleigh wave velocities in homogeneous half spaces of media I and II. The results have been separated into two figures because, since the substrate is always medium I, the top layer will be either medium I or II depending on whether the number of layers is even or odd. As expected, the following behavior is evident in Figs. 1 and 2: if $nkd \ll 1$, the velocity of the surface wave is determined almost entirely by the substrate. Conversely, if $kd \gg 1$, the velocity is essentially that in the top layer. In the intermediate

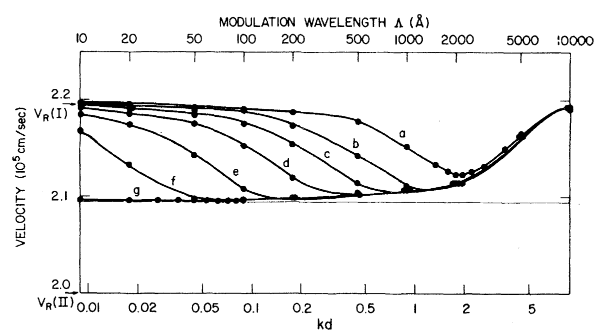

FIG. 2. Velocity of the lowest-order surface wave *vs* kd in laminated systems of even numbers of layers on a substrate. Curves are: a-2 layers, b-6 layers, c-10 layers, d-20 layers, e-50 layers, f-150 layers, and g-1000 layers.

region, however, where $kd < 1$ but $nkd > 1$, we see that a relatively flat region exists. It is in this region that we expect the effective-modulus theory to be applicable. The straight lines plotted in Figs. 1 and 2 are the results of such a calculation. Using the c_{ij} of the isotropic solids in Table I we computed those of the homogeneous solid as per Ref. 2. They are the elastic moduli of a hexagonal crystal. We then calculated the velocity of the surface wave in the basal plane of such a medium. It can be seen that in the flat portions of Figs. 1 and 2 the agreement is good. In particular, for 1000 layers and small kd values the agreement is excellent. Additionally, we note that there is no sign of any anomaly in the velocity of the surface wave at small kd values.

Figure 3 shows the velocity of a Rayleigh wave in a composite film on a substrate of medium I as a function of the thickness of the layers constituting the film. The film thickness is Δ, where $k\Delta = 8.95$, and it is made up of n layers so that $nd = \Delta$. The surface wave velocity is plotted as a function of d. When the layers are thick one sees the effect of the top layer quite clearly, but as they become thin the velocities converge to a value quite near to that of a surface wave in the effective-modulus solid. The velocity is not *equal* to that in the latter because of the finite thickness of the film.

From Figs. 1–3 we conclude that for our system, if $kd < 1$, the effective-modulus approximation yields results accurate to better than 1%. Our program does not allow us to calculate surface modes for a hexagonal homogeneous solid (obtained from the effective-modulus picture) on an isotropic substrate. However, replacing the hexagonal homogeneous solid by a similar isotropic one, we do obtain results that are in fair agreement with the modes obtained in a multilayered system provided $kd \ll 1$.

Some interesting properties of high-order modes in multilayer systems arise at large values of kd. These are most easily exemplified in the case of a two-layer system in which a softer material is sandwiched between the substrate and an outer layer. Figure 4 shows the velocity of the first few surface waves in such a system where the mode repulsion of the first two modes is clearly visible. We have calculated the amplitude profiles of these waves at various points along the dispersion curve. The amplitudes of the lowest mode in our two-layer system are shown in Fig. 5 and those of the next mode in Fig. 6. We see that the amplitudes of the lower mode resemble those of a Rayleigh wave even in the region where the velocity is depressed by the effect of the intermediate layer, but that as the velocity begins to rise again, the wave begins to become more localized in the second layer. In this region, the velocity of the second mode decreases with increasing kd, and when $kd \approx 10$, the modes are nearly degenerate. Here neither mode is a true Rayleigh wave. Beyond that point it is the higher mode which has the characteristic velocity of a Rayleigh wave in the outermost medium, and a look at the amplitude profiles shows that at this point the top mode has indeed become transformed into a true Rayleigh wave. The lower mode, on the other hand, is almost entirely confined to the second layer. For $kd > 15$ the velocity of the Rayleigh-type wave remains constant. Even at $kd \cong 23$, where the next higher mode crosses it, there is no sign of a mode repulsion within the accuracy of our calculations.

In conclusion, we have presented the results of numerical calculations of the velocities of Rayleigh waves in a layered system modeling Nb-Cu hetero-

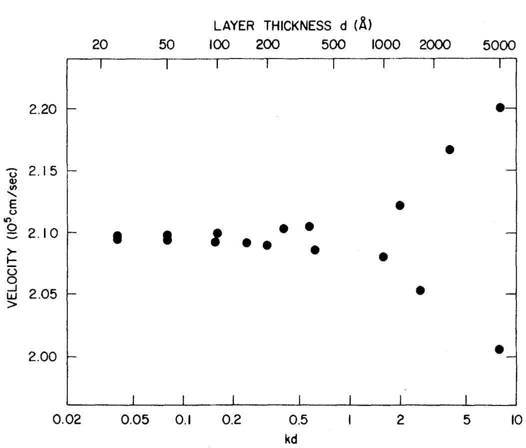

FIG. 3. Velocities of the lowest-order surface wave in a multilayered film of fixed thickness vs thickness of the constituent layers.

