



Local response theory of surface plasmons in the space-charge layer of GaAs (110)
by Bingruo Xu

A thesis submitted in partial fulfillment of the requirements for the degree of Master of Science in
Physics
Montana State University
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Abstract:

We study surface plasmons and phonons on n-type semiconductors, for non-uniform free-carrier density profiles, through use of the dielectric theory of electron-energy-loss spectroscopy and nonlocal description of the response of the electrons.

First, self-consistent calculations of the spatial variation of the conduction-electron density near the surface of n-type GaAs are presented. Second, the dielectric function and effective dielectric function are discussed, in which the Thomas-Fermi model and the Debye-Huckel model are introduced. Third, the energy loss spectra for bulk free-carrier densities of (1) $n_0=1.2 \times 10^{17} \text{ cm}^{-3}$ (2) $n_0=1.3 \times 10^{18} \text{ cm}^{-3}$ (3) $n_0=1.5 \times 10^{18} \text{ cm}^{-3}$ have been calculated. For each value of n_0 , we consider three values of the surface charge density, $Q_s=-0.08, 0.0, \text{ and } 0.08$ in thermal units, and plot the variation with wavevector of the maximum of the loss function. By varying these parameters we investigate a wide range of charge-density profiles and surface potentials; for example, our depletion layers have widths of 50Å, 75Å and 100Å. The results obtained with the local response theory are compared with Mills' results which come from a nonlocal theory.

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APPROVAL

of a thesis submitted by

Bingruo Xu

This thesis has been read by each member of the thesis committee and has been found to be satisfactory regarding content, English usage, format, citations, bibliographic style, and consistency, and is ready for submission to the College of Graduate Studies.

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June 9, 1989

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ABSTRACT

We study surface plasmons and phonons on n-type semiconductors, for non-uniform free-carrier density profiles, through use of the dielectric theory of electron-energy-loss spectroscopy and nonlocal description of the response of the electrons.

First, self-consistent calculations of the spatial variation of the conduction-electron density near the surface of n-type GaAs are presented. Second, the dielectric function and effective dielectric function are discussed, in which the Thomas-Fermi model and the Debye-Huckel model are introduced. Third, the energy loss spectra for bulk free-carrier densities of (1) $n_0=1.2 \times 10^{17} \text{cm}^{-3}$ (2) $n_0=1.3 \times 10^{18} \text{cm}^{-3}$ (3) $n_0=1.5 \times 10^{18} \text{cm}^{-3}$ have been calculated. For each value of n_0 , we consider three values of the surface charge density, $Q_s=-0.08, 0.0, \text{ and } 0.08$ in thermal units, and plot the variation with wavevector of the maximum of the loss function. By varying these parameters we investigate a wide range of charge-density profiles and surface potentials; for example, our depletion layers have widths of 50Å, 75Å and 100Å. The results obtained with the local response theory are compared with Mills' results which come from a nonlocal theory.

CHAPTER 1

INTRODUCTION

In the past century the studies of materials have been mainly focused on bulk properties. The understanding of surfaces and fundamental surface related processes has become feasible only in the last 20 years since modern technologies were developed.

During the past 20 years, electron-energy-loss spectroscopy (EELS) in the reflection geometry has emerged as a reliable technique for studying clean or contaminated surfaces. In this technique, monochromatized electrons backscattered from the surface of a target material are analyzed in energy to detect losses and gains characteristic of surface plasmons or vibrational excitations. First restricted to conducting targets, high resolution EELS experiments have recently been successfully performed with insulators and semiconductors,¹ so that this technique is now generally applicable as a powerful spectroscopic tool for the study of any material surface.

