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Spectra of Electromagnetic Plasmon Bands in an Infinite Superlattice Made of Lossless and Lossy Media

A. Al-Khateeb^a, I. Abu-AlJarayesh^a, A. El Ali (Al-Dairy)^a, R.W. Hasse^b and K. Khasawneh^c

^a Department of Physics, Faculty of Science, Yarmouk University, Irbid, Jordan.

^b GSI Darmstadt, Planckstr. 1, 64291 Darmstadt, Germany.

^c Al-Balqa Applied University, Faculty of Science and Information, Assalt, Jordan.

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Abstract: The dispersion relation of electromagnetic surface plasmon bands is calculated in closed form for an infinite metallic superlattice of two alternating arbitrary metallic layers. The well known electrostatic dispersion relation of plasmon bands is recovered. Inclusion of retardation effects and conductivity contributions give rise to the effect that the bands do not start at the plasma frequencies for low wave numbers. Furthermore, conductivity gives rise to damping, i.e. the spectra acquire imaginary parts, and for very large conductivities the waves are proved to be overdamped. The special case of an Al-Mg superlattice is discussed and the spectra and group velocities are calculated for various conductivities and layer thicknesses.

Keywords: Surface waves; Plasmon bands; Dispersion relation; Al-Mg superlattices.

Introduction

One dimensional superlattices are periodic structures consisting of alternating layers of different materials with sharp boundaries and layer thicknesses ranging from few to tens of Angstroms. The structural and physical properties of such structures have been investigated previously [1-8]. The investigation of collective plasmon modes has shown that the presence of surfaces in the superlattice introduces new modes of plasma oscillations with strong dependence on the properties of the surfaces [9, 10]. The elementary excitations of the various layers of the superlattice are coupled by the long range electric fields excited in each layer. The continuity of the fields at the interfaces introduces a coupling mechanism of the elementary excitations across the layers. Due to the lattice periodicity in the direction normal to the

interfaces, the Coulomb coupling of the elementary excitations results in a set of collective plasma excitations of the whole superlattice structure.

Evolution and splitting of plasmon bands in metallic superlattices have been investigated theoretically [6]. The dispersion relation for the collective excitations of an infinite superlattice consisting of alternating layers of four different materials has been derived within the local theory approximation. It was found that the number of bands is equal to the number of materials that make up the superlattice and the band gaps were found to be sensitive to the relative thicknesses of the insulating layers separating the two metallic layers in the superlattice. The dispersion relations of metal-dielectric superlattices have been solved by Sheng and Lue [11, 12]. Reflection peaks are observed only at

incident light frequencies near the plasma frequency ω_p , whereas a reflection minimum can occur at $\omega < (\omega_p/\sqrt{2})$ for sufficiently small values of the insulator thickness.

The electrodynamic properties of surface electromagnetic waves at the interface between two periodic dielectric superlattices have been studied by Bulgakov *et.al.* [13]. The interface was found to serve as a guide for electromagnetic waves with exponentially decaying fields on both sides of the plane of the interface. El Hassouani *et.al.* [14] investigated theoretically and experimentally the existence and behavior of the localized surface electromagnetic waves in Fibonacci superlattices. The experimental investigation was carried out by using coaxial cables in a frequency region of a few tens of MHz with the emphasis on the existence of various types of surface modes and their spatial localization.

In this work we study theoretically the spectra of electromagnetic surface waves in an infinite superlattice of two alternating metallic layers. The dispersion relation of this system will be obtained in closed form by accounting for retardation effects and conduction losses. Since the splitting of plasmon bands is small when the thicknesses of the two layers are different, we consider mostly the case of equal layer thicknesses. This allows the observation of the effect of pure screening on the evolution of the plasmon bands. The paper is organized as follows: In Sec. 2, we present the model

equations for the case of transverse magnetic modes (TM). In Sec. 3, we solve the wave equations and then obtain the dispersion relation of the electromagnetic surface waves. Here we make use of the lattice periodicity in the z -direction and of the Bloch wave nature of the solution. In Sec. 4, we use the general dispersion relation to discuss numerically the possible spectra of electromagnetic surface waves. Here we consider the special case in which the unit cell is assumed to be composed of two alternating layers of aluminum (Al) and magnesium (Mg). Finally, in Sec. 5, we present the main conclusions.

