

Interaction of Rayleigh waves with randomly distributed oscillators on the surface

E. A. Garova*

Institute of Radioengineering and Electronics, Russian Academy of Sciences, Fryazino, Moscow Region 141120, Russia

A. A. Maradudin

Department of Physics and Institute of Surface and Interface Science, University of California, Irvine, California 92697

A. P. Mayer[†]

Max-Planck-Institut für Physik komplexer Systeme, 01187 Dresden, Germany

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The attenuation of Rayleigh waves due to their interaction with resonating structures randomly distributed on the surface of a semi-infinite elastic medium is calculated along with the Rayleigh wave frequency. The resonating structures are modeled by single oscillators coupled to the displacement field at the surface of the elastic medium. Using the coherent potential approximation, the dependence of the frequency and damping constant of the Rayleigh waves on wave vectors are determined for various values of the concentration of oscillators on the surface. [S0163-1829(99)01719-1]

I. INTRODUCTION

Surface acoustic waves are known to be a versatile probe for various effects and physical properties at crystal surfaces. Their sensitivity to surface modifications along with the high accuracy, to which their frequencies can be measured in the ultrasonic regime, makes them attractive as a tool in surface science and as sensors in technical applications. For a theoretical description of the influence of surface modifications on Rayleigh waves,¹ simple perturbation theory is often sufficient. However, certain surface structures like protuberances, adsorbed crystallites, etc., may give rise to resonances in the interaction with a surface wave that are not accessible to low-order perturbation theory. The resonant interaction of surface acoustic waves with single resonating structures has been investigated in detail,²⁻⁹ partly with the aim of achieving high reflectivities in surface acoustic wave devices⁹ and in view of efficient protection against noise caused by railways in the macroscopic world. Here, concrete blocks are used as resonating surface structures.¹⁰

Internal oscillations of microscopic surface structures and their coupling to acoustic modes of the substrate have also been a focus of recent experimental work. The vibrational modes of periodic gold nanostructures on fused quartz substrates have been investigated by a picosecond ultrasonics technique and theoretically by the finite element method.¹¹ The percolation transition of gold islands on NaCl has been monitored via a Brillouin light-scattering analysis of the surface acoustic modes of this system.¹²

Recently, surface acoustic waves have been used to study the structural behavior of hydrogen films deposited on a surface of a LiNbO₃ crystal as a response to thermal treatment.¹³⁻¹⁵ Above a critical temperature, the homogeneous hydrogen film undergoes a transition to a state, where crystallites are formed spontaneously on the surface having their own vibrational resonances. These crystallites are distributed randomly on the surface. The transition has been

monitored by measuring the frequency and the attenuation of surface acoustic waves.

The goal of this paper is to study theoretically the effect of randomly distributed resonators on the frequency and the attenuation of Rayleigh waves. The resonators are modeled by masses and springs coupled to the displacement field at the surface and exerting a stress on the surface. Allowing the oscillators to randomly occupy the positions of a regular grid on the surface, one may use the well-established theory of the lattice vibrations in crystals with defects to calculate the self-energy of the surface modes. From this quantity, the frequency and attenuation constant of the surface waves is calculated as function of their wave number as well as the dependence of these quantities on the coupling strength between the oscillators and the substrate and on the concentration of oscillators on the grid.

II. GENERAL THEORY

A semi-infinite elastic medium is considered filling the half-space $z < 0$. For simplicity, this medium is assumed to be isotropic, which, however, is no restriction for the validity of the following general theory. On the surface of this medium ($z = 0$), we introduce a two-dimensional grid with gridpoints $\mathbf{Y}_{m,n} = (md, nd)$. On each of these gridpoints, a harmonic oscillator may be situated with probability p (Fig. 1). The oscillator degree of freedom $X_{m,n}$ obeys the equation of motion

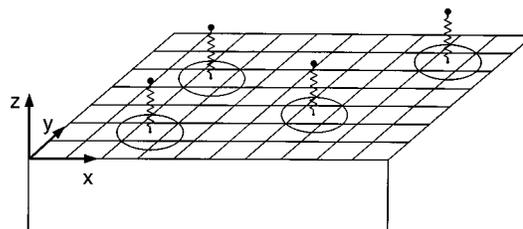


FIG. 1. Geometry of the system under consideration.