Near the surface of a doped semiconductor, the carrier density often differs dramatically from that in the bulk. Depletion layers may be encountered as thick as a few hundred angstroms, within which the free-carrier density drops dramatically below that in the bulk, or accumulation layers which contain an excess of carriers near the surface. In the first part of this thesis, self-consistent calculations of the

spatial variation of the conduction-electron density near the surface of n-type GaAs is presented, for the case where the surface is charge neutral, or bears net positive or negative charge. The model smears the charge density produced by ionized donors in the bulk into a jellium background, and introduces the effect of surface charge through a uniform electric field emanating from the surface. In this part, the Schrodinger equation subject to Poisson's equation and Fermi statistics is solved. The Hartree approximation is used to describe the electron-electron interaction.²

Recently, an adequate theoretical approach to EELS was developed within the so-called dielectric theory,^{3,4} where the electrons are considered as classical particles, while the absorption and emission of phonons or plasmons are treated quantum mechanically. In the theoretical description, the dielectric constant $\epsilon(k,\omega)$ depends on frequency and wave vector. With retardation ignored, the frequency ω_s of the surface plasmon is determined through the relation $\epsilon(\omega_s)=-1$. If ω_p is the plasma frequency of the free carriers, and ϵ_∞ the high-frequency dielectric constant, then^{5,10}

$$\epsilon(\omega)=\epsilon_\infty-\omega_p^2/(\omega^2+i\gamma\omega)$$

and

$$\omega_s=\omega_p/(\epsilon_\infty+1)^{1/2}.$$

Actually, ϵ depends not only on the frequency ω , but position z , since $\omega_p=4\pi n(z)e^2/m^*$ where m^* is the free-carrier effective mass. Calculations of $n(z)$, the conduction electron density, are described in the first part of this thesis. If the 2D wave vector k is not zero, but is very small, ϵ also depends on k . If we use the Thomas-Fermi model,⁶ then

$$\epsilon(k, \omega, z) = \epsilon_{\infty} - \omega_p^2 / [(\omega^2 - 0.6V_F^2 k^2) + i\omega\gamma]$$

where V_F is the Fermi velocity and γ is a damping factor.⁶

If we use the Debye-Huckel model,⁷ then

$$\epsilon(k, \omega, z) = \epsilon_{\infty} - \omega_p^2 / [(\omega^2 - 6k^2) + i\omega\gamma]$$

In fact, GaAs has an infrared active transverse optical phonon at long wavelengths. The background dielectric constant then is frequency dependent, and of the form⁸

$$\epsilon(\omega) = \epsilon_{\infty} + (\epsilon_0 - \epsilon_{\infty}) \omega_{TO}^2 / (\omega_{TO}^2 - \omega^2 - i\omega\gamma),$$

where ω_{TO} is the frequency of the long-wavelength transverse optical phonon, and ϵ_0 the static dielectric constant.

The dielectric theory can also be applied to anisotropic crystals, provided $\epsilon(\omega)$ in the loss function is replaced by an appropriate effective dielectric function $\xi(k, \omega)$. In Ref. 9, it is shown that the relevant effective dielectric function is equal to the surface value of the ratio of the displacement vector perpendicular to the surface, and the projection of the electric polarization field onto the direction of the surface wave vector k . The quantity is

$$\xi(k, \omega, z) = iD(k, \omega, z) \cdot n / [E(k, \omega, z) \cdot k/k],$$

with $D(k, \omega, z) = \epsilon(\omega, z)E(k, \omega, z)$, where $\epsilon(\omega, z)$, the long-wavelength dielectric constant

of the material, which may be a function of the coordinate z , is determined by $n(z)$.

In the regime of small-angle deflections, where surface plasmon contributions dominate the loss spectrum for back scattering from the surface of a simple semiconductor, the incident electron interacts with the excitations in the material through the fluctuating electric fields in the vacuum outside the material.¹¹ An incoming electron has an accompanying electric field which polarizes the medium. The induced field of polarization interacts back on the electron and damps its motion; in other words, the energy lost by the probing electron is dissipated by the medium. In this thesis the loss function will be dealt with classically. The amplitude of the induced field involves the factor $1/(\xi_0+1)$ where $\xi_0=\xi(z=0)$ is the effective surface dielectric function. The probability for energy loss will be proportional to this factor. A zero in the denominator of the loss function gives a peak in the loss spectrum.⁹

The position of the peak in the loss function is also calculated as a function of k , for the different values of the surface charge, for $T=300\text{K}$, and a carrier concentration of (1) $n_0=10^{18}\text{cm}^{-3}$ (2) $n_0=3*10^{17}\text{cm}^{-3}$. Dispersion curves, showing our results for the peak position vs. the wavevector, are plotted and compared with Mills' results.¹² In this thesis a local dielectric response description is applied, while Mills' results come from a full nonlocal description.

