that the carbon is a truly surface contaminant is undoubtedly an oversimplification. If, as we have argued, the carbon originates in the bulk of the target ribbon, it is entirely reasonable to suppose that sufficient concentrations of carbon can accumulate in the vicinity of the surface (i.e., the nearest few atomic layers) to cause the density-of-states function there to differ significantly from that for a pure Mo sample. Hence the changes observed in the shapes of the distributions here may reflect changes in bulk band structure as well as Auger transition probability.

SUMMARY

Measurements have been made of the Auger electron emission from polycrystalline molybdenum targets bombarded by He^+ and Ar^+. It has been found that carbon impurities present in the Mo sample reduce the value of the electron yield below that for an atomically clean surface. In accordance with previous work, it was found that the carbon could not be removed from the target by heating in vacuum, but that a short heat treatment in an O_2 atmosphere would remove it, producing an atomically clean surface. This contamination effect is thought to be responsible for some discrepancies in electron yields reported in the literature.

The differences between the Auger electron yields for the clean and carbon-contaminated surfaces can be at least qualitatively explained in terms of an increase of about 0.5 eV in work function of the contaminated surface relative to the clean-surface value. The measured increase of 0.4 eV supports this model. Measurements of the ejected electron-energy distributions for the two surfaces, however, show differences which do not seem interpretable on the basis of this simple model. Rather, it seems that in this case the carbon must be regarded as having a more subtle influence, perhaps involving alterations of the Mo band structure by impurity carbon in the bulk of the sample.

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Landau Damping and Dispersion of Phonon, Plasmon, and Photon Waves in Polar Semiconductors

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Landau damping results from the loss of energy of collective motion to the excitation of individual particles. Well known for plasmons, it can also occur for phonons and photons, as is shown herein. For a coupled longitudinal plasmon–optical-phonon wave, it can be significant both near the phonon resonance and near the plasmon resonance. It is generally insignificant for coupled transverse photon–optical-phonon waves. These results are important for infrared spectroscopy and Raman scattering involving plasmons and optical phonons.

I. INTRODUCTION

THE Landau damping of a plasma wave is due to the loss of energy from a collective motion to the individual particles, such as a plasmon decaying by exciting an electron below the Fermi energy. This occurs when the phase velocity of the wave becomes comparable to the thermal speed of the electrons,[1,2] i.e., when the wave number q of the plasmon is comparable to q_{Debye} of the electrons defined by $q_D = (\text{plasma frequency})/v_{\text{thermal}}$. In a coupled system of infrared active longitudinal optical phonons and plasmons, the optical phonons may also decay by exciting electrons. Thus, in addition to the usual optical-phonon loss due to lattice anharmonicity, we have the Landau damping of the optical phonons. The dispersion relations of a coupled system of longitudinal plasma waves and longitudinal optical and acoustic phonons have been examined by Tsu and White.[3] Due to the use of the moment equations of the Boltzmann transport equation, their results do not contain the effects of Landau damping. Varga[4] used the Drude model for the electron gas to derive dispersion relations which include the transverse case, one in which the transverse optical phonons interact with the dressed photons, i.e., photons dressed by electrons. More recently, Singwi and Tosi[5] used the electrostatic interaction Hamiltonian of a longitudinal optical phonon and an electron gas to obtain a dispersion relation similar to Varga's. However, because of the use of a power-series expansion of the dielectric response function in powers of the wave number, their results, like Varga's, also exclude Landau damping. In a coupled system, at frequencies near the optical-phonon resonant frequency, the condition of matching the phase velocity to the thermal speed of the

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electrons may be satisfied. Thus, Landau-damping losses may be significant near the optical-phonon frequencies in addition to the usual Landau-damping losses of the plasmons near the plasma frequency. However, if the optical-phonon damping due to lattice anharmonicity is taken into account, the condition for Landau damping can be met only for the longitudinal case, but not for the transverse case. Hence, in Raman[6,7] scattering involving plasmons and longitudinal optical phonons, Landau damping may be an important factor in the line broadening, whereas in experiments[8] involving reflection and transmission of infrared light near the optical-phonon frequencies, Landau damping in almost all cases may be ignored.

