Optical free-carrier absorption of an electron-hole plasma in silicon

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We present the expression for the free-carrier absorption in a multicomponent plasma, including the contributions from particle scattering, phonon absorption or emission, and impurity scattering. Numerical results are given for the absorption of an electron-hole plasma in silicon. It is found that the contribution from particle scattering dominates for high plasma densities and/or low photon energies.

I. INTRODUCTION

A completely homogeneous one-component plasma, like a homogeneous electron gas, cannot absorb light. The reason is that the perturbing potential

$$\frac{Ze}{mc}\sum_i(\mathbf{p}_i\cdot\mathbf{A}+\mathbf{A}\cdot\mathbf{p}_i)=\frac{Ze}{mc}(\mathbf{P}\cdot\mathbf{A}+\mathbf{A}\cdot\mathbf{P}) \tag{1.1}$$

that couples the light to the plasma and causes the absorption of light, commutes with the Hamiltonian. This is because **P**, the total momentum of the plasma, is a constant of motion. For absorption to take place, the Hamiltonian must contain terms not commuting with **P**, which arise, for instance, from the presence of impurities or coupling to phonons. The same arguments are valid for the electrical resistivity which cannot be induced by the scattering between the particles in the plasma.

The situation is different in a multicomponent plasma where not all components have equal charge-to-mass ratios Z/m, because in this case the perturbing potential in the absorption process is no longer proportional to **P**. Extra absorption processes occur in which two particles belonging to different components are excited. Also, collective excitations, plasmons, are possible. In what follows, we refer to this additional absorption as the absorption from particle scattering. This absorption is proportional to $\mathbf{n}^2$, where **n** is the plasma density, while the phonon contribution, as well as any impurity contribution, is proportional to **n**. This means that the particle-scattering contribution increases in relative importance with increasing plasma density.

A very-high-density plasma is created in experiments where silicon is irradiated by very short and intense laser pulses, and the absorption from particle scattering is bound to be important. The very heavy absorption during irradiation by femtosecond laser pulses has been proposed[1] to be due to this extra absorption process occurring in a multicomponent plasma. In these experiments one reaches extremely high plasma densities, higher than 10^{22} cm^{-3}.

These experiments involving high-density plasmas motivate a theoretical study of the particle-scattering contribution to the absorption. Furthermore, we will show here that the contribution from particle scattering can be important also for more modest plasma densities, in the range of $10^{17}-10^{18}$ cm^{-3}. The optical absorption of an electron-hole plasma is, as pointed out in Ref. 2, important for the following reasons: It can be used as a diagnostic tool to measure plasma concentrations, it affects the long-wavelength laser annealing of silicon, and it plays an important role in the performance of devices requiring a controlled ir absorption, such as thermophotovoltaic converters.

To our knowledge there have been two sets of experiments in which the absorption has been measured directly. In Ref. 2, the plasma was created by heavily forward biasing a specially constructed *p-i-n* diode. The absorption was measured at the wavelength $\lambda=2.5$ μm. In the second experiment[3] the plasma was created by optical excitation and the absorption was measured at $\lambda=10.6$ μm. This experiment was designed for studying the effect on the absorption resulting from a strong applied electric field. In both these works it was suggested that particle scattering was responsible for part of the absorption.

The free-carrier absorption is closely related to the dynamical conductivity which we derived for a multicomponent plasma in a recent paper.[4] Therefore, in this work we will use many of the results from that reference. Reference 4 is by no means the first work in which the conductivity for a multicomponent plasma is derived and in which the additional particle-scattering contribution is obtained. We refer to Ref. 5 and references therein for the gradual development of the early theory in this field. Many papers[6–12] have been concerned with the dynamical conductivity or absorption in degenerate semiconductors, which represent in many respects very similar situations. References 13 and 14 have treated the static conductivity for an electron-hole plasma by solving the Boltzmann equation, concentrating in particular on the transition between the classical and quantum limits.

In Sec. II we present numerical results for the absorption of an electron-hole plasma in Si. These results include the contributions from acoustical phonons and particle scattering. Since the band structure of Si near the band edges consists of six anisotropic conduction-band minima and two hole bands in the valence band, the particle scattering includes a set of different combinations of electron-electron, electron-hole, and hole-hole scattering processes. The results are obtained from using an expression for the free-carrier absorption arrived at in a derivation based on the Kubo formalism and diagrammatic perturbation theory. The expression, which we present in the Appendix, contains the contribution from impurities, phonons, and the additional particle-scattering contribution in a multicomponent plasma. The impurity contribution will not be needed here. It was included to make the expression general. Finally, in Sec. III we make a summary and draw conclusions.

