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Rayleigh waves in prestressed crystals

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Rayleigh waves in anisotropic, prestressed crystals have been investigated by a combination of lattice dynamics and elastic-wave theory. We derive an exact expression for the Rayleigh velocity as the root of a cubic equation involving the elastic constants of the prestressed material and the applied stress in the direction of propagation. Numerical calculations show that surface modes are softened by uniaxial tension or compression parallel to the direction of propagation. For the two-dimensional triangular lattice which is elastically isotropic in the unstressed state, we have calculated the dispersion of the surface waves by analytic lattice dynamics. We find the remarkable result that the frequency of the surface waves, at all wavelengths, is proportional to $\sin(2\pi d_x/\lambda)$, where $2d_x$ is the nearest-neighbor separation along the prestressed, close-packed x direction. We have made an estimate of the surface entropy which is in reasonable agreement with other calculations.

I. INTRODUCTION

The study of surface waves in solids has generated an extensive literature in many branches of physical science. After the pioneering work of Lord Rayleigh,[1] early applications and theoretical developments occurred in seismology.[2] A recent bibliography can be found in Ref. 3. Modern interest in surface waves has been centered on technological applications to microwave semiconductor devices.[4] Recent theoretical developments have extended the elastic-wave theory to arbitrary directions of propagation in anisotropic crystals[5] and studied the effects of simple defects.[6] Numerical lattice dynamics have been used to study short-wavelength surface modes and their effects on the surface properties of crystals.[4,7]

Our interest in Rayleigh waves arises from ongoing studies of crack propagation and dislocation dynamics.[8–10] The motion of cracks and dislocations in a finite-width strip results in the propagation of surface waves which are required to maintain the zero-stress condition at the free boundaries. According to the continuum theory of dislocation motion, the Rayleigh velocity is the limiting velocity for a steadily-moving edge dislocation in a finite-width slab.[11]

The classical two-dimensional close-packed triangular lattice, with nearest-neighbor Hooke's-law forces, is a convenient standard material for investigating the atomic dynamics of crack propagation, dislocation motion, and plastic flow.[8–10] The triangular lattice is a mechanically stable, elastically isotropic lattice which can support longitudinal and transverse waves. With nearest-neighbor Hooke's-law forces it has a close connection to the continuum mechanics of materials undergoing plane-stress or plane-strain deformation.[8,12] This connection provides a basis for relating the results of atomic simulations to the established continuum theories and suggests that this material is a useful standard for atomic studies of nonlinear solid mechanics. Its thermodynamic properties over a range of densities are now well characterized by a combination of lattice dynamics and molecular dynamics.[10,13]

It has been found desirable, especially for soft linear interparticle forces, to carry out atomic simulations of dislocation motion under slight compression rather than at the stress-free density in order to inhibit vacancy formation. In connection with these simulations, we have calculated by lattice dynamics the surface waves in a semi-infinite triangular lattice which has been subjected to a longitudinal stress parallel to the close-packed surface row. The boundary conditions require that any nonzero forces are parallel to the surface.

At long wavelengths, surface waves can be described by continuum elasticity theory. In this paper we describe calculations of the Rayleigh velocity in stressed crystals. The essential modification of the anisotropic stress-free theory[5] is to include the effects of stress on the coefficients that appear in the equations of motion.[14] Numerical calculations of the dependence of the Rayleigh velocity on initial stress have been carried out for some idealized but physically realistic crystals.

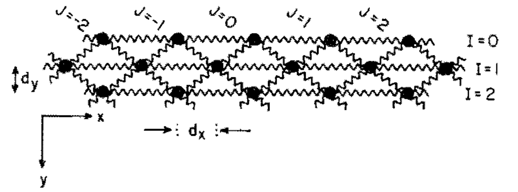

FIG. 1. Crystal geometry of the triangular lattice under tension. The top row of atoms is a free surface. The interplanar spacing d_x is one-half the interatomic spacing in the close-packed direction. The zero-force boundary condition requires that $d_x^2+d_y^2=d_0^2$.

II. THEORY OF SURFACE WAVES IN STRESSED SOLIDS

For isotropic materials, the long-wavelength surface waves are linear combinations of longitudinal and transverse waves. At shorter wavelengths and in anisotropic solids this is no longer true. Since the lattice dynamics and continuum mechanics calculations have many features in common, it is instructive to describe both calculations in parallel, thus highlighting the similarities and differences.

For simplicity we will consider only surfaces that either are mirror planes or contain mirror planes. In the latter case the propagation direction must lie in the mirror plane. On the basis of the known anisotropic theory we then expect the Rayleigh wave to be a plane wave perpendicular to the surface.[5] In our calculations we take the xz plane to be the surface plane and the x axis as the direction of propagation. The positive y axis penetrates the elastic half-space. The elastic constants defined in Eq. (A9) in the Appendix refer to this coordinate system which is not necessarily coincident with the usual choice. The symmetry requirements imply that C_{xxxy} and C_{xyyy} are zero.

For a monochromatic wave traveling in the x direction, the displacements can be written as

$$(u,v)_{I,J}=(U,iV)\exp[-qI+i\theta(I+2J)-i\omega t] \,, \quad \text{(1a)}$$

$$(u,v)=(U,iV)\exp(-\kappa\nu_p^{1/2}y+ikx-i\omega t) \,. \quad \text{(1b)}$$

In Eq. (1a) the atoms are labeled as shown in Fig. 1; the wavelength $\lambda=2\pi d_x/\theta$. In Eq. (1b), $\nu_p=S_{yyxx}/S_{yyyy}$ is a Poisson's ratio for plane strain in the xy plane. The constants $S_{\alpha\beta\gamma\delta}$ [see Eq. (A1)] are derivatives of the stress with respect to unsymmetrized first-order strains, and are related to the adiabatic elastic constants described in the Appendix. For the triangular lattice $\nu_p=d_x^2/d_y^2$ so $\kappa d_x=q$ and $kd_x=\theta$. At long wavelengths, all the quantities in Eqs. (1a) and (1b) are real, corresponding to a wave propagating in the x direction that is exponentially damped in the y direction. At short wavelengths, q, and consequently U and V, are complex, corresponding to a damped periodic disturbance in the y direction.