$$M(\ddot{X}_{m,n} + \gamma \dot{X}_{m,n}) + \kappa[X_{m,n} - u_3(\mathbf{Y}_{m,n}, 0)] = 0, \quad (2.1)$$

where $u_\alpha(\mathbf{R}, z)$ is the α component of the displacement field and $\mathbf{R} = (x, y)$. When taking these oscillators as a simple model for crystallites with their vibrational resonances, the damping constant γ represents dissipation inside the crystallites. The oscillators exert the stress

$$T_{33}^{(os)}(\mathbf{R}, 0) = \sum_{m,n} c_{m,n} S(\mathbf{R} - \mathbf{Y}_{m,n}) \kappa[X_{m,n} - u_3(\mathbf{Y}_{m,n}, 0)] \quad (2.2)$$

on the surface. Here we have introduced the random variable $c_{m,n}$, which is equal to 1 with probability p and equal to 0 with probability $1-p$. The function $S(\mathbf{R})$ characterizes the stress distribution on the surface generated by a single oscillator. Energy conservation in the case $\gamma=0$ requires

$$\int d^2R S(\mathbf{R}) = 1. \quad (2.3)$$

The equation of motion for the displacement field reads

$$\rho \ddot{u}_\alpha = \sum_\beta \frac{\partial}{\partial x_\beta} T_{\alpha\beta} \quad (2.4)$$

with the mass density ρ and the constitutive equation

$$T_{\alpha\beta} = \sum_{\mu,\nu} C_{\alpha\beta\mu\nu} \frac{\partial}{\partial x_\mu} u_\nu. \quad (2.5)$$

For the isotropic material under consideration, the elastic moduli $C_{\alpha\beta\mu\nu}$ can be expressed by two Lamé constants λ and μ via

$$C_{\alpha\beta\mu\nu} = \lambda \delta_{\alpha\beta} \delta_{\mu\nu} + \mu (\delta_{\alpha\mu} \delta_{\beta\nu} + \delta_{\alpha\nu} \delta_{\beta\mu}). \quad (2.6)$$

Equation (2.2) has to be regarded as a boundary condition for the displacement field at the surface.

When applying an external surface stress of the form

$$T_{\alpha 3}^{(ex)}(\mathbf{R}, 0; t) = I_\alpha(\mathbf{k}, \omega) e^{i(\mathbf{k} \cdot \mathbf{R} - \omega t)}, \quad (2.7)$$

oscillating with a fixed frequency ω , the displacement field responding to this surface stress can be represented as

$$u_\alpha(\mathbf{R}, z; t) = (2\pi)^{-2} \int d^2q W_\alpha(z|\mathbf{q}) e^{i(\mathbf{q} \cdot \mathbf{R} - \omega t)}. \quad (2.8)$$

To satisfy the equations of motion in the isotropic substrate, the functions W_β , $\beta=1,2,3$, describing the depth dependence of the displacement field have to be of the form

$$\begin{aligned} \begin{pmatrix} W_1(z|\mathbf{q}) \\ W_2(z|\mathbf{q}) \\ W_3(z|\mathbf{q}) \end{pmatrix} &= \frac{1}{q} \begin{pmatrix} q_1 \\ q_2 \\ -i\alpha_L(q, \omega) \end{pmatrix} e^{\alpha_L(q, \omega)z} A_L(\mathbf{q}, \omega) \\ &+ \frac{1}{q} \begin{pmatrix} q_1 \\ q_2 \\ -i\frac{q_2^2 + q_1^2}{\alpha_T(q, \omega)} \end{pmatrix} e^{\alpha_T(q, \omega)z} A_{T1}(\mathbf{q}, \omega) \\ &+ \frac{1}{q} \begin{pmatrix} -q_2 \\ q_1 \\ 0 \end{pmatrix} e^{\alpha_T(q, \omega)z} A_{T2}(\mathbf{q}, \omega), \end{aligned} \quad (2.9)$$

where

$$\alpha_{L,T}(q, \omega) = \left[q_2^2 + q_1^2 - \left(\frac{\omega}{v_{L,T}} \right)^2 \right]^{1/2} \quad (2.10)$$

and v_L and v_T are the velocities of longitudinal and transverse bulk sound waves in the isotropic medium. The roots in Eq. (2.10) are the ones with positive real part or, if the expression in the square brackets is negative, the ones with negative imaginary part to satisfy the boundary conditions of exponential decay or the Sommerfeld radiation conditions at $z \rightarrow -\infty$.