II. DISPERSION RELATIONS

The coupled system is represented by putting the free electrons of density n_0 into an infrared active crystal. For simplicity, it is assumed that the crystal may be represented by scalar dielectric constants, a high-frequency one which measures the atomic polarizations, and a low-frequency one which measures the polarizations of the optical phonons. The effects of the free carriers are accounted for by using the currents induced by a self-consistent field. Using these currents in Maxwell-Lorentz equations together with the relations[9] for the polarization and displacement vectors for optical phonons at long wavelengths, the dispersion relations become

$$\epsilon_t+4\pi\sigma/i\omega-\epsilon_\infty+(\epsilon_0-\epsilon_\infty)\omega_0^2/(\omega^2-\omega_0^2+i\gamma\omega)=0, \quad (1)$$

where $\epsilon_t=0$, $\sigma=\sigma_l$ for the longitudinal case, and $\epsilon_t=q^2c^2/\omega^2$, $\sigma=\sigma_t$ for the transverse case. In Eq. (1), c is the speed of light, γ is the optical-phonon linewidth due to damping mechanisms other than Landau damping (e.g., lattice anharmonicity), ω_0 is the optical-phonon resonant frequency, ϵ_∞ and ϵ_0 are the high- and low-frequency limits of the dielectric constants, and σ_l and σ_t are the longitudinal and transverse conductivities, respectively.

III. CURRENTS DUE TO THE SELF-CONSISTENT FIELDS

The conductivities σ_l and σ_t due to a time-dependent self-consistent field have been treated by several authors.[10–12] In order to obtain expressions most readily useful for the dispersion relations including quantum effects, charge bunching, Landau damping, and collision damping arising from collisions of electrons with thermal phonons and impurities, we shall briefly derive these conductivities from the self-consistent equation of motion of the single particle density matrix ρ,

$$i\hbar\dot{\rho}=[H_0+H_1,\ \rho]-i\hbar(\partial\rho/\partial t)_c, \quad (2)$$

with $H_0=P^2/2m$, $H_1=-(e/2mc)(\mathbf{P}\cdot\mathbf{A}+\mathbf{A}\cdot\mathbf{P})+e\phi$, in which $\mathbf{A}$ and ϕ are the self-consistent vector and scalar potentials, and $\mathbf{P}$ and m are the momentum and effective mass of the electrons.

For the longitudinal case, the collision term $(\partial\rho/\partial t)_c$ is described by a phenomenological frequency independent ν to account for the finite lifetime of the electrons due to collision with thermal phonons and impurities. In order to account for the charge bunching described by a local density n_1, we let[13]

$$(\partial\rho/\partial t)_c=[\rho-\rho_0(1+n_1/n_0)]\nu, \quad (3)$$

in which $\rho\equiv\rho_0+\rho_1$, and n_0 is the electron density. The average current and density are calculated from $\mathbf{J}=\mathrm{Tr}(\mathbf{S}\rho)$ and $n_1=\mathrm{Tr}[\delta(\mathbf{x}-\mathbf{x}')(\rho-\rho_0)]$, with the current operator $\mathbf{S}$ defined by $\mathbf{S}=(e/2m)[(\mathbf{P}-(e/c)\mathbf{A}),\delta(\mathbf{x}-\mathbf{x}')]_+$. For the transverse case, a simple way to account for the effects of collision is to set $\rho=\rho_0+\rho_1(t)e^{\nu t}$, $\mathbf{A}=\mathbf{A}(t)e^{\nu t}$, and $(\partial\rho/\partial t)_c=0$.[14] Although these forms suggest processes involving adiabatic turning on of the perturbations, ν is finite in our case.

We shall not go into a detailed treatment in view of the fact that Spector[15] has done a similar calculation without collision damping. (Spector's conductivity, represented by his Eq. (213a), has an error in sign.) Neglecting the term $H_1\rho_1$ and taking

$$\rho_0\,|\,k\rangle=f(k)\,|\,k\rangle, \qquad H_0\,|\,k\rangle=(\hbar^2k^2/2m\,|\,k\rangle,$$

with $|\,k\rangle$ the free particle wave function of the electron momentum $\mathbf{k}$, we obtain for the transverse and longitudinal current densities