The equations of motion for the two problems are

$$\begin{aligned}-(m/K)\ddot{u}_{00}=-F_x/K&=(2u_{00}-u_{01}-u_{0-1})+(d_x/d_0)^2(4u_{00}-u_{10}-u_{-10}-u_{1-1}-u_{-11})\\&\quad-(d_xd_y/d_0^2)(v_{10}+v_{-10}-v_{1-1}-v_{-11})\,,\\-(m/K)\ddot{v}_{00}=-F_y/K&=[1-(d_0/2d_x)](2v_{00}-v_{01}-v_{0-1})+(d_y/d_0)^2(4v_{00}-v_{10}-v_{-10}-v_{1-1}-v_{-11})\\&\quad-(d_xd_y/d_0^2)(u_{10}+u_{-10}-u_{1-1}-u_{-11})\,,\end{aligned} \quad \text{(2a)}$$

$$\begin{aligned}\rho\ddot{u}&=S_{xxxx}\frac{\partial^2u}{\partial x^2}+S_{xyxy}\frac{\partial^2u}{\partial y^2}+(S_{xxyy}+S_{xyyx})\frac{\partial^2v}{\partial x\,\partial y}\,,\\\rho\ddot{v}&=S_{yxyx}\frac{\partial^2v}{\partial x^2}+S_{yyyy}\frac{\partial^2u}{\partial y^2}+(S_{yxxy}+S_{yyxx})\frac{\partial^2u}{\partial x\,\partial y}\,,\end{aligned} \quad \text{(2b)}$$

where $\vec{F}$ is the force on particle (0,0), K is the force constant, and ρ is the mass density.

Since there is an initial stress, the antisymmetric parts of the strain tensor corresponding to an infinitesimal rotation also change the stress tensor. The symmetry of the stress tensor requires that $S_{\alpha\beta\gamma\delta}$ is symmetric with respect to permutation of the first two suffixes, i.e., $S_{\alpha\beta\gamma\delta}=S_{\beta\alpha\gamma\delta}$. The assumption of mirror symmetry in the xz or yz planes means that S_{xxxy}, S_{xyyy}, etc., are zero.

Using the displacements given in Eqs. (1) and the equations of motion from Eqs. (2), we obtain two dispersion relations in each case which can be written as

$$\Delta_L=\frac{(m/K)(\omega^2-\omega_L^2)}{4(d_x/d_0)^2}=\cos\theta(1-\cosh q)-R^{-1}\sin\theta\sinh q\ ,$$

$$\Delta_T=\frac{(m/K)(\omega^2-\omega_T^2)}{4(d_y/d_0)^2}=\cos\theta(1-\cosh q)+R\sin\theta\sinh q\ , \tag{3a}$$

$$\rho\Delta_L=\frac{\rho(\omega^2-\omega_L^2)}{v_p S_{xyxy}}=-\kappa^2-\Delta_1 R^{-1}k\kappa\ ,$$

$$\rho\Delta_T=\frac{\rho(\omega^2-\omega_T^2)}{S_{yyxx}}=-\kappa^2+\Delta_2 Rk\kappa\ , \tag{3b}$$

where ω_L and ω_T are the frequencies of pure (q or $\kappa=0$) longitudinal and transverse waves parallel to the surface, and $R=v_p^{1/2}U/V$. The frequencies ω_L and ω_T are

$$(m/K)\omega_L^2=2(1-\cos 2\theta)+4(d_x/d_0)^2(1-\cos\theta)\ ,$$
$$(m/K)\omega_T^2=[2-(d_0/d_x)](1-\cos 2\theta)+4(d_y/d_0)^2(1-\cos\theta)\ , \tag{4a}$$

$$\rho\omega_L^2=S_{xxxx}k^2\ ,\qquad \rho\omega_T^2=S_{yxyx}k^2=S_{xyyx}k^2\ . \tag{4b}$$

The quantities Δ_1 and Δ_2 are ratios of stress derivatives,

$$\Delta_1=(S_{xxyy}+S_{xyyx})/S_{xyxy}\ ,\qquad \Delta_2=(S_{xyxy}+S_{yyxx})/S_{yyxx}\ . \tag{5}$$

Using the expressions for $S_{\alpha\beta\gamma\delta}$ appropriate to the triangular lattice [Eqs. (A13), (A14)], it can be seen that Eqs. (3b) and (4b) are the long-wavelength limits of Eqs. (3a) and (4a) for this material.

The dispersion relations can be combined to eliminate R, resulting in a quadratic equation in $\cosh q$ or κ^2:

$$\cosh^2 q+[(\Delta_L+\Delta_T)\cos\theta-2\cos^2\theta]\cosh q+[\Delta_L\Delta_T-(\Delta_L+\Delta_T)\cos\theta+\cos^2\theta-\sin^2\theta]=0\ , \tag{6a}$$

$$\kappa^4+[\rho(\Delta_L+\Delta_T)+\Delta_1\Delta_2 k^2]\kappa^2+\rho^2\Delta_L\Delta_T=0\ . \tag{6b}$$

Surface waves can be constructed from linear combinations of two waves with the same wavelength and frequency but different damping factors. It will be seen that a particular linear combination satisfies the boundary conditions.