Basic Equations

The general wave equations satisfied by the magnetic induction \vec{B} , and electric field \vec{E} , in a source free conducting medium of conductivity S , permittivity ϵ and permeability μ_0 are obtained from Faradays and Amperes laws, namely,

$$\left. \begin{aligned} \nabla^2 \mathbf{B}(\mathbf{r}, t) - \mu_0 \epsilon \frac{\partial^2 \mathbf{B}(\mathbf{r}, t)}{\partial t^2} - \mu_0 S \frac{\partial \mathbf{B}(\mathbf{r}, t)}{\partial t} &= 0 \\ \nabla^2 \mathbf{E}(\mathbf{r}, t) - \mu_0 \epsilon \frac{\partial^2 \mathbf{E}(\mathbf{r}, t)}{\partial t^2} - \mu_0 S \frac{\partial \mathbf{E}(\mathbf{r}, t)}{\partial t} &= 0 \end{aligned} \right\} \quad (1)$$

Let the lattice be infinite in the x and y directions according to Fig. 1 with the surface wave propagation being in the xy -plane. Then the scalar Maxwell's equations in conducting media take the following form,

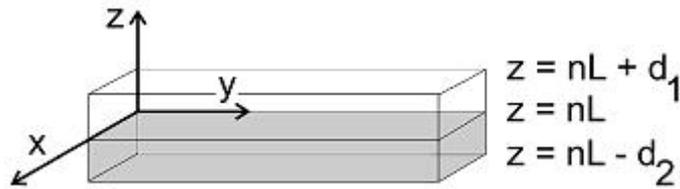


FIG.1. Geometry of the n^{th} unit cell.

$$\left. \begin{aligned} ik_y E_z - \frac{\partial E_y}{\partial z} &= i\omega B_x \\ ik_x E_y - ik_y E_x &= i\omega B_z, \\ \frac{\partial E_x}{\partial z} - ik_x E_z &= i\omega B_y, \\ ik_y B_z - \frac{\partial B_y}{\partial z} &= -i\mu_0 \omega \left(\epsilon + i \frac{S}{\omega} \right) E_x, \\ \frac{\partial B_x}{\partial z} - ik_x B_z &= -i\mu_0 \omega \left(\epsilon + i \frac{S}{\omega} \right) E_y, \\ ik_x B_y - ik_y B_x &= -i\mu_0 \omega \left(\epsilon + i \frac{S}{\omega} \right) E_z \end{aligned} \right\} \quad (2)$$

Without loss of generality, we consider TM surface wave modes ($\mathbf{k} \cdot \mathbf{B} = 0$) that are propagating along the x -axis. Upon setting $k_y = 0$ and $B_x = 0$, the only non-vanishing electromagnetic field components are E_x , E_z and B_y [1]. The corresponding scalar wave equations become,

$$\left. \begin{aligned} \frac{d^2 E_{x,z}}{dz^2} - \left(k^2 - \frac{\omega^2}{c^2} \epsilon(\omega) - i\omega\mu_0 S \right) E_{x,z} &= 0 \\ \frac{d^2 B_y}{dz^2} - \left(k^2 - \frac{\omega^2}{c^2} \epsilon(\omega) - i\omega\mu_0 S \right) B_y &= 0 \end{aligned} \right\} \quad (3)$$

where $\epsilon = \epsilon_0 \epsilon(\omega)$ has been used with $\epsilon(\omega)$ being the longitudinal dielectric function at frequency ω . Upon solving the Maxwell's curl equations simultaneously for E_z and B_y in terms of E_x , we obtain the following equations,

$$\left. \begin{aligned} E_z &= -i \frac{k}{k^2 - \frac{\omega^2}{c^2} \epsilon(\omega) - i\omega\mu_0 S} \frac{dE_x}{dz}, \\ B_y &= -i \frac{\mu_0}{k} (S - i\omega\epsilon_0) E_x \end{aligned} \right\} \quad (4)$$