In summary, surface plasmons on n-type semiconductors are studied, for non-uniform free-carrier density profiles, through the use of a formalism describing electron-energy-loss spectroscopy. In the calculation of the inelastic cross section, the loss function $\text{Im}[-1/(\xi(k,\omega)+1)]$ is required as input. To derive the effective dielectric function, the dielectric function $\epsilon(k,\omega,z)$ needs to be calculated first. But $\epsilon(k,\omega,z)$ is directly related to $n(z)$. Thus we must first determine the free-carrier density profile.

The thesis is organized as follows. Chapter 2 presents self-consistent calculations of depletion-and accumulation-layer profiles for a range of carrier concentrations in n-type GaAs, at room temperature. Many figures are presented for several cases. In Chapter 3 and Chapter 4, we discuss the theory of the dielectric function and the effective surface dielectric function. In Chapter 5 we present the theory of the electron-energy-loss cross section and results for the dispersion relation, and Chapter 6 is devoted to a summary of our many results and principal conclusions.

CHAPTER 2

SELF-CONSISTENT CALCULATION OF DEPLETION-AND
ACCUMULATION-LAYER PROFILES

A uniformly doped n-type GaAs slab with thickness near 1400 Å is considered. The undoped crystal is to be regarded as a neutral medium whose electrical effect is simply to provide a background dielectric constant ϵ_{∞} . We consider an electric field E outside the material and normal to its surface, due to surface charges. The electric field just inside the material will be E/ϵ . When we consider boundary conditions on the potential, we will use the fact that the field outside the material is larger by a factor ϵ than that used in the boundary condition for the field inside.

The dynamic system we consider is the sea of conduction electrons which are free to move under the influence of various forces. There are two types of force¹³ that act on a conduction electron. The first type is the electrostatic force arising from the charge density of other conduction electrons, the uniform background of ionized donors, and the externally imposed uniform field. The second type is the exchange and correlation force. Exchange and correlation forces arise among conduction electrons due to dynamic and statistical correlations of their motion. We do not consider these forces here, since they are weak in our case.¹⁴

The system of equations includes Schrodinger's equation for the state of the conduction electrons, a constitutive equation giving the charge density in terms of

wavefunctions for the occupied states, and Poisson's equation giving the potential in terms of the charge density.

The single-particle wave functions are solutions² of an effective Schrodinger equation

$$\left[-\frac{\hbar^2}{2m^*} \nabla^2 + V(z) \right] \Psi_\alpha(\mathbf{r}) = E_\alpha \Psi_\alpha(\mathbf{r}) \quad (2.1)$$

where m^* is the effective mass; for GaAs, $m^*=0.069m$, with m the free-electron mass. $V(z)$ is the self-consistent potential. The solution of this equation is of the form

$$\Psi_{\mathbf{k},i}(\mathbf{r}) = [\exp(i\mathbf{k} \cdot \mathbf{r}) / A^{1/2}] \chi_i(z) \quad (2.2)$$

where \mathbf{k} is the wave vector parallel to the surface, A is the area of the sample and the index α represents the combination (\mathbf{k}, i) , where i labels a particular solution for wave vector \mathbf{k} . In Eq. (2.1), the energy zero is the conduction band edge.

$$E_\alpha = E_{\mathbf{k},i} = (\hbar^2 k^2 / 2m^*) + \epsilon_i$$

The value of ϵ_i is discrete and can be positive or negative; we have then

$$\left[-\frac{\hbar^2}{2m^*} \frac{d^2}{dz^2} + V(z) \right] \xi(z) = \epsilon_i \chi_i(z) \quad (2.3)$$

The solutions of Eq.(2.3) are subject to the boundary conditions

$$\chi_i(0) = 0 \quad (2.4a)$$

$$\chi_i(L) = 0 \quad (2.4b)$$

where L is the thickness of the slab.

The calculation is carried out in the Hartree approximation. It is assumed that the potential energy $V(z)$ appearing in Schrodinger's equation is just the energy of an electron in the electrostatic potential $\Phi(z)$ set up by all the conduction electrons. The electrostatic potential satisfies Poisson's equation:

$$V(z) = -e\Phi(z) \quad (2.5)$$

$$-\frac{d^2\Phi(z)}{dz^2} = \frac{4\pi}{\epsilon_s} \delta n(z), \quad (2.6)$$

where ϵ_s is the static dielectric constant, and $\delta n(z)$ is the deviation of the electron density from its bulk value. We chose the zero of energy such that $\Phi(L/2)=0$.