Inserting Eq. (2.8) with Eq. (2.9) into the boundary conditions

$$T_{\alpha 3}(\mathbf{R}, 0) = T_{\alpha 3}^{(os)}(\mathbf{R}, 0) + T_{\alpha 3}^{(ex)}(\mathbf{R}, 0) \quad (2.11)$$

and choosing $I_1 = I_2 = 0$, $I_3(\mathbf{q}, \omega) \equiv I(\mathbf{q}, \omega)$, we obtain the following equations for the amplitudes A_L , A_{T1} , and A_{T2} :

$$A_{T1}(\mathbf{q}, \omega) = -\frac{2\alpha_L(q, \omega)\alpha_T(q, \omega)}{\alpha_T^2(q, \omega) + q^2} A_L(\mathbf{q}, \omega), \quad (2.12a)$$

$$A_{T2}(\mathbf{q}, \omega) = 0, \quad (2.12b)$$

$$\begin{aligned} A_L(\mathbf{q}, \omega) &= R_0(q, \omega) I(\mathbf{q}, \omega) \\ &+ R_0(q, \omega) \int d^2q' V(\mathbf{q}, \mathbf{q}', \omega) A_L(\mathbf{q}', \omega). \end{aligned} \quad (2.12c)$$

In writing Eq. (2.12c) we have introduced the bare Green function

$$R_0(q, \omega) = \frac{q[\alpha_T(q, \omega)^2 + q^2]}{4q^2\alpha_T(q, \omega)\alpha_L(q, \omega) - [\alpha_T(q, \omega)^2 + q^2]^2}, \quad (2.13)$$

which, for given wave number q , has a pole at the frequency $\omega = v_R q$, where v_R is the Rayleigh wave velocity of the substrate. We have also introduced an interaction potential

$$V(\mathbf{q}, \mathbf{q}', \omega) = a(\mathbf{q}, \omega) b(q', \omega) \sum_{m,n} c_{m,n} e^{i(\mathbf{q}' - \mathbf{q}) \cdot \mathbf{Y}_{m,n}}, \quad (2.14)$$

where

$$a(\mathbf{q}, \omega) = \frac{\kappa}{\mu} \frac{\omega^2 + i\gamma\omega}{\omega_0^2 - \omega^2 - i\gamma\omega} \int d^2R e^{i\mathbf{q}\cdot\mathbf{R}} S(\mathbf{R}), \quad (2.15)$$

$$b(q, \omega) = \frac{1}{4\pi^2} \frac{\alpha_L(q, \omega)[q^2 - \alpha_T^2(q, \omega)]}{q[\alpha_T(q, \omega)^2 + q^2]}. \quad (2.16)$$

Introducing now the Green function $R(\mathbf{q}, \mathbf{q}', \omega)$ of the disordered system via

$$A_L(\mathbf{q}, \omega) = \int d^2q' R(\mathbf{q}, \mathbf{q}', \omega) I(\mathbf{q}', \omega), \quad (2.17)$$

one may obtain from Eq. (2.12c) the Dyson equation

$$\begin{aligned} R(\mathbf{q}, \mathbf{q}', \omega) &= R_0(q, \omega) \delta(\mathbf{q} - \mathbf{q}') \\ &+ R_0(q, \omega) \int d^2q'' V(\mathbf{q}, \mathbf{q}'', \omega) R(\mathbf{q}'', \mathbf{q}', \omega). \end{aligned} \quad (2.18)$$