From equation (4) we see that it is sufficient to solve for the field component E_x . For an infinite lattice of two alternating layers of thicknesses d_1 and d_2 the x component of the electric field E_x in each layer is,

$$\left. \begin{aligned} E_x^{(I)} &= A_1 e^{\tau_1 z} + A_2 e^{-\tau_1 z} \\ E_x^{(II)} &= A_3 e^{\tau_2 z} + A_4 e^{-\tau_2 z} \\ \tau_\alpha^2 &= k^2 - \frac{\omega^2}{c^2} \epsilon_\alpha(\omega) - i\omega\mu_0 S_\alpha, \quad \alpha = 1, 2 \end{aligned} \right\} \quad (5)$$

where $\epsilon_\alpha(\omega) = 1 - \omega_\alpha^2/\omega^2$, and ω_α is the corresponding bulk plasma frequency.

Lattice Periodicity and Bloch Solutions

Due to the lattice periodicity along z , the solution that satisfies the boundary conditions at each interface of the two layers L_I and L_{II} represents Bloch waves with respect to the translations in the direction normal to the interfaces. We consider also a primitive unit cell of two layers of lengths d_1 and d_2 such that $L = d_1 + d_2$ being the length of the primitive unit cell of the direct lattice, see Fig.1.

In analogy to the Bloch theorem of electrons that move in periodic potentials and that have wavefunctions in the form of plane waves multiplied by a function that has the periodicity of the direct lattice, we require a solution of the form,

$$\left. \begin{aligned} E_x(k, z, \omega) &= e^{iqz} U_q(k, z, \omega) \\ U_q(k, z, \omega) &= U_q(k, z + nL, \omega) \end{aligned} \right\} \quad (6)$$

where n is an integer and q is a wavevector in the direction of the periodicity.

Applying the boundary conditions at the interfaces at $z = nL$ and $z = nL + d_1$, namely the continuity of E_x and B_y at $z = nL$ and $z = nL + d_1$, we obtain the following dispersion relation for the spectra of the electromagnetic surface waves in an infinite superlattice of two alternating metallic layers,

$$\left. \begin{aligned} &4 \frac{\tau_2}{\tau_1} \frac{S_1 - i\omega\epsilon_0\epsilon_1(\omega)}{S_2 - i\omega\epsilon_0\epsilon_2(\omega)} \cos qL = \\ &\left(1 + \frac{\tau_2}{\tau_1} \frac{S_1 - i\omega\epsilon_0\epsilon_1(\omega)}{S_2 - i\omega\epsilon_0\epsilon_2(\omega)} \right)^2 \cosh(\tau_1 d_1 + \tau_2 d_2) - \\ &\left(1 - \frac{\tau_2}{\tau_1} \frac{S_1 - i\omega\epsilon_0\epsilon_1(\omega)}{S_2 - i\omega\epsilon_0\epsilon_2(\omega)} \right)^2 \cosh(\tau_2 d_2 - \tau_1 d_1) \end{aligned} \right\} \quad (7)$$

where ω in equation (7) represents the frequency of the electromagnetic collective excitation of the whole superlattice.