II. FREE-CARRIER ABSORPTION OF AN ELECTRON-HOLE PLASMA IN SILICON

In this section we present numerical results for the absorption of an electron-hole plasma in silicon. Before going into the details of the specific system we make a brief discussion of the free-carrier absorption of a multicomponent plasma in general.

The absorption $\alpha(\Omega)$ is related to the real part of the dynamical conductivity $\sigma_1(\Omega)$, according to the relation

$$\alpha(\Omega)=\frac{4\pi\sigma_1(\Omega)}{c\sqrt{\kappa(\Omega)}} , \qquad (2.1)$$

where Ω, c, and $\kappa(\Omega)$ are the photon frequency, the speed of light, and the background dielectric function, respectively. The dynamical conductivity was derived in Ref. 4 and we will make use of some of the expressions obtained in that reference below.

The absorption has contributions from processes where a photon is absorbed at the same time as various excitations occur in the system. Phonons and impurities or defects are sources for such excitations. In a multicomponent plasma where not all components have equal charge-to-mass ratios, Z/m, absorption can take place even in the absence of phonons and defects. Pairs of particles belonging to different components can be excited, as well as plasmons. The full result for σ_1 in a multicomponent plasma, in absence of impurities, was given in Eq.

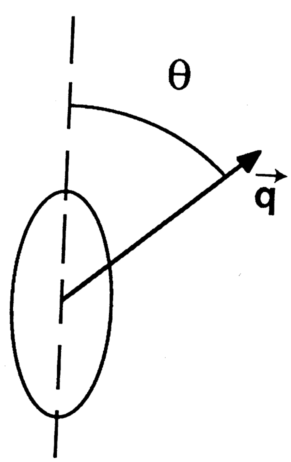

FIG. 1. The definition of the angle θ appearing in the electron-phonon coupling as the angle between the vector **q** and the main symmetry axis for each conduction-band ellipsoid.

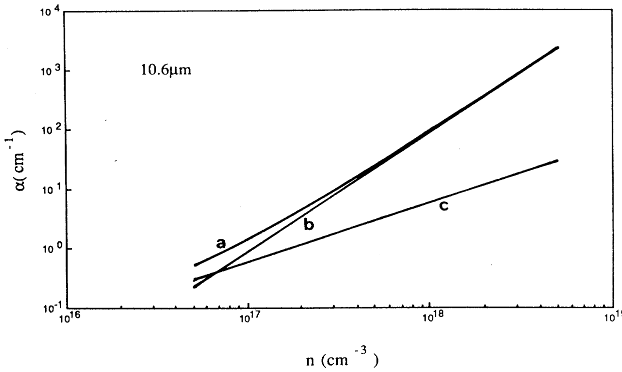

FIG. 2. The absorption as a function of plasma density for an electron-hole plasma in silicon at the wavelength 10.6 μm. The curves a, b, and c represent the full result, the contribution from particle scattering, and the phonon contribution, respectively.

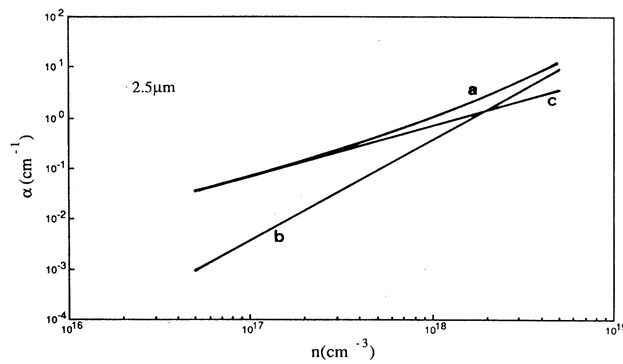

FIG. 3. The same as Fig. 2 but now for the wavelength 2.5 μm.

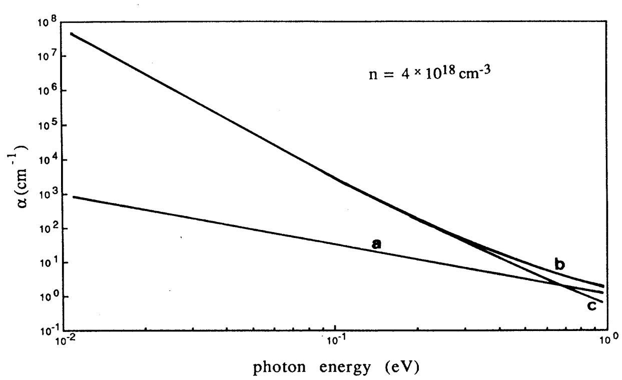

FIG. 4. The absorption as a function of photon energy for an electron-hole plasma in silicon with density 4×10^{18} cm^{-3}. The curves a, b, and c represent the phonon contribution, the full result, and the contribution from particle scattering, respectively.