The boundary condition on the potential is

$$-\left(\frac{d\Phi}{dz}\right)_{z=0} = E_0 \quad (2.7)$$

There are two contributions to $\delta n(z)$,² so $\delta n(z)=\delta n_c(z)+\delta n_d(z)$. The first is from the free carriers in the conduction band:

$$\delta n_c(z) = \frac{2}{(2\pi)^2} \int d^2k \sum_i f \left[\frac{\hbar^2 k^2}{2m^*} + \epsilon_i - \mu \right] \chi_i^2(z) - n_0 \quad (2.8)$$

where $f \left[\frac{\hbar^2 k^2}{2m^*} + \epsilon_k - \mu \right] = \left[\exp \left(\beta \left(\frac{\hbar^2 k^2}{2m^*} + \epsilon_k - \mu \right) \right) + 1 \right]^{-1}$

is the Fermi-Dirac function with $\beta = (k_B T)^{-1}$, n_0 is the bulk free-carrier concentration and μ is the chemical potential.

The second contribution is

$$\delta n_D(z) = n_D \left[f \left(E_D - e\Phi(z) - \mu \right) - f \left(E_D - \mu \right) \right]$$

where n_D is the concentration of donor impurities. Except at the highest concentrations, we can assume that $\delta n_D(z) = 0$, a constant. The self-consistent solution of Eqs. (2.3) and (2.6) proceeds as follows.

First, an initial potential is employed in the Schrodinger equation, which may then be solved straightforwardly by a series approach. Then $\delta n(y)$ may be constructed from these solutions. Finally, the potential $\Phi(z)$ is calculated. We repeat the procedure again and again until the new potential and old potential agree within the desired precision.

Before proceeding further, it is convenient to introduce the dimensionless units which will be employed for most of what follows. All energies will be expressed as multiples of $k_B T$ and all lengths will be expressed as multiples of the thermal wave length

$$\lambda = (h^2/2m^*k_B T)^{1/2}$$

which assumes the value 46.2Å for GaAs at room temperature. That is, we have

$$-e\Phi(y) = \Phi(y)k_B T \quad (2.8a)$$

$$z = y\lambda \quad (2.8b)$$

$$k \rightarrow k\lambda^{-1} \quad (2.8c)$$

$$\chi_i \rightarrow \chi_i\lambda^{-1/2} \quad (2.8d)$$

Schrodinger's equation (2.3) now takes the form

$$\left(-\frac{d^2}{dy^2} + \Phi(y)\right) \chi_i(y) = \epsilon \chi_i(y) \quad (2.9)$$

Poisson's equation (2.6) becomes

$$-\frac{d^2\Phi}{dy^2} = -8\pi \frac{\lambda}{a_0} \delta n(y) \quad (2.10)$$

where $a_0 = \epsilon_0 h^2/m^* e^2$ is the Bohr radius.

The boundary conditions and constraint on the charge density become

$$\Phi(y=L/2) = 0 \quad (2.11)$$

$$\left(\frac{d\Phi}{dy} \right)_{y=0^+} = -8\pi \frac{\lambda}{a_0} Q \quad (2.12)$$

$$\text{where } Q = -1/2 \int_0^L \delta n(y) dy \quad (2.13)$$

is the charge displaced by virtue of the presence of a depletion layer, or an accumulation layer. If we assume Q_s is the charge per unit area trapped on the surface, then Q_s must equal $-Q$ to satisfy electrical neutrality. We can also obtain the electrostatic potential by integrating Eq. (2.10), noting the boundary conditions

$$\left[\frac{d\Phi(y)}{dy} \right]_{y=y} - \left[\frac{d\Phi(y)}{dy} \right]_{y=0^+} = A \int_0^y \delta n(y') dy' \quad (2.14)$$

where $A = -8\pi\lambda/a_0$ and according to (2.12),

$$\Phi'(y) \Big|_{y=0^+} = -8\pi Q \lambda / a_0 = A Q = -A \int_0^\infty \delta n(y) dy \quad (2.15)$$

$$\begin{aligned} \Phi'(y) &= A \int_0^y \delta n(y') dy' + \Phi' \Big|_{y=0^+} \\ &= A \int_0^y \delta n(y') dy' - A \int_0^\infty \delta n(y') dy' \\ &= -A \int_y^\infty \delta n(y') dy' \end{aligned}$$