In the electrostatic limit such that $\omega/c \rightarrow 0$ and $\omega S_{1,2} \rightarrow 0$, we have $\tau_1 = \tau_2 = \kappa$, and therefore, Eq. (7) reduces into the following electrostatic dispersion relation,

$$4 \frac{\varepsilon_1(\omega)}{\varepsilon_2(\omega)} \cos qL = \left. \begin{aligned} &\left(1 + \frac{\varepsilon_1(\omega)}{\varepsilon_2(\omega)}\right)^2 \cosh k(d_1 + d_2) - \\ &\left(1 - \frac{\varepsilon_1(\omega)}{\varepsilon_2(\omega)}\right)^2 \cosh k(d_2 - d_1) \end{aligned} \right\} \quad (8)$$

In order to reduce equation (8) into a well known form we rewrite it as follows,

$$2 \cos qL = \left. \begin{aligned} &\frac{1}{2} \frac{\varepsilon_2(\omega)}{\varepsilon_1(\omega)} \left(1 + \frac{\varepsilon_1(\omega)}{\varepsilon_2(\omega)}\right)^2 \cosh k(d_1 + d_2) - \\ &\frac{1}{2} \frac{\varepsilon_2(\omega)}{\varepsilon_1(\omega)} \left(1 - \frac{\varepsilon_1(\omega)}{\varepsilon_2(\omega)}\right)^2 \cosh k(d_2 - d_1) \end{aligned} \right\} \quad (9)$$

Upon using $2 \cosh \theta = e^\theta + e^{-\theta}$ to rewrite $\cosh[k(d_1 + d_2)]$ and $\cosh[k(d_2 - d_1)]$, and then by using $2 \sinh \theta = e^\theta - e^{-\theta}$, the electrostatic dispersion relation (Eq. 9) takes the following familiar form [6, 15],

$$\cos qL = \cosh kd_1 \cosh kd_2 + \left. \frac{1}{2} \frac{\varepsilon_2(\omega)}{\varepsilon_1(\omega)} \left[1 + \frac{\varepsilon_1^2(\omega)}{\varepsilon_2^2(\omega)}\right] \sinh kd_1 \sinh kd_2 \right\} \quad (10)$$

In the absence of retardation effects, the surface response is expressed in terms of the bulk longitudinal dielectric function $\varepsilon_\alpha(\omega)$. While equation (10) focuses on the surface wave electrostatic regime, it should be noted that electromagnetic surface waves are generally of hybrid character where both transverse and longitudinal parts do exist. An electrostatic treatment is valid for surface modes having phase velocities much less than the speed of light and the response of the medium is of continuum character and is local so that it is only valid in the long-wavelength limit [16].

Numerical Examples

The implicit dispersion relation Eq. (7) is solved numerically by complex Newton's iteration scheme with carefully choosing the initial values [17-19]. In the electrostatic case and for $d_1 = d_2$, the dispersion relation has only two real solutions corresponding to $qL = \pi$ in the region $kd_1 \sim 0$. This is due to the fact that for $kd_1 \sim 0$, the wavelength of the plasmon mode is much larger than the periodicity of the superlattice. In this case the effect of the interface is not observed and a continuum (band) extending from the characteristic plasmon energy of Mg to that of Al is expected. For more details, the reader is referred to refs. [6, 15]. As an example, we consider a superlattice consisting of Al and Mg, because each of these metals has a single, well defined plasmon, and the energies of the two plasmons are appreciably different ($\omega_{p,Al} = 15 \text{ eV}$, $\omega_{p,Mg} = 10 \text{ eV}$). Also, we consider the case of equal layer thicknesses of Al and Mg, since in the absence of retardation and conductivity, this choice leads to a single-unsplit plasmon bands. Consequently, we can associate any change with these effects when it is included. Fig. 2 shows the plasmon spectra of superlattices consisting of alternating layers of aluminum and magnesium.

In the electrostatic limit the spectra are identical, and we only show the representative spectrum for the cases $d_2 = 10d_1$ and $d_2 = 1.5d_1$. A broad unsplit band between the characteristic plasmon energies of the two metals appears at $kd_1 \sim 0$, which subsequently narrows down with increasing kd_1 and converges to the characteristic value of the interface plasmon between Al and Mg layers given by $\omega_I = \sqrt{[\omega_{p,Al}^2 + \omega_{p,Mg}^2]/2}$. This is due to the fact that for $kd_1 \gg 1$, the hyperbolic terms in the dispersion relation become exponentially large, and thus the term containing $\cos qL$ becomes negligible. Accordingly, all solutions converge.