In the atomic calculations the boundary conditions require that the forces between particles in the surface row ($I=0$) and hypothetical particles in the row above it ($I=-1$) vanish. In the continuum calculations the normal and shear stresses must vanish at the surface, i.e., $\sigma_{xy}=\sigma_{yy}=0$ at $y=0$. (See note added in proof.) The boundary conditions can be expressed as

$$-F_x^0/K=(d_x/d_0)^2(2u_{00}-u_{-10}-u_{-11})-(d_xd_y/d_0^2)(v_{-10}-v_{-11})=0\ , \tag{7a}$$

$$-F_y^0/K=(d_y/d_0)^2(2v_{00}-v_{-10}-v_{-11})-(d_xd_y/d_0^2)(u_{-10}-u_{-11})=0\ ,$$

$$\frac{\partial u}{\partial y}+\frac{\partial v}{\partial x}=0,\quad v_p\frac{\partial u}{\partial x}+\frac{\partial v}{\partial y}=0\ . \tag{7b}$$

The boundary conditions cannot be satisfied by a single wave that has the dispersion described in Eqs. (3). We therefore take a fixed linear combination of the two waves that have the same wavelengths and frequency. The relative amplitude of the waves is described by the ratio $\mathscr{R}=V_1/V_2$, and from the boundary conditions we have

$$\mathscr{R}=-\frac{R_2(e^{q_2}\cos\theta-1)+e^{q_2}\sin\theta}{R_1(e^{q_1}\cos\theta-1)+e^{q_1}\sin\theta}=-\frac{R_2e^{q_2}\sin\theta-(e^{q_2}\cos\theta-1)}{R_1e^{q_1}\sin\theta-(e^{q_1}\cos\theta-1)}\ , \tag{8a}$$

$$\mathscr{R}=-\frac{R_2\kappa_2+k}{R_1\kappa_1+k}=-\frac{R_2k-\kappa_2}{R_1k-\kappa_1}\ . \tag{8b}$$

Thus, in order to have a surface-wave solution it is required that

$$(1+R_1R_2)(e^{q_1}-e^{q_2})\sin\theta -(R_1-R_2)[e^{q_1}e^{q_2}-(e^{q_1}+e^{q_2})\cos\theta+1]=0\ , \tag{9a}$$

$$(1+R_1R_2)(\kappa_1-\kappa_2)k-(R_1-R_2)(\kappa_1\kappa_2+k^2)=0\ . \tag{9b}$$

Since quadratic equations in ω^2 and either θ or k can be deduced for R and q or κ from the dispersion relations given in Eqs. (3), the conditions expressed in Eqs. (9) are sufficient to determine the frequency of the Rayleigh waves as a function of wavelength. The algebraic steps required to determine the exact form of the dispersion relation are outlined below.

An expression for the ratios R_1 and R_2 can be obtained from the second equation of the pairs (3a) and (3b) and substituted into the surface condition Eqs. (9). In the continuum case there is obviously a common factor $(\kappa_1-\kappa_2)$; in the atomic case a little manipulation is required to show that $(e^{q_1}-e^{q_2})$ is a common factor. Removing these factors gives

$$\Delta_T^2+(\cosh q_1\cosh q_2+\sinh q_1\sinh q_2-2\cos\theta+1)\Delta_T+\sinh q_1\sinh q_2 +(\cosh q_1+\cosh q_2-\cosh q_1\cosh q_2-\sinh q_1\sinh q_2-1)\cos\theta=0\ , \tag{10a}$$

$$(\rho\Delta_T)^2+(\kappa_1^2+\kappa_2^2+\Delta_2k^2+\Delta_2\kappa_1\kappa_2)(\rho\Delta_T)+\Delta_2(\Delta_2-1)k^2\kappa_1\kappa_2-(\Delta_2-1)\kappa_1^2\kappa_2^2=0\ . \tag{10b}$$

$\cosh q$ and κ^2 can be most easily eliminated from Eqs. (10) by using the expressions for the sums and products of roots of quadratic equations in Eqs. (6). Eliminating the square-root term gives an equation for the frequency of surface waves as a function of wavelength,

$$\{\Delta_T^2+[2\cos^2\theta-2\cos\theta-\cos\theta(\Delta_T+\Delta_L)+\Delta_T\Delta_L]\Delta_T-\Delta_T\Delta_L\cos\theta\}^2 -\{(\Delta_T\Delta_L)[4\cos^2\theta-2\cos\theta(\Delta_T+\Delta_L)+\Delta_T^2\Delta_L^2]\}(1-\cos\theta+\Delta_T)^2=0\ , \tag{11a}$$

$$[(\rho\Delta_T)(\rho\Delta_L)+(\Delta_1-1)k^2(\rho\Delta_T)]^2-[(\rho\Delta_T)(\rho\Delta_L)][(\rho\Delta_T)+(\Delta_2-1)k^2]^2=0\ . \tag{11b}$$

The reduction of these equations to more tractable expressions is somewhat different in the two problems, so they will be considered separately, taking the atomic case first.