On the other hand, we also have

$$\begin{aligned}\Phi|_y^\infty &= \int_y^\infty d\Phi(y') = \int_y^\infty \Phi'(y') dy' \\ &= -A \int_y^\infty dy' \int_{y'}^\infty \delta n(y'') dy''\end{aligned}$$

since $\Phi(\infty) = 0$, and thus

$$\begin{aligned}\Phi(y) &= A \int_y^\infty dy' \int_{y'}^\infty \delta n(y'') dy'' \\ &= A \int_y^\infty dy'' \delta n(y'') \int_y^{y''} dy' \\ &= A \int_y^\infty dy'' \delta n(y'') (y'' - y)\end{aligned}$$

Now let $x = y'' - y$, $dy'' = dx$; then

$$\begin{aligned}\Phi(y) &= A \int_0^\infty dx \delta n(x+y) x \\ &= -8\pi\lambda/a_0 \int_0^\infty dy' y' \delta(y+y')\end{aligned}\tag{2.16}$$

Finally we let $x = y'$. Eq.(2.16) is equivalent to Eq.(2.6).

The charge density or, more correctly, the number density appropriate to this unit of length is expressed by

$$\delta n(y) = 2 \int_{-\infty}^{\infty} \frac{d^2k}{4\pi^2} \sum_i \frac{1}{\exp(\epsilon_i + k - \mu) + 1} \chi_i^2(y) - n_0\tag{2.17}$$

Since the electrostatic potential is symmetric,

$$\begin{aligned}\delta n(y) &= \frac{1}{2\pi^2} \sum_i \int_{-\infty}^{\infty} \frac{d^2k}{\exp(\epsilon_i + k^2 - \mu) + 1} \chi_i^2(y) - n_0 \\ &= \frac{1}{2\pi} \sum_i \ln [(\exp(\mu - \epsilon_i) + 1) \chi_i^2(y) - n_0]\end{aligned}\quad (2.18)$$

The Fermi level is found by requiring charge neutrality:

$$\int_0^L \delta n(y) dy = -2Q \quad (2.19)$$

or

$$\frac{1}{2\pi} \sum_i \log [\exp(\mu - \epsilon_i) + 1] = n_0 L - 2Q \quad (2.20)$$

In the numerical calculation, first a step charge density is used, with the thickness D of the depletion or accumulation layer determined by Q , from the definition $n_0 D = Q$. Then this charge density is put into the equation

$$\Phi_i(y) = -8\pi\lambda/a_0 \int_0^{L/2-y} dy' y' \delta(y+y'),$$

where i means initial. After integration, the initial potential can be obtained.

This potential is put into the Schrodinger equation (2.9); then, the wave function and the eigenvalues which can be positive or negative and also discrete are calculated. According to Eq. (2.18), the deviation of the electron density from its bulk value will be obtained.

In the next step, using the equation

$$\Phi_n(y) = - 8\pi\lambda/a_0 \int_0^{L/2-y} dy'y'\delta(y+y'),$$

where n means "new", again and integrating it, we obtain a new potential. Comparing the new potential with the initial potential, if the value $[\Phi_n(y)-\Phi_i(y)]$ is larger than the precision which we desire, we use some linear combination of these two potentials as input into the Schrodinger equation and repeat the procedure again and again until the value $[\Phi_n(y)-\Phi_i(y)]$ is equal or smaller than the precision which we desire. This concludes the self-consistent calculation.

Several bulk charge densities, namely $1*10^{17}/\text{cm}^3$, $3*10^{17}/\text{cm}^3$, $1.2*10^{18}/\text{cm}^3$ and $1.5*10^{18}/\text{cm}^3$ have been used in our calculations. For each charge density, different thicknesses of depletion and accumulation layers, namely 50A, 75A and 100A were used. Also, the potentials for different cases were calculated. These potentials describe the band bending in the surface region.