In this way, the problem of determining the response of the displacement field to an external stress is transformed into a standard multiple-scattering problem. We finally introduce the ensemble-averaged Green function

$$\langle R(\mathbf{q}, \mathbf{q}', \omega) \rangle = G(q, \omega) \delta(\mathbf{q} - \mathbf{q}'). \quad (2.19)$$

In letting G depend on the modulus of the wave vector only, we have assumed that the function S is sufficiently symmetric that isotropy in the x - y plane is restored after averaging over the ensemble of oscillator configurations on the surface. This means in particular that $a(\mathbf{q}, \omega) = a(q, \omega)$. For the Green function G , we write the Dyson equation

$$G(q, \omega) = R_0(q, \omega) + R_0(q, \omega) \Sigma(q, \omega) G(q, \omega) \quad (2.20)$$

involving the self-energy Σ . It is the determination of Σ that we are addressing in Sec. III.

III. FREQUENCY SHIFT AND ATTENUATION OF RAYLEIGH WAVES

In determining the self-energy, we apply standard approximations used in the theory of phonons in crystals with lattice defects.^{16,17} For convenience, we define

$$\Sigma(q, \omega) = a(q, \omega) b(q, \omega) \left(\frac{2\pi}{d} \right)^2 w(q, \omega). \quad (3.1)$$

In a concentration expansion, i.e., an expansion with respect to p , the first-order term is found to be

$$w^{(1)}(\omega) = \frac{p}{1 - K_0(\omega)}, \quad (3.2)$$

where

$$K_0(\omega) = 2\pi \int_0^\infty dq q a(q, \omega) b(q, \omega) R_0(q, \omega). \quad (3.3)$$

In this approximation, the self-energy is proportional to the average density p/d^2 of the oscillators on the surface.

An approach that goes beyond the first-order theory and may be applied to higher values of p is the coherent-potential

approximation (CPA). It is known to reproduce correctly the first-order results in p and $1-p$ (Ref. 17), and it is widely used as an interpolation scheme between low-concentration and high-concentration limits. Within this approximation, the function w is calculated from the implicit equation

$$w(\omega) = \frac{p}{1 - K(\omega)[1 - w(\omega)]} \quad (3.4)$$

with

$$K(\omega) = 2\pi \int_0^\infty dq q a(q, \omega) b(q, \omega) G(q, \omega). \quad (3.5)$$

From Eqs. (3.4) and (3.5) together with Eqs. (2.20) and (3.1), the self-energy may be calculated. Note that as in Eqs. (3.2) and (3.4), w is a function of the frequency ω only.

IV. NUMERICAL RESULTS

Surface localized modes of the system under consideration that can be excited by an external surface stress component $T_{33}^{(\text{ex})}$ manifest themselves as (complex) poles $\omega_p = \Omega(q) - i\Gamma(q)$ of the Green function $G(q, \omega)$ for given real q . The real part Ω as a function of q gives the dispersion relation for the surface modes of the system, while $\Gamma(q)$ may be identified with the damping constant of a mode with wave number q . The complex poles have been determined numerically. For the function S , a Gaussian has been chosen: $S(\mathbf{R}) \propto \exp[-0.5(R/a)^2]$. The integral occurring in the CPA iteration procedure [right-hand side of Eq. (3.5)] has been carried out numerically on appropriate contours in the complex plane slightly off the real axis.

In the following, we use $\omega_0 = \sqrt{\kappa/M}$ as frequency unit and $q_0 = \omega_0/v_R$ as wave-vector unit, where v_R is the velocity of Rayleigh waves of the substrate. The reduced frequencies Ω/ω_0 and reduced damping constants Γ/ω_0 depend on the following dimensionless system parameters: The Poisson ratio σ of the substrate, the ratio a/d of the width of the interaction area and the nearest-neighbor distance between oscillators, the quantity $q_0 a$, the coupling constant $\varepsilon = \kappa/(\mu a)$, the reduced internal damping constant of the resonators $\eta = \gamma/\omega_0$, and the concentration p of resonators on the surface. In all calculations reported on here, we have chosen $\sigma = 0.17$, which corresponds to fused quartz, $q_0 a = \pi/16$ and $a/d = 0.5$, while the parameters ε , η , and p have been varied. The above choice of relative lengths, i.e., $q_0 a$ and a/d , implies that for wave numbers near the resonance value q_0 , effects resulting from the discreteness of the latticelike Bragg reflection are unimportant.