$$\mathbf{J}_t=-\frac{\omega_p^2}{4\pi i(\omega+i\nu)}\{\hat{t}\hat{t}-n_0^{-1}\sum_{\mathbf{k}}D^{-1}\times[f(k)-f(k+q)](\mathbf{k}+\mathbf{q}/2)(\mathbf{k}+\mathbf{q}/2)\}\cdot\mathbf{E}_t, \quad (4a)$$

$$\mathbf{J}_l=\sum_k\frac{\omega_p^2}{4\pi iq}\frac{m}{\hbar n_0}D^{-1}\times[f(k)-f(k+q)][\hat{z}(k_z+q/2)+\hat{t}k_t]E_l-i\sum_k\frac{e\nu n_1}{n_0D}f(k)[\hat{z}(k_z+q/2)+\hat{t}k_t], \quad (4b)$$

$$n_1=-\frac{iem}{\hbar^2q}\sum_{\mathbf{k}'}D^{-1}[f(k')-f(k'+q)]E_l, \quad (4c)$$

$$D\equiv\mathbf{k}\cdot\mathbf{q}+\tfrac{1}{2}q^2-m(\omega+i\nu)/\hbar, \quad (4d)$$

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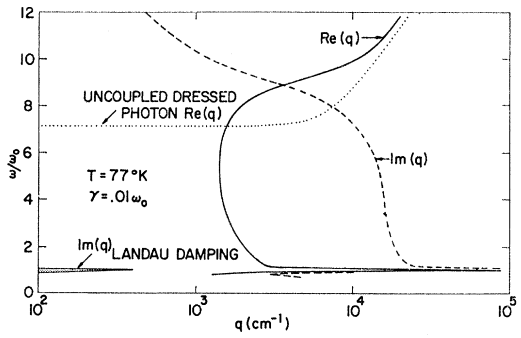

FIG. 1. Dispersion relation for SnTe for a coupled system of transverse optical phonons and dressed photons. The constants used are $\epsilon_0=1200$, $\epsilon=45$, $\omega_0=10^{13}$, $\omega_p=4.78\times10^{14}$, $\nu=10^{13}$, $\gamma=0.01\omega_0$, and $m=0.07m_e$ [taken from G. Pawley, *et al.*, Phys Rev. Letters, **17**, 753 (1966); H. R. Riedl, J. R. Dixon, and R. B. Schoolar, Solid State Commun. **3**, 323 (1965); R. Tsu, W. E. Howard, and L. Esaki, *ibid.* **5**, 167 (1967)]. Shaded region shows the $(\mathrm{Im}q)_{\mathrm{L.D.}}$.

where $\omega_p^2=4\pi n_0e^2/m$, $\mathbf{E}_l=-\nabla\phi$, $\mathbf{E}_t=(i\omega/c)\mathbf{A}$, and, $\hat{l}$ and $\hat{z}$ are the unit vectors transverse to and parallel to q. In the second term of Eq. (4b), the electric-field factor is contained in the density function n_1. It looks as if the conductivity tensors derived from Eqs. (4) would have off-diagonal components. Actually these off-diagonal terms will vanish when the sum over k is performed. After the sums over k are replaced by integrals, we have integrals of the form

$$I(Z)=\int_{-\infty}^{\infty}\frac{g(k_z)\,dk_z}{k_z-Z}, \tag{5}$$

where $Z=X+iY=(m\omega/\hbar q-\frac{1}{2}q)-i(m\nu/\hbar q)$. Because ν is not infinitesimal, the path of integration should be moved up the imaginary Z plane to

$$-\infty+iY\rightarrow+\infty+iY.$$

Therefore, Eq. (5) may be written as[16]

$$I(Z)=\sum_{n=0}^{\infty}(n!)^{-1}(iY)^n\left[\mathcal{P}\int_{-\infty}^{\infty}\frac{g^{(n)}(k_z)\,dk_z}{k_z-X}+i\pi g^{(n)}(X)\right], \tag{6}$$

where $g^{(n)}(X)=\partial^n g/\partial k_z^n\,|_X$. For simplicity, we shall calculate up to $n=1$, which is sufficient for a comparison of the imaginary parts involving ν with those not involving ν, i.e., the Landau-damping contribution to the losses. Further, we shall neglect the second term in Eq. (4b), which is only important for very high ν, electric field and carrier concentration. Upon using the Maxwellian distribution function for $f(k)$, we obtain the longitudinal conductivity