CHAPTER 3

BULK DIELECTRIC FUNCTION

Classical Plasma Frequency³³

We now discuss collective electron motions based on a purely classical and elementary treatment of plasma oscillations. Let the uniform background density of positive charge be n_0 , and let $n(\mathbf{r},t)$ be the density of electrons at position \mathbf{r} at time t .

The excess positive charge is given by $(n_0 - n)$ and hence from Maxwell's equations

$$\nabla \cdot \mathbf{E} = 4\pi e (n_0 - n) \quad (3.1.1)$$

where \mathbf{E} is the electric field.

Now, suppose the electron gas is displaced by \mathbf{x} to give a current density $n\mathbf{v}$; then according to the equation of continuity

$$\nabla \cdot (n\mathbf{v}) = - \partial n / \partial t \quad (3.1.2)$$

It is assumed that the displacement \mathbf{x} is small. Then the plasma oscillations are small in amplitude and Eq. (3.1.2) may be written as

$$n_0 \nabla \cdot \mathbf{v} = - \partial n / \partial t \quad (3.1.3)$$

which can be integrated to give

$$n_0 - n = n_0 \nabla \cdot \mathbf{x} \quad (3.1.4)$$

since $n = n_0$, at $x=0$. Thus, we have the result, from Eq.(3.1.1),

$$\nabla \cdot \mathbf{E} = 4\pi e n_0 \nabla \cdot \mathbf{x} \quad (3.1.5)$$

and hence

$$\mathbf{E} = 4\pi e n_0 \mathbf{x} \quad (3.1.6)$$

which satisfies the boundary condition that $\mathbf{E}=0$ when $x=0$. Combining this with the Newtonian equation of motion for an electron in an electric field \mathbf{E} , namely

$$m\mathbf{x}'' = - e\mathbf{E} \quad (3.1.7)$$

we have

$$m\mathbf{x}'' + 4\pi e^2 n_0 \mathbf{x} = 0 \quad (3.1.8)$$

This immediately shows that oscillations in the electron gas can occur, with angular frequency ω_p , given by

$$\omega_p = (4\pi n_0 e^2/m)^{1/2} \quad (3.1.9)$$

ω_p is called the plasma frequency

Frequency dependent dielectric constant $\epsilon(\omega)$

Consider the jellium model, and apply a time-varying external field E . Under these circumstances, the equation of motion for an electron is, classically,

$$m \frac{d^2x}{dt^2} + m\gamma \frac{dx}{dt} = -eE \quad (3.2.1)$$

where m is the electronic mass and e is the magnitude of the electronic charge. E is the electric field acting on the electron as a driving force. The term $m\gamma(dx/dt)$ represents viscous damping and provides for an energy loss mechanism. The electric field E can be taken to vary in time as $e^{-i\omega t}$, thus the solution to Eq. (3.2.1) is

$$x = \frac{eE/m}{\omega^2 + i\gamma\omega} \quad (3.2.2)$$

and the induced dipole moment is

$$P = -ex = -\frac{e^2E}{m(\omega^2 + i\gamma\omega)} \quad (3.2.3)$$

Note that it is important to be consistent in the form of the time variation used to describe time-dependent fields. The use of a time variation $e^{i\omega t}$ leads to a complex

refractive index $n=n-ik$, as we now show.

If there are n atoms per unit volume, the polarization is

$$\mathbf{P} = -np = \frac{ne^2}{m(-\omega^2 - i\gamma\omega)} \mathbf{E} = \chi\mathbf{E} \quad (3.2.4)$$

The complex dielectric function ϵ is defined by

$$n^2 = \epsilon = \epsilon_\infty + 4\pi\chi \quad (3.2.5)$$

Using Eq. (3.2.4), this yields

$$\begin{aligned} \epsilon(\omega) &= \epsilon_\infty - \frac{4\pi ne^2}{m(\omega^2 + i\gamma\omega)} \\ &= \epsilon_\infty - \frac{\omega_p^2}{\omega^2 + i\gamma\omega} \end{aligned} \quad (3.2.6)$$

From Eq.(3.2.6)¹⁶

$$\epsilon_1(\omega) = n^2 - k^2 = \epsilon_\infty - \frac{\omega_p^2(\omega^2)}{(\omega^2)^2 + \gamma^2\omega^2} \quad (3.2.7)$$

$$\epsilon_2(\omega) = 2nk = \frac{\omega_p^2\gamma\omega}{(\omega^2)^2 + \gamma^2\omega^2} \quad (3.2.8)$$