Figure 2 shows the reduced dispersion relation of surface modes at fixed values of $\varepsilon = 0.2$ and $\eta = 0.1$ for various concentrations p of oscillators on the surface. For small values of p , only one branch of surface modes is found, namely the Rayleigh branch. It is slightly perturbed near the resonance wave vector q_0 and crosses the straight line of the Rayleigh wave dispersion curve for a free surface at a wave number slightly smaller than q_0 . When approaching this wave number from below, the surface waves of our system are first slowed down and then accelerated as compared to Rayleigh waves of the free surface.

From a critical concentration of resonators on, the disper-

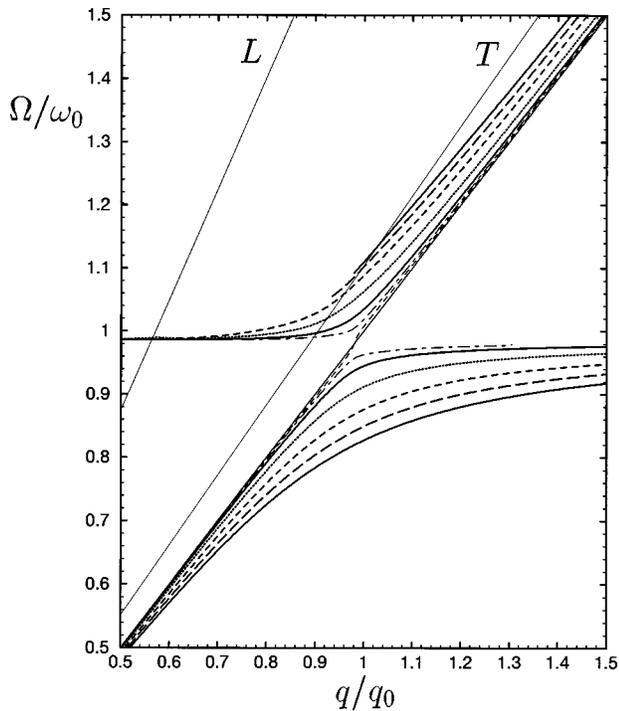


FIG. 2. Dispersion relation of surface modes for various concentrations of oscillators on the surface: $p=1$ (outer thick solid line), $p=0.75$ (thick long-dashed line), $p=0.5$ (thick short-dashed line), $p=0.25$ (dotted line), $p=0.1$ (inner thick solid line), $p=0.05$ (thin dash-dotted line), $p=0.025$ (thin short-dashed line), and $p=0.001$ (thin solid line). The upper thin solid straight lines marked by L and T correspond to longitudinal and transverse sound waves of the substrate, respectively. Further parameters: $\varepsilon=0.2$, $\eta=0.1$.

sion relation splits into two branches. The lower one bends off from the straight line $\omega=v_Rq$ leading to wave slowing. It is bounded above by ω_0 . With increasing concentration, the lower branch bends away from the Rayleigh branch more strongly.

The upper branch starts off at $q=0$ as a leaky wave at a

frequency slightly below ω_0 , leaves the radiating region of the ω - q plane at a wave number $q \approx \omega_0/v_T$, and bends up to approach asymptotically the Rayleigh branch of the free surface. The typical mode repulsion behavior is found resulting from the coupling of the Rayleigh mode of the substrate and the vibrational mode of a film of oscillators on the surface. We note that the limiting case $p=1$ of a perfect lattice of oscillators on the surface had already been considered earlier. It occurs as the special case of vanishing interaction between the oscillators in Refs. 18 and 20 and has been treated for a one-dimensional array of resonating elements in Ref. 19. For larger values of p , the upper branch cannot be pursued all the way from the nonradiative region to $q=0$. In fact, it has been found that for vanishing internal damping of the oscillators ($\eta \rightarrow 0$), the leaky branch in the radiative region disappears, and the upper branch of the surface modes terminates at the boundary $\omega=v_Tq$ of the nonradiative region.