Equation (11a) can be extensively factorized, with the result

$$\Delta_T(\Delta_T-\Delta_L)(\Delta_T-2\cos\theta)[2(\Delta_T-\cos\theta)(\Delta_L-\cos\theta)+(\Delta_T+\Delta_L-2\cos\theta)(1+\cos^2\theta)+2\cos^2\theta]=0\ . \tag{12}$$

There are four solutions of this equation, and the one corresponding to a Rayleigh wave is most easily found by considering the long-wavelength limit at the stress-free density. In this case, the lattice is elastically isotropic and $c_L^2=3c_T^2$. The Rayleigh velocity is given by $c_R^2=(2-2/\sqrt{3})c_T^2$, and from this it can be seen that the required solution is a root of the quadratic term in Eq. (12). The final substitution is

$$\begin{aligned}\Omega_L^2&=(d_0^2/d_x^2)[\tfrac{1}{4}(m/K)\omega^2-\sin^2\theta]\\&=\Delta_L+1-\cos\theta\ ,\\ \Omega_T^2&=(d_0^2/d_y^2)\\&\quad\times\{\tfrac{1}{4}(m/K)\omega^2-[1-(d_0/2d_x)]\sin^2\theta\}\\&=\Delta_T+1-\cos\theta\ ,\end{aligned} \tag{13}$$

and the quadratic term in Eq. (12) becomes

$$2\Omega_T^2\Omega_L^2-(\Omega_T^2+\Omega_L^2)\sin^2\theta=0\ . \tag{14}$$

This equation only has solutions if $\omega^2\propto\sin^2\theta$. Since the wavelength $\lambda=(2\pi d_x/\theta)$, we have the remarkably simple dispersion relation for surface waves in a triangular lattice,

$$\omega=(c_R/d_x)\sin\theta\ , \tag{15}$$

which is the same form as the dispersion relation for a nearest-neighbor one-dimensional chain. This dispersion relation has been correctly deduced for the isotropic stress-free lattice from numerical calculations.[8]

The Rayleigh velocity is the root of a quadratic equation,

$$(m/Kd_0^2)c_R^2=5(d_x/d_0)^2-(d_x/d_0) -[4(d_x/d_0)^5+(d_x/d_0)^4 -2(d_x/d_0)^3+(d_x/d_0)^2]^{1/2}\ . \tag{16}$$

At the stress-free density $(d_x/d_0)=\frac{1}{2}$ and $(m/Kd_0^2)c_R^2=(\frac{1}{4})(3-\sqrt{3})$, in agreement with previous results.[8] At long wavelengths $\omega=c_Rk$ and from Eq. (11b), using the results of Eq. (A11), we obtain a cubic equation for c_R^2:

$$(\rho c_R^2-S_{xyyx})[S_{yyyy}(\rho c_R^2-S_{xxxx})+S_{yyxx}^2]^2 - S_{xyxy}S_{yyyy}(\rho c_R^2-S_{xxxx}) \times[(\rho c_R^2-S_{xyyx})+S_{xyxy}]^2=0 \;. \quad (17)$$

This equation has the same structure as the frequency equation derived by Hayes and Rivlin[15] for the propagation of Rayleigh waves along a principal stress direction of an elastically isotropic material. Other authors have considered Rayleigh-wave propagation in stressed isotropic materials,[16–18] but some of them do not include the effects of an initial stress on the elastic constants.[16,18] The other authors consider small initial stresses by including the third-order elastic constants.[17]

It is sometimes convenient to express this equation for the Rayleigh velocity in terms of the ratios

$$\begin{aligned}
\gamma_L &= S_{yyyy}(\rho c_R^2-S_{xxxx})/S_{xyyx}^2 \\
&= (c_L^{\perp})^2(c_R^2-c_L^{\|2})/(c_T^{\|})^4 \;, \\
\gamma_T &= S_{xyxy}(\rho c_R^2-S_{xyyx})/S_{xyyx}^2 \\
&= (c_T^{\perp})^2(c_R^2-c_T^{\|2})/(c_T^{\|})^4 \;, \\
S_1 &= S_{xyxy}^2/S_{xyyx}^2=(c_T^{\perp})^4/(c_T^{\|})^4 \;, \\
S_2 &= S_{yyxx}^2/S_{xyyx}^2 \;,
\end{aligned} \quad (18)$$

where the sound speeds are the same as in Eq. (A7). Then Eq. (17) can be written as

$$\gamma_L(\gamma_T+S_1)^2=\gamma_T(\gamma_L+S_2)^2 \;. \quad (19)$$

It is shown in the Appendix that for materials with pairwise-additive forces at low temperatures (compared with the melting temperature), $S_{xyxy}=S_{yyxx}$, i.e., $S_1=S_2$. This is a statement of the Cauchy relations and as a result the Rayleigh velocity if a root of the quadratic equation $\gamma_L\gamma_T=S_1^2$ and is completely determined by the four sound speeds parallel to and perpendicular to the surface:

$$c_R^2=\frac{1}{2}(c_L^{\|2}+c_T^{\|2}) -\frac{1}{2}[(c_L^{\|2}-c_T^{\|2})^2+4(c_T^{\perp})^6/(c_L^{\perp})^2]^{1/2} \;. \quad (20)$$

Using the expressions given in the Appendix for the sound speeds appropriate to the triangular lattice, the expression for the Rayleigh velocity given in Eq. (16) is obtained again.

In an unstressed material the stress derivatives are equal to the elastic constants, and the equation for $\gamma=\rho c_R^2/C_{44}$ reduces to (in Voigt notation)

$$\gamma^2(\gamma-C_{11}/C_{44})=(C_{22}/C_{44})(\gamma-1) \times[\gamma-C_{11}/C_{44}+C_{12}^2/(C_{22}C_{44})]^2 \;, \quad (21)$$

which is identical to an expression given by Dobrzynski and Maradudin.[19]

The damping factors q and κ can be determined from the roots of the quadratic equations (6) once the Rayleigh velocity is known. Then, from Eqs. (3) and (8), the displacement ratios R_1, R_2, and $\mathscr{R}$ can be obtained, which together with θ and q or κ describe the displacements produced by a surface wave.

III. RESULTS

A. Rayleigh velocity of stressed crystals

For a given force law the Rayleigh velocity depends on the crystal structure, the orientation of the surface plane, the direction of propagation, and the applied stress, which can only be in the same plane as the surface. Though only the component of stress in the direction of propagation σ_{xx}^0 enters directly into the calculation of the Rayleigh velocity, the velocity also depends on the effects of σ_{xz}^0 and σ_{zz}^0 on the elastic constants.