$$\sigma_l=-\omega_p^2B/4\pi iq, \tag{7}$$

where

$$B=v^{-1}[1+\tfrac{3}{2}(v_r/v)^2]-(2\sqrt{\pi})(m\nu/\hbar v_r)(v/v_r)^2\times[\exp(\hbar\omega/2KT)-\exp(-\hbar\omega/2KT)]\times\exp[-(v/v_r)^2]-iv^{-1}(\nu/\omega)(1+\tfrac{9}{2}(v_r/v)^2)-(i\sqrt{\pi})(m/\hbar q)(v/v_r)[\exp(\hbar\omega/2KT)-\exp(-\hbar\omega/2KT)]\exp[-(v/v_r)^2],$$

and $v=\omega/q$, $v_r^2=2KT/m$. The terms involving exponentials come from the $i\pi g^n(X)$ term in Eq. (6) and have been integrated exactly. The imaginary exponential term is the Landau-damping contribution to the losses. The condition stated previously that the Landau damping becomes significant as $v\rightarrow v_{\mathrm{thermal}}$ derives from the factor $\exp[-(v/v_r)^2]$ in Eq. (7). This condition is actually not exact, since for very large q, the pole of the integrand in Eq. (6) gives the condition for Landau damping which is also the condition for pair creation. The other terms which come from the principal-value integrals are integrated approximately. We caution that our results are only valid for small but finite ν, e.g., $\nu\ll\omega$, because we have terminated the series at $n=1$ in Eq. (6). For large ν, the classical moment equations of the Boltzmann equation give far simpler expressions.[3] Similarly, the transverse conductivity is

$$\sigma_t=-[\omega_p^2/4\pi i(\omega+i\nu)](1+B_t), \tag{8}$$

with

$$B_t=[(v_r/v)]^2[1-i(2\nu/\omega)]-[(2\sqrt{\pi})(\nu/qv_r)(v/v_r)+i\sqrt{\pi}]\times[\exp(\hbar\omega/2KT)-\exp(-\hbar\omega/2KT)]\exp[-(v/v_r)^2].$$

If $B_t=0$, then σ_t is identical to that of the Drude theory including damping.

IV. DISCUSSION

If we take $B=v^{-1}(1-iv/\omega)$, and $B_t=0$ for σ_l and σ_t in Eq. (1), we obtain two dispersion relations similar to Varga's.[4] The dressed photon-transverse optical phonon coupled mode has q dependence, and thus has

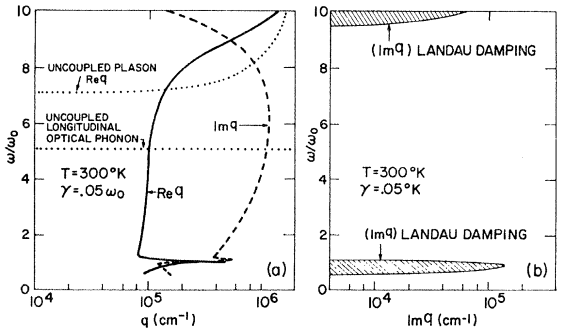

FIG. 2. Dispersion relation for SnTe for a coupled system of longitudinal optical phonons and plasmons for $\gamma=0.05\omega_0$.

[16] J. D. Jackson, J. Nucl. Energy: Pt. C, **1**, 171 (1960).

dispersion. However, because of this simple form of B, the longitudinal expression is only a frequency equation, being independent of q. Because our B has q dependence, the longitudinal expression is also a dispersion relation, an expression for ω as a function of q. At this point, a brief mention on the comparison of the dispersion relations obtained here and those by Tsu and White[3] is in order, particularly because both the forms and methods used are different. Neglecting the Landau damping and terms involving ν in σ_l, the dispersion relation for the longitudinal optical phonon-plasmon coupled mode may be written as

$$[\omega^2-\omega_p^2/\epsilon_\infty-\tfrac{3}{2}v_r^2q^2(\omega_p^2/\epsilon_\infty\omega^2)](\omega^2-\omega_0^2)$$
$$=(\epsilon_0/\epsilon_\infty-1)\omega_0^2\omega^2. \quad (9)$$

On the other hand, Eq. (26) of Tsu and White

$$[1+iD_a+i(\omega_p^2/\epsilon_\infty)(1/\omega\nu)](\omega^2-\omega_0^2)=g\omega_0^2(1+iD_a),$$

with $D_a=(\omega/\nu)(3v_r^2q^2/\omega^2-1)$, and $\omega\gg\nu$, may be written identical to Eq. (9) if $g=\epsilon_0/\epsilon_\infty-1$. It is interesting to note that Tsu and White used $g=e_1^2/C_1\epsilon_\infty$, with e_1 and C_1 being the appropriate piezoelectric constant and elastic constant, respectively, for CdS crystal.