It has to be noted that only parts of the two branches in the dispersion relation are relevant for propagation experiments, while in other regions of the dispersion relation the group velocity of the modes is too small to be applicable in such experiments. To illustrate this, we have displayed in Fig. 3 the power flow along the surface at $z=0$ generated by an external surface stress (2.7) with $I_\alpha(\mathbf{k}, \omega) = \delta_{\alpha 3} I_0$ as a function of k and ω , where I_0 is a constant. The concentration of oscillators on the surface has been chosen to be $p=0.5$. In a certain range of wave numbers (corresponding to a certain range of periodicities in a transducer), the two modes are both visible in Fig. 3.

The attenuation of the surface modes in our system is shown in Fig. 4. For small concentrations of resonators, the damping constant Γ has a well-defined maximum as a function of wave numbers slightly below q_0 . This maximum sharpens with increasing p , but changes its position very little. Beyond the critical concentration, when the modes have split into two branches, the Γ - q curves become much broader. For the lower mode [Fig. 4(a)], the maximum occurs at wave numbers q_{\max} larger than q_0 , and q_{\max} slightly

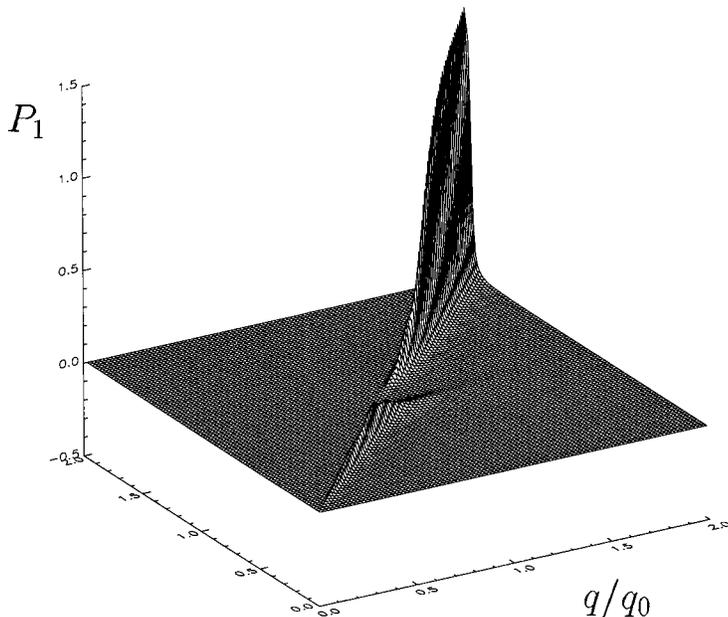


FIG. 3. Power flow P_1 in the x direction at the surface generated by an external surface stress (2.7) with constant amplitude (arbitrary units). $\eta=0.1$, $\varepsilon=0.2$, $p=0.5$.