Lindhard screening

Lindhard screening

Here, Lindhard screening¹⁷ is discussed briefly. The plasma oscillations can exist because for small k , the dielectric function does not always act as a screening factor. The long-range Coulomb interactions then make possible collective oscillations of large numbers of electrons. The dielectric constant in the limit of long wavelengths has the Drude form

$$\epsilon(\omega) = \epsilon_{\infty} - \frac{\omega_p^2}{\omega^2 + i\gamma\omega}$$

But this is for the case $k=0$. If the phenomenon of screening is considered, the general dielectric constant is

$$\epsilon(k) = 1 - \frac{4\pi}{k^2} \frac{\rho^{\text{ind}}(k)}{\Phi(k)} \quad (3.3.1)$$

where ρ^{ind} is the charge density induced in the electron gas by the external particle and $\Phi(k)$ is the total potential. If Φ varies slowly, we can use the Thomas-Fermi approximation; then the dielectric constant becomes

$$\epsilon(k) = 1 + k_0^2/k^2 \quad (3.3.2)$$

where $k_0^2 = 4\pi e^2(\partial n_0/\partial\mu)$ and n_0 is the charge density of the uniform positive background which is given by

$$n_0(\mu) = \int \frac{dk}{4\pi^3} \frac{1}{\exp[\beta(hk^2/2m) - \mu]} \quad (3.3.3)$$

where μ is the chemical potential.

Another theory is due to Lindhard. In this case the induced density is required only to be of linear order in the total potential Φ . The dielectric constant is

$$\epsilon(k) = 1 - \frac{4\pi e^2}{k^2} \int \frac{dq}{4\pi^3} \frac{f(\epsilon_{q+k}) - f(\epsilon_q)}{(\epsilon_{q+k} - \epsilon_k)} \quad (3.3.4)$$

where f denotes the equilibrium Fermi function for a free electron with energy $h^2k^2/2m$.

If the external field has time dependence $e^{-i\omega t}$, then the induced potential and charge density will also have such a time dependence, and the dielectric constant will depend on frequency as well as on wave vector. It can be generalized by using time-dependent rather than stationary perturbation theory. The Lindhard dielectric constant then becomes

$$\epsilon(k, \omega) = \epsilon_\infty + \frac{4\pi e^2}{k^2} \int \frac{dq}{4\pi^3} \frac{f(\epsilon_{q+k}) - f(\epsilon_q)}{(\epsilon_{q+k} - \epsilon_q) + h\omega} \quad (3.3.5)$$

For the real part of this constant, following the procedure derived by Wooten,¹⁸ the result is

$$\text{Re } \epsilon(k, \omega) = \epsilon_\infty - \frac{\omega_p^2}{\omega^2} \frac{1}{\omega^2} \quad (3.3.6)$$

$$\omega^2 - 1 - \frac{\hbar^2 k^2 (3/5 k_F^2)}{m^2 \omega^2}$$

Using $\hbar k_F/m = v_F$ where v_F is the velocity of an electron on the Fermi surface and assuming

$$\frac{\hbar^2 k^2 (3/5 k_F^2)}{m^2 \omega^2} \ll 1,$$

Eq.(3.3.6) becomes

$$\begin{aligned} \text{Re}\epsilon(k, \omega) &\approx \epsilon_\infty - \frac{\omega_p^2}{\omega^2} \left(1 + \frac{3k^2 v_F^2}{5\omega^2} \right) \\ &\approx \epsilon_\infty - \frac{\omega_p^2}{(\omega^2 - 3k^2 v_F^2/5)} \end{aligned} \quad (3.3.7)$$

In the numerical work, this formula will be used. It is called the Thomas-Fermi model.

Dielectric function including lattice vibrations

To describe the long wavelength optical vibrations, a coordinate specifying the relative displacement between the positive and negative ions is required. For an elastic motion, the effective inertial mass for a unit volume is the density; for the optical type of motion, on the other hand, the corresponding mass is the reduced mass of the positive and negative ions $M = (M_+ * M_-) / (M_+ + M_-)$ divided by the volume of a lattice cell. It has been found that the most convenient parameter to choose for

describing the optical type of motion is the displacement of the positive relative to the negative ions multiplied by the square root of this effective mass per unit volume, which we denote by W :

$$W = \rho^{1/2} (\mathbf{u}_+ - \mathbf{u}_-),$$

where $\rho = M/\Omega$, and Ω is the volume of a lattice cell.