Using the full B and B_t in σ_l and σ_t, we have computed Req and Imq from Eq. (1) as shown in Figs. 1 and 2. First we neglect parts of q due to Landau damping for the dispersion relations, then these values of ω and q are used to compute Landau damping. For the transverse case, note that $(\mathrm{Im}q)_{\mathrm{LD}}$, imaginary part of q due to Landau damping, is much smaller than the Req and Imq. However, as shown in Fig. 2, $(\mathrm{Im}q)_{\mathrm{LD}}$ may be comparable to Req for the longitudinal case. Also, because of screening, the longitudinal optical phonon mode is lowered to $\omega\sim\omega_0$. Fig. 3 shows another example for SnTe. The shaded region bordered by two parabolic functions, denoted as the pair-creation region (electron below the Fermi surface excited above the Fermi surface), is the region of ω–q where Landau damping may be significant. The longitudinal branch crosses into this region twice, once near ω_0, and the second time slightly above the plasma frequency. The latter one produces the usual Landau damping of the plasmon, a plasmon decaying by exciting an electron. The former represents the decay of an optical phonon by exciting an electron. The broader parts of the ω–q curve indicates where $(\mathrm{Im}q)_{\mathrm{LD}}$ are significant, such as the example shown in Fig. 2. However, the dispersion curve for the coupled mode of dressed photon and transverse optical phonon is not anywhere near the pair-production region. In principle, if the losses due to lattice anharmonicity are negligible, then even for the transverse case as in Fig. 1, near ω_0, q will have large enough values to approach the shaded region. As the dispersion curve for the transverse case in Fig. 3 has

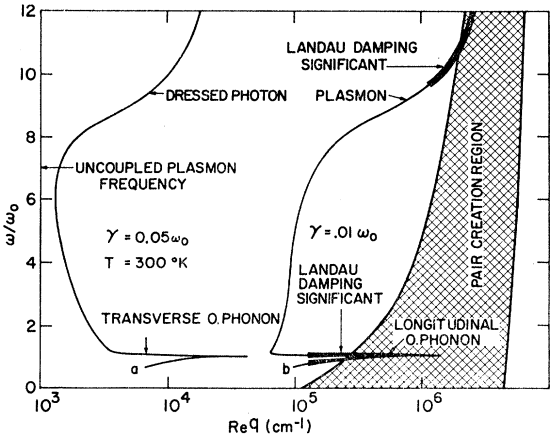

FIG. 3. Dispersion relation for SnTe, $\gamma=0.05\omega_0$ for the transverse case and $\gamma=0.01\omega_0$ for the longitudinal case. The shaded region shows where Landau damping may be significant. (This region, denoted by pair creation region, refers to the excitation of electrons from below the Fermi surface as contrary to usual excitation of electron-hole pairs across the valence and conduction bands.)

a lattice damping five times greater than the example used for Fig. 1, Landau damping for this case is almost zero. It is frequently true in practice that the lattice damping is large enough so that Landau damping may be ignored for the transverse case. In the case of Raman scattering from longitudinal optical phonons, the line broadening due to Landau damping will be important for infrared active materials with low lattice anharmonicity and relatively high mobility. At the moment, low carrier concentration SnTe materials are not available, so that we do not know the pure optical-phonon damping due to lattice anharmonicity. Consequently, experiments involving SnTe cannot separate Landau damping from others.

The coupling of the phonon and plasma waves does shift the resonant frequencies of these waves. Due to the inclusion of an electron-collision term, phonon modes are damped through coupling to the plasmons even without lattice anharmonicity. However, it is important to realize that the Landau damping of the phonon results from its interaction to the individual electrons. As pointed out by Platzman and Buchsbaum[13] for the case of plasmons, collision is only necessary to maintain a steady-state Landau damping.

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