To illustrate these effects we have calculated the Rayleigh velocity for the (100) plane of a face-centered-cubic lattice, for propagation in both the [100] and [110] directions. The stress in the xz plane is hydrostatic, i.e., $\sigma_{xx}^0=\sigma_{zz}^0=\sigma^0$. For simplicity we consider only nearest-neighbor pairwise-additive forces. We have used the soft harmonic potential

$$\phi_H(r)=\frac{1}{2}Kd_0^2[(r/d_0)^2-1] \;, \quad (22)$$

and the hard and very anharmonic Lennard-Jones (12-6) potential,

$$\phi_{LJ}(r)=\frac{1}{72}Kd_0^2[(d_0/r)^{12}-2(d_0/r)^6] \;. \quad (23)$$

The sound speeds as a function of stress are shown in Table I for the Lennard-Jones potential, and graphs of the Rayleigh velocities are shown in Fig. 2.

The Rayleigh velocity has qualitatively the same

TABLE I. Sound speeds in a face-centered-cubic lattice with nearest-neighbor Lennard-Jones (12-6) forces. The stress σ^0 is applied hydrostatically in the surface xz plane. The nearest-neighbor spacing in the surface plane is d. The sound speeds are in units of $(\kappa d_0^2/m)^{1/2}$.

d/d_0	$\sigma^0 V/\kappa d_0^2$	$c_L^{\parallel 2}$ [100]	$c_L^{\parallel 2}$ [110]	$c_T^{\parallel 2}$	$c_L^{\perp 2}$	$c_T^{\perp 2}$	c_R^2 [100]	c_R^2 [110]
0.88	−0.4139	3.8599	7.6839	0.0607	1.5021	0.4746	0.0420	0.0513
0.89	−0.3394	3.3564	6.5816	0.1390	1.4590	0.4784	0.1158	0.1273
0.90	−0.2765	2.9279	5.6403	0.2054	1.4161	0.4819	0.1767	0.1909
0.91	−0.2233	2.5634	4.8358	0.2619	1.3733	0.4852	0.2263	0.2438
0.92	−0.1784	2.2535	4.1481	0.3098	1.3308	0.4882	0.2658	0.2871
0.93	−0.1406	1.9902	3.5598	0.3503	1.2885	0.4909	0.2961	0.3220
0.94	−0.1086	1.7668	3.0566	0.3846	1.2463	0.4932	0.3182	0.3491
0.95	−0.0817	1.5777	2.6262	0.4135	1.2045	0.4952	0.3325	0.3689
0.96	−0.0591	1.4180	2.2581	0.4378	1.1629	0.4969	0.3400	0.3816
0.97	−0.0401	1.2836	1.9434	0.4581	1.1217	0.4983	0.3411	0.3873
0.98	−0.0242	1.1711	1.6747	0.4750	1.0808	0.4992	0.3370	0.3857
0.99	−0.0110	1.0774	1.4454	0.4888	1.0402	0.4998	0.3285	0.3765
1.00	0.0000	1.0000	1.2500	0.5000	1.0000	0.5000	0.3170	0.3596
1.01	0.0091	0.9367	1.0839	0.5089	0.9602	0.4998	0.3035	0.3352
1.02	0.0166	0.8857	0.9430	0.5158	0.9208	0.4992	0.2893	0.3043
1.03	0.0227	0.8454	0.8240	0.5208	0.8819	0.4981	0.2751	0.2685
1.04	0.0276	0.8144	0.7237	0.5243	0.8435	0.4967	0.2615	0.2301
1.05	0.0316	0.7915	0.6398	0.5263	0.8055	0.4947	0.2491	0.1912
1.06	0.0347	0.7757	0.5699	0.5270	0.7681	0.4924	0.2380	0.1537
1.07	0.0371	0.7662	0.5123	0.5266	0.7312	0.4895	0.2283	0.1189
1.08	0.0388	0.7623	0.4653	0.5250	0.6949	0.4862	0.2200	0.0874
1.09	0.0401	0.7632	0.4276	0.5224	0.6592	0.4823	0.2130	0.0597
1.10	0.0410	0.7684	0.3978	0.5189	0.6241	0.4780	0.2072	0.0358

dependence on compressive stress as the velocity of transverse waves propagating parallel to the surface. The reason for this can be seen by expanding the square-root term in the expression for the Rayleigh velocity given in Eq. (20),

$$c_R^2 \approx (c_T^{\parallel})^2 - [(c_T^{\perp})^6]/[(c_L^{\perp})^2(c_L^{\parallel 2} - c_T^{\parallel 2})] + \cdots \quad . \tag{24}$$

The second term is typically $\sim 10^{-1}$ K/m and decreases as the crystal is compressed. In fact $c_T^{\parallel}$ is a rigorous upper bound to the Rayleigh velocity, as can be seen from the requirement that the product of the roots $\kappa_1\kappa_2$ in Eq. (6b) is positive. The transverse sound speed $c_T^{\parallel}$ decreases monotonically under compression until the onset of a mechanical shear instability. Consequently all the Rayleigh velocities have the same qualitative behavior under compression, vanishing just before the onset of this shear instability. The maximum compressive strains are about 10% for the Lennard-Jones potential and about 40% for the unrealistically soft harmonic potential. The stresses required for significant surface-mode softening are generally large, i.e., $10^9 - 10^{11}$ N m^{-2}, but these are quite easily realized in shock-loaded solids.