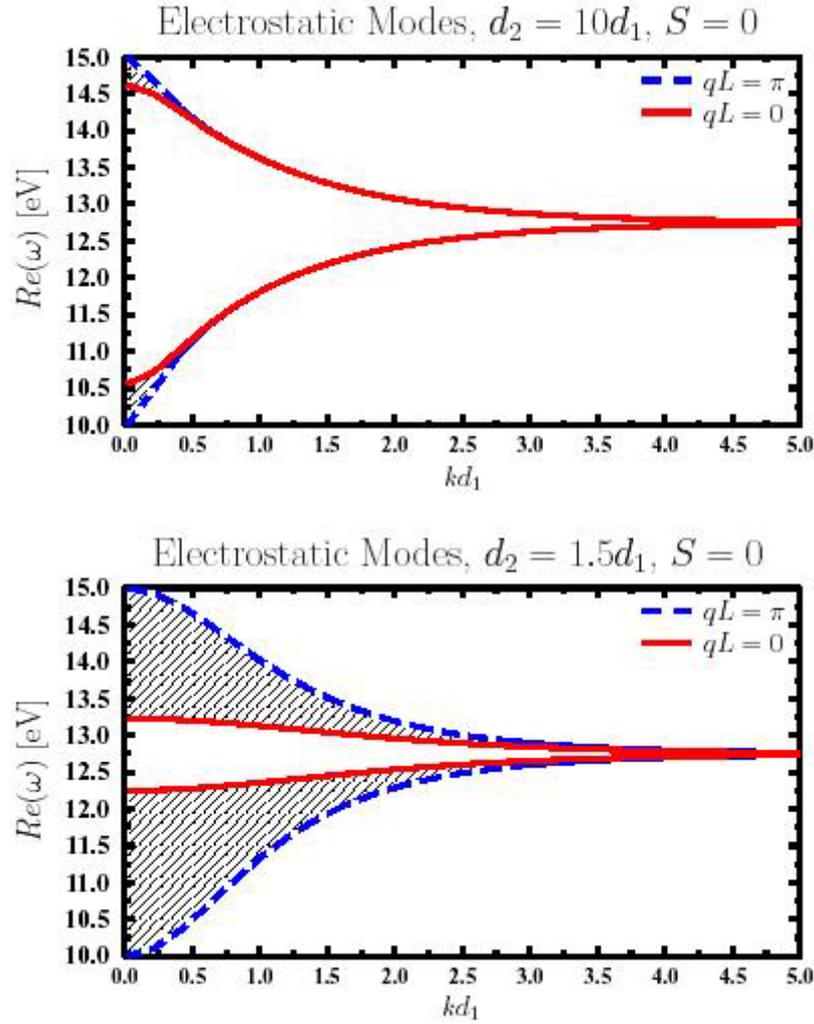


FIG.2. Energy of electrostatic surface modes versus kd_1 for $qL=0$ and $qL=\pi$.

The long range Coulomb fields produced within the layers of the superlattice couple the elementary excitations of various layers with each other. The coupled layers of the whole superlattice produce collectively the plasmon modes described by the dispersion relation for $qL = \pi$ for the bulk mode and $qL = 0$ for the surface mode. Due to the periodicity of the superlattice in the z -direction and to the dependence of the

collective modes on the vertical wavenumber q , energy can be transmitted normal to the interfaces by the excited surface modes. This explains the downward and upward shifting in Fig. 3 of the energies of the plasmon modes of Al (15 eV) and Mg (10 eV), respectively. In addition, they acquire imaginary parts by virtue of the finite conductivity.