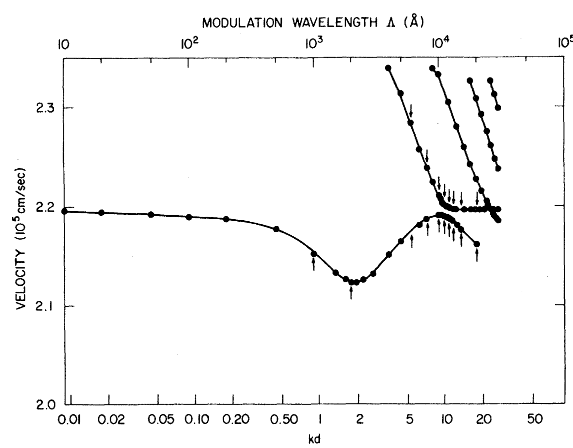

FIG. 4. Velocities of the five lowest surface waves vs *kd* in a two-layer system.

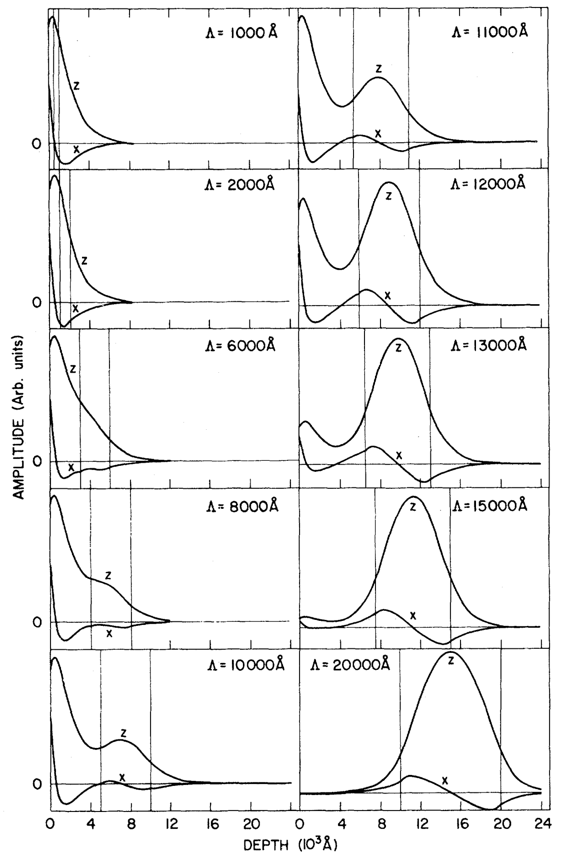

FIG. 5. Transverse ($\hat{z}$) and longitudinal ($\hat{x}$) amplitudes of lowest-order surface waves in a two-layer system vs depth at selected values of kd (arrows, Fig. 4).

structures. We have compared these velocities with those in an effective-modulus model and found the agreement to be good where $kd \ll 1$. We found no evidence that the anomalous surface wave velocity reported earlier can be explained within a purely classical elasticity theory. In addition, we have presented some interesting features of surface waves in a simple layered system.

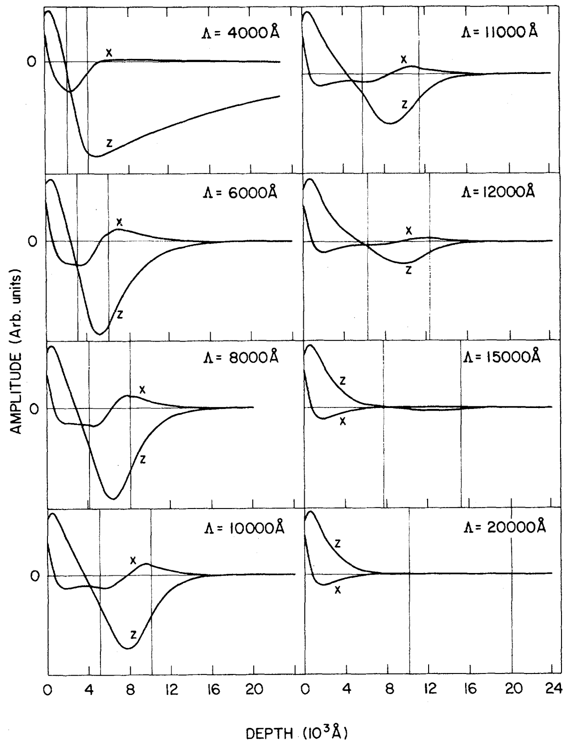

FIG. 6. Transverse ($\hat{z}$) and longitudinal ($\hat{x}$) amplitudes of second-order surface waves vs depth in a two-layer system at selected values of kd (arrows, Figs. 4).

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