Under tension the Rayleigh velocity is no longer governed by $c_T^{\parallel}$, and in anharmonic crystals the velocities of waves propagating in the [100] and [110] directions are qualitatively different. Surface waves in the [110] direction propagate a little faster than those in the [100] direction when the lattice is compressed, but under tensile stress the velocity decreases very rapidly. The softening of modes under tension is qualitatively different from the compressive case in that it is not directly associated with a bulk instability, although the longitudinal sound speeds are about one-half of their stress-free value. In a stress-free face-centered-cubic crystal there is a softening of the surface modes when $C_{11} \sim C_{12}$ [Eq. (21)], which occurs, for instance, near the structural phase transition in Nb_3Sn (Ref. 20). It would seem that in a stress-free crystal, surface-mode softening is always associated with bulk-mode softening but this is not necessarily true in a stressed crystal. The strains

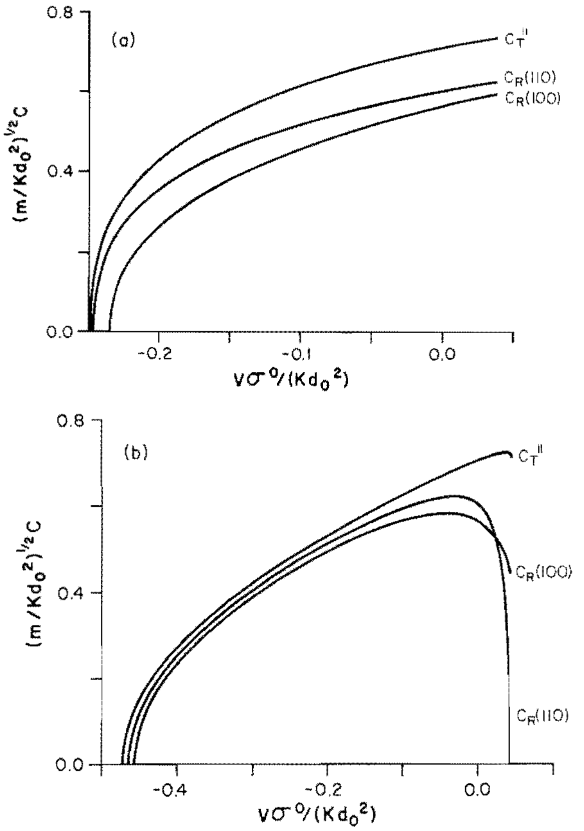

FIG. 2. Sound speeds in a face-centered-cubic lattice as a function of the applied stress in the surface plane σ^0. The results are qualitatively the same for uniaxial stress $\sigma^0_{xx}=\sigma^0$ and hydrostatic stress $\sigma^0_{xx}=\sigma^0_{zz}=\sigma^0$. The results for hydrostatic stress are shown here. (a) Harmonic forces, (b) Lennard-Jones forces.

involved are again of the order of 10%, which is slightly less than the theoretical yield strain of the Lennard-Jones crystal but this requires much less stress ($\sim 10^8$ N m^{-2}) than equivalent compression. In the earth's crust, the typical deviatoric stresses of about 3×10^7 N m^{-2} might change the Rayleigh velocity by a few percent. For the purely harmonic potential, the surface modes do not soften under tension.

It is interesting to compare these results with the calculations of Brunelle,[16] who considered surface-wave propagation in stressed isotropic materials, ignoring the effects of stress on the elastic constants themselves. He found an essentially linear relation between the square of the Rayleigh velocity and the unaxial stress leading to an instability at large compressions, which he suggested might provide mechanisms for earthquake initiation and prehistoric land-mass formation. Our results for compressive stresses are in qualitative agreement with his, though the change in elastic constants hastens the onset of the instability. For tensile stresses the results are quite different, which is to be expected since his calculation neglects the softening of the longitudinal modes.

B. Dispersion and displacements in the triangular lattice

At short wavelengths, surface waves can be described by numerical lattice dynamics.[7] The triangular lattice is of some interest since it encompasses many of the features of surface-wave propagation in three-dimensional crystals, but is sufficiently tractable for us to find an analytic solution to its dispersion relation. We were able to show that the dispersion relation was a remarkably simple sine wave, regardless of the initial stress.

For a given wavelength and frequency, the displacements are determined, to within an arbitrary amplitude, by the damping factors q or κ and the ratios R_1, R_2, $\mathscr{R}$. We have computed the displacements corresponding to various values of $\theta=kd_x$ for a triangular lattice subjected to a range of longitudinal stresses. Since the displacements are qualitatively independent of the applied stress, we show only a selection from the stress-free density in Fig. 3. For small values of θ the damping factor q is real and the wave-like displacements are similar to those deduced from continuum mechanics. The damping of these waves is relatively slow, there being noticeable displacements nine layers into the crystal for $\theta=\pi/20$. As θ increases, the damping of the displacements becomes more rapid and at sufficiently large values of θ, about $\pi/8$ at the stress-free density, q becomes complex. There is no qualitative change in the displacements during the transition from real to complex values of q, which takes place at progressively larger values of θ as the lattice is compressed.

When the wavelength is of the order of the interatomic spacing, i.e., $\theta\approx1$, the displacements are no longer wavelike. At the highest frequency when $\theta=\pi/2$ the displacements in successive rows alternate between purely y and purely x components.