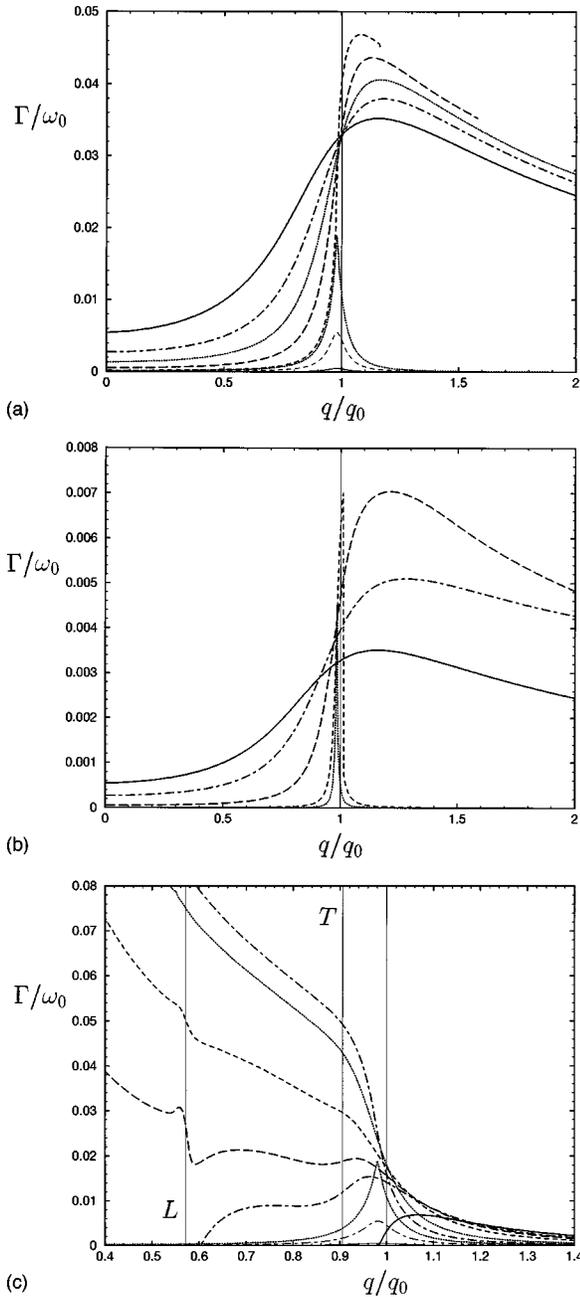


FIG. 4. Damping constant Γ of surface modes as a function of the modulus q of the wave vector, $\varepsilon=0.2$. (a) Lower mode in the dispersion relation, $\eta=0.1$. $p=1$ (upper solid line), $p=0.5$ (dash-dotted line), $p=0.25$ (upper dotted line), $p=0.1$ (long-dashed line), $p=0.03$ (upper short-dashed line), $p=0.025$ (lower dotted line), $p=0.01$ (lower short-dashed line), and $p=0.001$ (lower solid line). (b) Lower mode in the dispersion relation, $\eta=0.01$. $p=1$ (solid line), $p=0.5$ (dash-dotted line), $p=0.1$ (long-dashed line), $p=0.005$ (short-dashed line), and $p=0.001$ (dotted line). (c) Upper mode in the dispersion relation, $\eta=0.1$. $p=1$ (thick solid line), $p=0.5$ (lower thick dash-dotted line), $p=0.4$ (long-dashed line), $p=0.25$ (short-dashed line), $p=0.1$ (upper dotted line), $p=0.05$ (upper thick dash-dotted line), $p=0.025$ (lower dotted line), $p=0.01$ (thin dash-dotted line), and $p=0.001$ (thin solid line). The vertical lines marked by L and T correspond to $q/q_0=v_R/v_L$ and $q/q_0=v_R/v_T$, respectively.

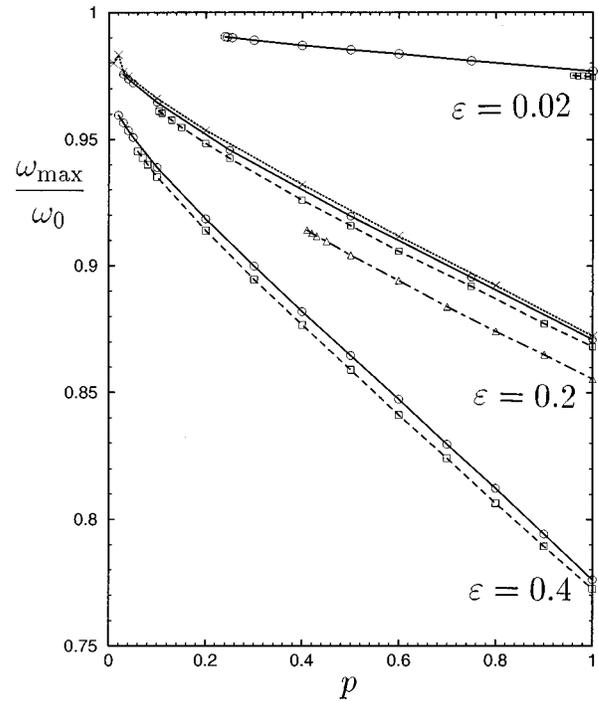


FIG. 5. Frequency of maximal attenuation as a function of concentration p of oscillators on the surface for three different values of the coupling constant ε . $\eta=0.05$ (\times , dotted line); $\eta=0.1$ (\circ , solid line), $\eta=0.2$ (\square , dashed line), $\eta=0.4$ (\triangle , dash-dotted line).