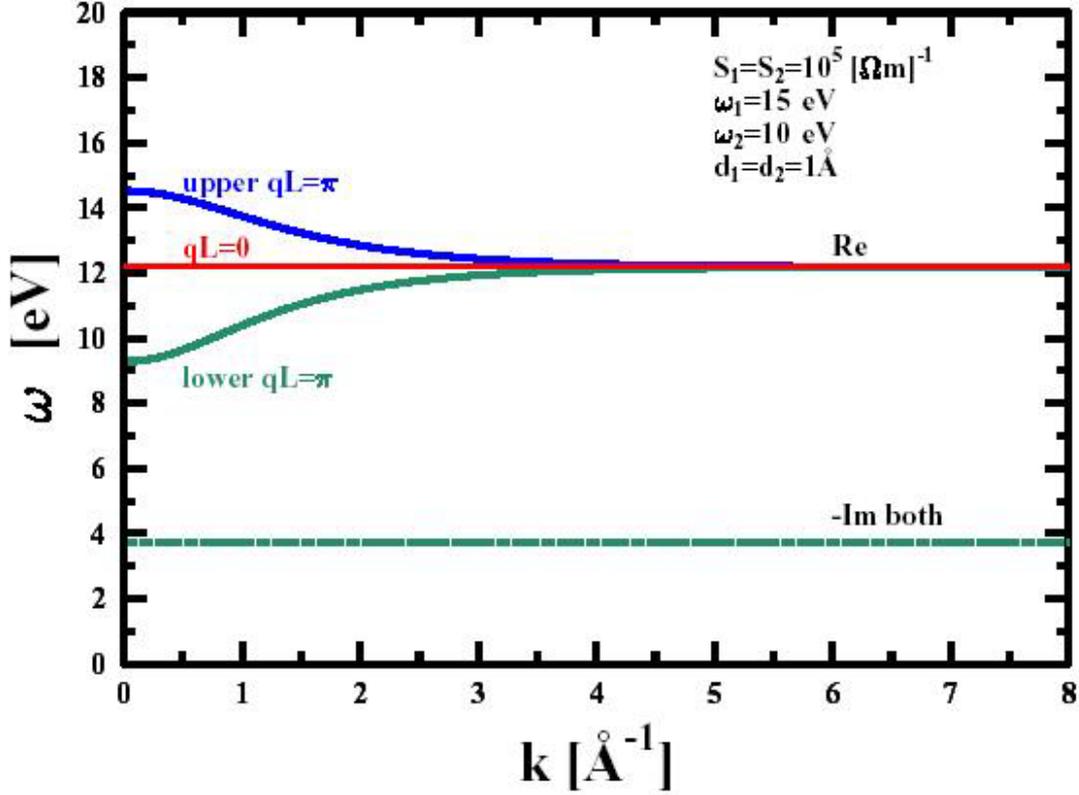


FIG.3. Spectra of Al (15 eV)-Mg (10 eV) superlattices

As shown in Fig. 4, this shift depends strongly on the thicknesses of the layers, in particular of the lower $qL = \pi$ mode. Fig. 5 shows that the splitting continues with increasing conductivity. At critical values, different for each branch, running waves cease to exist. For conductivities above threshold only overdamped and exponentially increasing modes exist. Due to the symmetries, $d_1 = d_2$ and $S_1 = S_2$ in Fig.5, in the underdamped region all branches have the same imaginary parts. Finally Fig.6 shows the spectrum of the group velocity $\partial\omega/\partial k$ in units of the speed of light. The upper branch of Fig. 3 turns out to correspond to a backwards running wave

whereas the lower branch is the forward wave.

The branch $qL = 0$ can be forward or backward running depending on the layer thicknesses and the conductivities. A wave in which phase and group velocities have opposite signs is known as a backward wave [20]. Conditions for these waves are found in many periodic structures which support equal numbers of forward and backward space harmonics. As can be seen from Fig. 3, the imaginary part of ω is constant; hence the imaginary part of the group velocity is zero.