C. Surface entropy of the triangular lattice

In the bulk crystal, waves propagating parallel to the close-packed direction can be separated into longitudinal and transverse modes. In the presence of a free surface, half of these modes become surface waves and the other half form some unknown

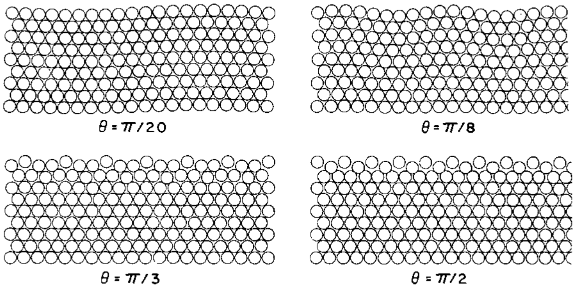

FIG. 3. Surface-wave displacements in a triangular lattice at various reduced wave vectors $\theta = kd_x$. The wavelength dependence of the displacements is discussed in the text.

bulk excitations. An estimate of the surface entropy can be obtained by assuming that these latter excitations have the same entropy per mode as the bulk crystal. The surface entropy per atom S_s is then given by (in units of k_B)

$$S_s = \langle \ln(\omega_L \omega_T/\omega_0^2) \rangle - \langle \ln(\omega_R/\omega_0) \rangle - \langle \ln(\omega_B/\omega_0) \rangle \ , \qquad (25)$$

where $\omega_0 = (K/m)^{1/2}$. The expressions for the longitudinal and transverse frequencies at the stress-free density can be obtained from Eqs. (4a). The average entropy per mode in the bulk lattice has been calculated by Huckaby,[21] and combining these results gives

$$S_s = \tfrac{1}{2}\ln 3 - \tfrac{1}{2}\ln(3/4 - \sqrt{3}/4) - 0.412\,6784 \simeq 0.711 \ . \qquad (26)$$

The Brillouin-zone average is $0 \le \theta \le \pi$ and the required integrals, which are of the form $\pi^{-1}\int_0^{\pi} \ln(a + b\cos\theta)d\theta$ are listed in Ref. 22. This result ($S_s = 0.71$) is in reasonable agreement with numerical lattice dynamics[23] ($S_s = 0.66$) and cell cluster theory[24] ($S_s = 0.62$).

The dominant contribution to the surface entropy comes from the region of the Brillouin zone around $\theta = \pi$ where $\omega_R = 0$ and $\omega_L\omega_T$ is a maximum. This suggests that a calculation based on the low-frequency elastic waves will be a very poor approximation to the surface entropy.

Note added in proof. The boundary conditions require that the stressers in a co-moving, or Lagrangian, coordinate system vanish at the surface. Equation (7b) only involves the symmetric components of $S_{\alpha\beta\gamma\delta}$.

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APPENDIX: STRESS DERIVATIVES, SOUND SPEEDS, AND ELASTIC CONSTANTS

In this section we consider the relationships between the stress derivatives $S_{\alpha\beta\gamma\delta}$ that appear in the expressions for the Rayleigh velocity, Eqs. (17) and (20), the speeds of longitudinal and transverse sound waves, and the adiabatic elastic constants. These relations have been discussed by Wallace,[14] but we use a slightly different approach and consider mainly the case of initial stresses that are purely in the surface xz plane.

Hooke's law for a prestressed material is

$$\sigma_{\alpha\beta} = \sigma^0_{\alpha\beta} + S_{\alpha\beta\gamma\delta}\epsilon_{\gamma\delta} \ , \qquad (A1)$$

where the coefficients $S_{\alpha\beta\gamma\delta}$ are derivatives of the stress with respect to unsymmetrized strains evaluated at the initial prestressed state. The strain tensor $\epsilon_{\alpha\beta} = \partial u_\alpha/\partial x_\beta$ can be split into symmetric and antisymmetric parts,

$$\epsilon_{\alpha\beta} = \epsilon^+_{\alpha\beta} + \epsilon^-_{\alpha\beta}, \quad \epsilon^\pm_{\alpha\beta} = \tfrac{1}{2}(\epsilon_{\alpha\beta} \pm \epsilon_{\beta\alpha}) \ , \qquad (A2)$$

and Hooke's law Eq. (A1) becomes

$$\sigma_{\alpha\beta} = \sigma^0_{\alpha\beta} + S^+_{\alpha\beta\gamma\delta}\epsilon^+_{\gamma\delta} + S^-_{\alpha\beta\gamma\delta}\epsilon^-_{\gamma\delta} \ , \qquad (A3)$$
$$S^\pm_{\alpha\beta\gamma\delta} = \tfrac{1}{2}(S_{\alpha\beta\gamma\delta} \pm S_{\alpha\beta\delta\gamma}) \ .$$

If the initial stress is nonhydrostatic, it is rotated by the antisymmetric component of the strain tensor. Thus $S^-_{\alpha\beta\gamma\delta}$ can be obtained from the rotational properties of the stress tensor. Consider a material that is prestressed in the xz plane and subjected to an antisymmetric strain $-\epsilon_{xy} = \epsilon_{yx} = \epsilon$. This corresponds to an infinitesimal counterclockwise rotation ϵ about the z axis. To first order only the shear stress is affected,

$$\sigma_{xy} = -(S^-_{xyxy} - S^-_{xyyx})\epsilon = \sigma^0_{xx}\epsilon \ , \qquad (A4)$$

and from this it follows that $S^-_{xyyx} = -S^-_{xyxy} = \tfrac{1}{2}\sigma^0_{xx}$, with all other components of $S^-_{\alpha\beta\gamma\delta}$ (not including z) being zero. This is in agreement with the general expression in Ref. 14:

$$S^-_{\alpha\beta\gamma\delta} = \tfrac{1}{2}(\sigma^0_{\alpha\delta}\delta_{\beta\gamma} - \sigma^0_{\alpha\gamma}\delta_{\beta\delta} + \sigma^0_{\beta\delta}\delta_{\alpha\gamma} - \sigma^0_{\beta\gamma}\delta_{\alpha\delta}) \ . \qquad (A5)$$

The linearized equations of motion describing elastic-wave propagation in a prestressed material are

$$\rho\ddot{u}_\alpha=\nabla_\beta\sigma_{\alpha\beta}=S_{\alpha\beta\gamma\delta}\frac{\partial^2 u_\gamma}{\partial x_\beta \partial x_\delta} . \quad (A6)$$