increases with increasing p . On the other hand, the maximal values of Γ decrease as p approaches 1. We note that for $p=1$, attenuation of the surface modes is only due to the internal damping of the oscillators on the surface. In the limit $\eta \rightarrow 0$, the surface modes would be undamped for $p=1$. To illustrate the influence of the internal damping constant γ of the oscillators on the attenuation of the surface modes, Γ - q curves for the lower branch with $\eta=0.01$, which is smaller than the value of η in Fig. 4(a) by a factor of 10. The attenuation of the surface modes is generally reduced as compared to the corresponding curves for $\eta=0.1$. Especially the difference between the attenuation for $p=0.5$ and $p=0.1$ and for the totally covered surface ($p=1$) has become much larger, and for small p , the resonance peak in the Γ - q curve has become much sharper.

When Γ is plotted as a function of frequency rather than of wave number, the frequency ω_{\max} with maximal damping varies largely linearly with concentration p as demonstrated for various sets of parameters in Fig. 5.

The damping constants of the modes belonging to the upper branch of the dispersion relation are shown in Fig. 4(c). In the radiative region, the damping due to radiation into the bulk is very large as compared to attenuation of the true surface modes, and it decreases with increasing concentration p . The onset of conversion into longitudinal bulk waves near the left vertical line in Fig. 4(c) gives rise to a rapid variation of the Γ - q curve.

The qualitative dependence of the dispersion curves and attenuation of the surface modes on the coupling constant ε at fixed concentration p of oscillators may be characterized as follows and is easily understood: with increasing ε , the

two branches in the dispersion relation repel each other more strongly. The Γ - q curves become broader, and the damping of the Rayleigh branch increases at finite γ as the Rayleigh modes are more strongly coupled to the dissipative oscillators at the surface.

A simplified treatment of the randomly distributed oscillators on the surface would be to replace the system under consideration by one with an oscillator situated on each grid-point $\mathbf{Y}_{m,n}$ having an effective reduced coupling constant $\varepsilon^{(\text{eff})} = \varepsilon p$. This would correspond to the virtual crystal approximation in the theory of vibrations in disordered crystals. This simplified description would lead to a dispersion relation in qualitative agreement with the CPA results, although quantitative differences exist. However, the attenuation of the surface modes cannot be described correctly in this approach since radiation damping due to conversion into bulk waves is not included.

V. CONCLUSIONS

In summary, we have calculated the dispersion curves and the attenuation of surface acoustic modes in a semi-infinite isotropic half-space with a surface covered by randomly distributed damped harmonic oscillators. The oscillators model surface structures that give rise to surface shape resonances. The randomness has been treated within the coherent-potential approximation. For small intrinsic damping of the single oscillators, the attenuation of the surface modes shows a strong sensitivity to the concentration of oscillators on the

surface. A particularly interesting feature is the almost linear dependence on the concentration of the frequency at which maximal damping occurs. This finding can perhaps be used for the determination of the density of resonating surface elements with the help of surface acoustic waves.

We hope that the results presented in this work are helpful in the interpretation of experiments like the ones reported in Refs. 13–15. Up to now, a comparison between theory and experiment can only be a qualitative one because the system treated here can only be regarded as a very simplified model of the situation encountered in the experiments. Hydrogen crystallites forming on a LiNbO_3 substrate have been modeled by oscillators that all have equal frequencies, coupling constants to the surface, and internal damping. For a quantitative comparison with experiment, a better modeling of the shape of the surface elements, their size distribution, their internal structure, and their coupling to the substrate would be necessary, and the elastic anisotropy of the substrate would have to be taken into account.

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*Present address: Siemens Matsushita Components GmbH & KG, 81617 Munich, Germany.

[†]On leave from Institut für Theoretische Physik, Universität Regensburg, 93040 Regensburg, Germany.

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