For diatomic ionic crystals, the macroscopic theory is fully embodied in the following pair of equations:

$$d^2W/dt^2 = -r_{11}W + r_{12}E \quad (3.4.1)$$

$$P = r_{12}W + r_{22}E \quad (3.4.2)$$

where P and E are the dielectric polarization and electric field as defined in the usual way in Maxwell's theory.

The coefficients r_{11}, r_{12}, r_{22} are related to the dielectric function. The dielectric function for any particular frequency ω can be deduced directly from (3.4.1) and (3.4.2) by considering periodic solutions:

$$E = E_0 e^{-i\omega t} \quad (3.4.3a)$$

$$P = P_0 e^{-i\omega t} \quad (3.4.3b)$$

$$W = W_0 e^{-i\omega t} \quad (3.4.3c)$$

Thus the results can be obtained from these equations

$$-\omega^2 \mathbf{W} = -r_{11} \mathbf{W} + r_{12} \mathbf{E} \quad (3.4.4)$$

$$\mathbf{P} = r_{12} \mathbf{W} + r_{22} \mathbf{E} \quad (3.4.5)$$

When \mathbf{W} is eliminated from these equations, it is seen that \mathbf{P} and \mathbf{E} are related by

$$\mathbf{P} = [r_{22} + r_{12}^2/(r_{11}-\omega^2)] \mathbf{E} \quad (3.4.6)$$

Comparing it with the definition of the dielectric displacement,

$$\mathbf{D} = \mathbf{E} + 4\pi \mathbf{P} = \epsilon \mathbf{E},$$

the dielectric function is obtained:

$$\epsilon(\omega) = 1 + 4\pi[r_{22} + r_{12}^2/(r_{11}-\omega^2)] \quad (3.4.7)$$

If $\omega^2 = \omega_0^2 = r_{11}$, there is a pole in this function, so r_{11} can be determined by this pole. ω_0 is in the infrared region. When $\omega \ll \omega_0$, $\epsilon(\omega)$ reduces to the well-known static dielectric constant ϵ_0

$$\epsilon_0 = 1 + 4\pi(r_{22} + r_{12}^2/r_{11}) \quad (3.4.8)$$

When $\omega \gg \omega_0$, $\epsilon = \epsilon_\infty$, where ϵ_∞ is the high-frequency dielectric constant

$$\epsilon_\infty = 1 + 4\pi r_{22} \quad (3.4.9)$$

Now, these coefficients can be found as

$$r_{11} = \omega_0^2 \quad (3.4.10a)$$

$$r_{12} = [(\epsilon_0 - \epsilon_\infty)/4\pi]^{1/2} \omega_0 \quad (3.4.10b)$$

$$r_{22} = (\epsilon_\infty - 1)/4\pi \quad (3.4.10c)$$

Finally, the result is

$$\epsilon(\omega) = \epsilon_\infty + (\epsilon_0 - \epsilon_\infty) \omega_0^2 / (\omega_0^2 - \omega^2) \quad (3.4.11)$$

If a simple damping term is considered, then Eq. (3.4.1) can be modified as

$$d^2W/dt^2 = -r_{11}W - \gamma W + \gamma_{12} \quad (3.4.12)$$

where γ is a positive constant with the dimension of frequency; the additional term represents a force always opposed to the motion. So, Eq. (3.4.12) reduces to

$$-\omega^2 W = (-r_{11} + i\omega\gamma)W + \gamma_{12}E \quad (3.4.13)$$

The addition of the damping term is equivalent to the replacement of $-r_{11}$ by $r_{11} + i\omega\gamma$. Hence the dispersion formula (3.4.11) becomes^{8,31}

$$\epsilon(\omega) = \epsilon_\infty + \frac{(\epsilon_0 - \epsilon_\infty) \omega_0^2}{\omega_0^2 - \omega^2 - i\omega\gamma} \quad (3.4.14)$$