The symmetry properties of the coefficients $S_{\alpha\beta\gamma\delta}$ are not the same as those of the elastic-wave propagation coefficients derived by Wallace.[14] This is due to the differences between differentiating in Eulerian and Lagrangian coordinate systems, but it will be shown that the equations of motion for $\ddot{u}_\alpha$ are exactly the same, as would be expected in the linearized case. Some of these coefficients are directly related to the propagation velocities of bulk acoustic waves parallel to $[\vec{k}=(k,0,0)]$ and perpendicular to $[\vec{k}=(0,k,0)]$ the surface:

$$\rho^{-1}S_{xxxx}=c_L^{\parallel 2},\ \ \rho^{-1}S_{yyyy}=c_L^{\perp 2} ,$$
$$\rho^{-1}S_{xyyx}=c_T^{\parallel 2},\ \ \rho^{-1}S_{xyxy}=c_T^{\perp 2} . \quad (A7)$$

It is sometimes useful to relate the stress derivatives $S_{\alpha\beta\gamma\delta}$ to the adiabatic elastic constants $C_{\alpha\beta\gamma\delta}$ which are usually defined as derivatives with respect to symmetric Lagrangian strains,

$$\eta_{\alpha\beta}=\tfrac{1}{2}(\epsilon_{\alpha\beta}+\epsilon_{\beta\alpha}+\epsilon_{\gamma\alpha}\epsilon_{\gamma\beta}) , \quad (A8)$$

since the energy is rotationally invariant. For a small but finite strain, the internal energy can be expanded in a power series of Lagrangian strains,

$$E=E_0+(V\sigma_{\alpha\beta})_0\eta_{\alpha\beta}+\tfrac{1}{2}(VC_{\alpha\beta\gamma\delta})_0\eta_{\alpha\beta}\eta_{\gamma\delta}+\cdots , \quad (A9)$$

where the subscript 0 indicates the initial prestressed state. All the strains are measured from this state. The relation between the stress and the internal energy can be obtained from a consideration of the work done during a finite deformation[14] with the result

$$V\sigma_{\alpha\beta}=\frac{\partial E}{\partial\eta_{\alpha\beta}}+\epsilon_{\alpha\epsilon}\frac{\partial E}{\partial\eta_{\beta\epsilon}}+\epsilon_{\beta\epsilon}\frac{\partial E}{\partial\eta_{\alpha\epsilon}}+O(\epsilon^2)+\cdots . \quad (A10)$$

The stress derivative is then given by

$$S_{\alpha\beta\gamma\delta}=\left[\frac{\partial\sigma_{\alpha\beta}}{\partial\epsilon_{\gamma\delta}}\right]_0=\sigma^0_{\alpha\delta}\delta_{\beta\gamma}+\sigma^0_{\beta\delta}\delta_{\alpha\gamma}-\sigma^0_{\alpha\beta}\delta_{\gamma\delta}+C_{\alpha\beta\gamma\delta} , \quad (A11)$$

where we have used the relation $V=V_0(1+\epsilon_{\alpha\alpha})$. This agrees with the stress-strain coefficients derived by Wallace,[14] but is different from the elastic-wave propagation coefficients $A_{\alpha\beta\gamma\delta}=\sigma_{\beta\delta}\delta_{\alpha\gamma}+C_{\alpha\beta\gamma\delta}$ for the reason discussed earlier. The equations of motion, though, only require a symmetric combination of $S_{\alpha\beta\gamma\delta}+S_{\alpha\delta\gamma\beta}=A_{\alpha\beta\gamma\delta}+A_{\alpha\delta\gamma\beta}$ and are thus identical.

If the solid is at sufficiently low temperatures, the fluctuation contributions to the elastic constants[25] can be ignored. If, in addition, the forces are pairwise additive, the Cauchy conditions are satisfied and the elastic constants are symmetric with respect to any permutation of suffixes. The expression for the Rayleigh velocity then reduces to the root of a quadratic equation (20). In general, the static lattice contribution to the stress and adiabatic elastic constants for pairwise additive forces is

$$V\sigma_{\alpha\beta}=\sum_{i>j}\frac{r_\alpha r_\beta}{r^2}(r\phi'),\ \ r_\alpha=r^i_\alpha-r^j_\alpha ,$$
$$VC_{\alpha\beta\gamma\delta}=\sum_{i>j}\frac{r_\alpha r_\beta r_\gamma r_\delta}{r^4}(r^2\phi''-r\phi') . \quad (A12)$$

These expressions together with (A11) were used to calculate the stress derivatives in the triangular and face-centered-cubic lattices. In the case of the triangular lattice the stress derivatives were also calculated from the velocities of elastic waves using the equations of motion (2a). The results agree, and are summarized below,

$$S_{xxxx}-\sigma^0_{xx}=C_{xxxx},\ \ S_{yyyy}=C_{yyyy} ,$$
$$S_{xxyy}+\sigma^0_{xx}=S_{yyxx}=C_{xxyy}=C_{xyxy}$$
$$=S_{xyxy}=S_{xyyx}-\sigma^0_{xx} , \quad (A13)$$

$$V\sigma^0_{xx}=Kd_0^2[4(d_x/d_0)^2-2(d_x/d_0)] ,$$
$$VC_{xxxx}=Kd_0^2[2(d_x/d_0)+2(d_x/d_0)^4] ,$$
$$VC_{yyyy}=Kd_0^2[2-4(d_x/d_0)^2+2(d_x/d_0)^4] . \quad (A14)$$
$$VC_{xyxy}=Kd_0^2[2(d_x/d_0)^2-2(d_x/d_0)^4] .$$

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