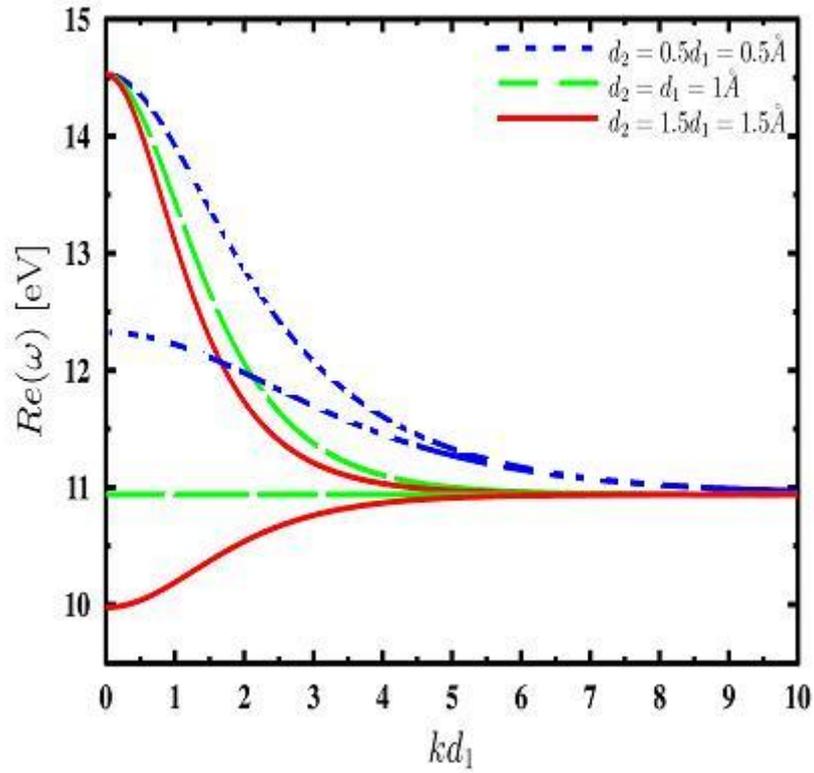


FIG.4. Influence of different layer thicknesses on the spectra $qL=\pi$ for $S_1=10^5/\Omega\text{m}$ and $S_2=2.5S_1$.

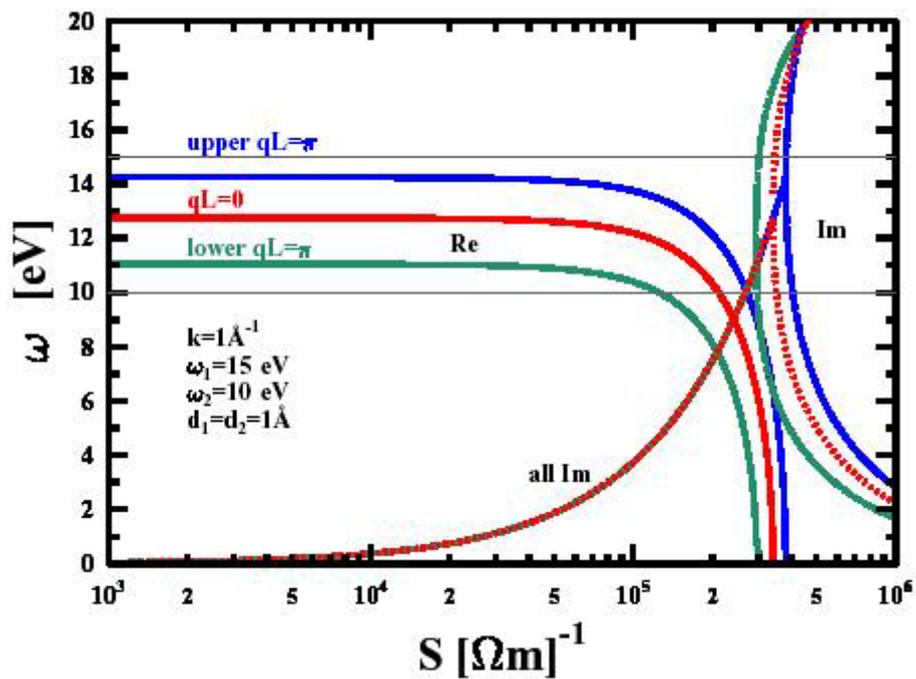


FIG.5. Dependence of the spectra on the conductivity $S = S_1 = S_2$.

