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PHONONS AT METAL SURFACES

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Abstract. - We examine phonons at metal surfaces using hydrodynamic equations. The principle focus is on the strength of the electric field produced outside the metal by such oscillations. We find that the magnitudes of these coupling strengths for both surface and bulk modes depend crucially on the boundary conditions imposed at the surface.

1. Hydrodynamic model. - Our linearized continuum model of the coupled motion of electrons and ions is defined by the equations:

$$\frac{\partial \vec{E}_i}{\partial t} = \frac{\Omega_i^2}{4\pi} \vec{E}_i + \rho_0 \left[ c_L^2 \vec{\nabla} \cdot (\vec{\nabla} \vec{E}_i) - c_T^2 \vec{\nabla} \times (\vec{\nabla} \times \vec{E}_i) \right]$$  \hspace{1cm} (1a)

$$\frac{\partial \vec{E}_e}{\partial t} = \frac{\omega_p^2}{4\pi} \vec{E}_e - \rho_0 \left[ \beta_e^2 \vec{\nabla} \cdot (\vec{\nabla} \vec{E}_e) \right]$$  \hspace{1cm} (1b)

$$\vec{\nabla} \cdot \vec{E}_i = 4\pi \rho_0 (\vec{\nabla} \cdot \vec{E}_i) - \vec{\nabla} \cdot \vec{E}_e$$  \hspace{1cm} (1c)

where e and i subscripts refer, respectively, to electrons and ions; $\vec{E}$ is the (longitudinal) electric field; $\rho_0$ the (constant) equilibrium ion charge density, $\Omega_i$ and $\omega_p$ are the ion and electron plasma frequencies; and the $c$'s and $\beta$'s are short range restoring forces; and the $\vec{E}$'s are displacement fields related by a time derivative to the current densities $\vec{j}_i = \omega_0 \frac{\partial \vec{E}_i}{\partial t}$ and $\vec{j}_e = -\rho_0 \frac{\partial \vec{E}_e}{\partial t}$. Note that we have neglected retardation and discrete lattice effects and that only the ions sense transverse forces, via $c_T$. In bulk material at a general frequency $\omega$, one has electronic longitudinal waves and ionic longitudinal and transverse waves. When one considers excitations near a surface, where $\rho_0$ drops discontinuously to zero, linear combinations of these bulk modes plus excitations varying as $\exp(\text{ik}\cdot x - \omega t)$ must be used. Here $\chi$ (and the wavevector $Q$) lies in the surface plane while $x$ is normal to it. The coupled modes are labeled by $\omega$, $Q$, and polarization indices. To determine the eigenmodes of (1) requires in general the imposition of five independent surface boundary conditions. For the first two, we use continuity of the potential $\Phi$ ($\vec{E} = -\vec{\nabla} \Phi$) and continuity of the normal component of the displacement field. This last is equivalent to $\Delta (\vec{E} \cdot \hat{x}) = 4\pi \sigma_s$, where $\sigma_s$ is the induced surface charge density and $\Delta (\ldots)$ means the discontinuity in (\ldots). For the other boundary conditions we have examined several possibilities. Consideration of metal or plasma physics suggests we set $c_T = 0$, which eliminates the transverse modes and
one boundary condition, and for the remaining two conditions require at the surface,
\[ \mathbf{j} \cdot \mathbf{x} = 0 = \mathbf{j}_e \cdot \mathbf{x}, \]  
which we call case C. Note that (2) implies \( \sigma = 0 \). On the other hand, elasticity theory suggests we keep \( c_T \neq 0 \) and instead require (case S)
\[ \sigma_1 \cdot \mathbf{x} = 0 = \sigma_e \cdot \mathbf{x}, \]  
where \( \sigma_{1, e} \) is the stress tensor that leads to (1).

2. Results. — The different boundary conditions (2) and (3) lead to dramatically different predictions. Consider first possible surface modes. With (2) there is a surface mode just below (at each \( Q \)) the bulk longitudinal modes. This mode has been found also in less general \( (c_L = 0) \) models.\[1,2\] With (3) a surface mode only appears below the bulk transverse modes. This surface mode is in essence a (stiffened) Rayleigh wave. It requires a finite \( c_T \) and the effective longitudinal sound speed is \( v_L = c_L^2 + c_T^2 \) where \( \Omega_{p} = \pi k_{x} \) with \( k_{x} = \frac{\omega}{\beta} \). To discuss the possible external coupling to these modes we have quantized \( \sigma \) and write the external potential as \( \Phi(x) = \sum_0 Q \Lambda_0 e^{iQ \cdot x} e^{-Q \cdot x} (a^+ + a) \) where \( a^+ (a) \) is a creation (annihilation) operator for the surface mode \( Q \). A similar expression holds for the coupling to bulk modes. In figure 1 we plot \( \Lambda_0 \) vs. \( Q \) for the cases C and S and also an analogous quantity from the theory of Rahman and Mills\[3\], case R.

![Fig. 1: External coupling strength parameter \( \Lambda \) for surface modes resulting from different boundary conditions versus surface wavevector \( Q \). All \( \Lambda \)'s are in the same arbitrary units. Other symbols are defined in the text.](image)

In figure 2 we plot a quantity \( b \), proportional to the sum of the squares of all the finite \( \Lambda \)'s for the bulk modes at each \( \omega \) and \( Q \). Simple integrals of \( b \) determine experimental quantities such as image potentials, electron loss spectra, or thermal diffuse scattering.
The most striking feature of both figures (1) and (2) is the small relative size of the $A$'s for case S. They are reduced by roughly $\frac{\Omega_p^2}{\omega^2}$ compared to those for cases C or R. Closer study shows that the condition $\sigma_{e,x=0}$ is the cause of this reduction. Requiring the electrons to sense zero stress at the surface essentially suppresses any external fields at frequencies comparable to $\Omega_p \ll \omega$. This work was supported in part by the NSF through grant DMR 78-10235.

References