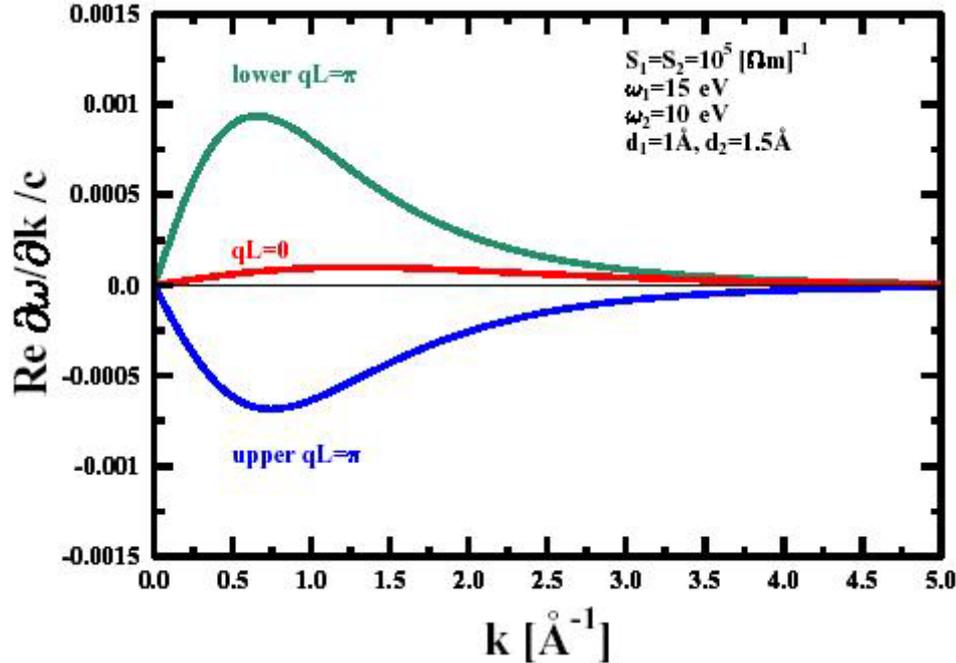


FIG.6. Spectra of the group velocity.

Discussion and Conclusions

We presented detailed calculations of a closed form dispersion relation of the electromagnetic surface modes in an infinite superlattice of two alternating metallic layers. The geometry of the system shown in Fig. 1 is a multilayer slab waveguide. The dispersion relation includes both retardation effects from the magnetic field and finite conductivities, and recovers the well known electrostatic dispersion relation [6, 15]. Since the splitting of plasmon bands is small when the thicknesses of the two layers are different, we consider mostly the case of equal layer thicknesses. This allows the observation of the effect of pure screening on the evolution of the plasmon bands. The special case of an Al-Mg superlattice is discussed and the spectra and group velocities are calculated for various conductivities and layer thicknesses.

The electromagnetic surface wave spectra have been calculated numerically for the $qL = 0$ and $qL = \pi$ modes. The main effect is that the spectra in the static

limit do no longer start at the respective plasma frequencies of the layer materials as in the electrostatic case. The conductivity gives rise to damping, i.e. the spectra acquire imaginary parts. For very large conductivities, the waves are proved to be overdamped. As can be seen from Fig.1 and Fig. 3, the terminology of bands is still applicable when plotting frequency ω versus wavenumber k up to a threshold value of conductivity. Extensions of this work under way will include three or four layers because the interfaces between the double sheets experimentally are not well separated and behave as an extra sheet.

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