(2.30) of Ref. 4. We can copy that result here. The impurity contribution, however, was only given for a one-component plasma in Eqs. (3.10)–(3.14). Hence we need to generalize that result. Since the final result is rather complicated, we have deferred its presentation to the Appendix.

Now let us turn to the electron-hole plasma in silicon. We assume that the system is pure enough for the absorption to be dominated by carrier-carrier and carrier-phonon scattering. Thus the three last terms in Eq. (A1) are not used here. They were included to make the presentation general. We study the density and frequency dependence of the absorption. As the expressions presented in Eq. (A1) are very complicated, it is difficult to obtain general results. Furthermore, the expressions were derived under the assumption of isotropic, parabolic bands. Both the electron and hole bands in silicon are parabolic in all directions, but not isotropic. The problems are drastically reduced in the limit $\Omega \gg E_F, k_B T$, in which the experiments in Refs. 2 and 3 were performed. In this limit, one can use a simplified dielectric function for the carriers, viz., one obtained by assuming that all particles are at $\mathbf{k}=0$. By using this approximation one can include the anisotropy of the conduction-band valleys and the heavy- and light-hole bands. The anisotropy of the conduction bands gives rise to an extra absorption in which electrons in different valleys are scattered. In this approximation the polarizability for a component i is given by

$$\chi_i(\mathbf{q},\omega)=\frac{2\mathbf{n}_i}{\hbar}\frac{\dfrac{\hbar q^2}{2m_i(\mathbf{q})}}{\omega^2-\left[\dfrac{\hbar q^2}{2m_i(\mathbf{q})}\right]}-i\frac{\pi\mathbf{n}_i}{\hbar}\left[\delta\left[\omega-\frac{\hbar q^2}{2m_i(\mathbf{q})}\right]-\delta\left[\omega+\frac{\hbar q^2}{2m_i(\mathbf{q})}\right]\right] . \tag{2.2}$$

When putting this approximate expression for the polarizability into Eq. (A1) and noting that the integrands give contributions only for relatively large q values, one finds that χ_i has nonnegligible value only very close to the curves defined by $\omega=\pm\hbar q^2/2m_i(\mathbf{q})$. Using these facts, Eq. (A1) reduces to

$$\alpha(\Omega)=\alpha_{\text{part}}(\Omega)+\alpha_{\text{phon}}(\Omega) , \tag{2.3}$$

where

$$\begin{aligned}\alpha_{\text{part}}(\Omega)=&-\frac{2\pi e^2\hbar}{c[\kappa(\Omega)]^{5/2}3\Omega^3}\int_0^\infty d\omega\frac{1}{2\pi}\frac{\sinh\left[\dfrac{\hbar\beta\Omega}{2}\right]}{\sinh\left[\dfrac{\hbar\beta}{2}\left[\omega+\dfrac{\Omega}{2}\right]\right]\sinh\left[\dfrac{\hbar\beta}{2}\left[\omega-\dfrac{\Omega}{2}\right]\right]}\\&\times\int d\mathbf{q}\frac{1}{(2\pi)^3}v(q)^2q^2\sum_{i,j}Z_i^2Z_j^2\left[\frac{Z_i}{m_i(\mathbf{q})}-\frac{Z_j}{m_j(\mathbf{q})}\right]^2\\&\times\left[\operatorname{Im}\chi_i\left[\mathbf{q},\omega+\frac{\Omega}{2}\right]\operatorname{Im}\chi_j\left[\mathbf{q},\omega-\frac{\Omega}{2}\right]+\operatorname{Im}\chi_i\left[\mathbf{q},\omega-\frac{\Omega}{2}\right]\operatorname{Im}\chi_j\left[\mathbf{q},\omega+\frac{\Omega}{2}\right]\right]\end{aligned} \tag{2.4}$$

and

$$\begin{aligned}\alpha_{\text{phon}}(\Omega)=&-\frac{4\pi e^2\hbar}{c\sqrt{\kappa(\Omega)}3\Omega^3}\int_0^\infty d\omega\frac{1}{2\pi}\frac{\sinh\left[\dfrac{\hbar\beta\Omega}{2}\right]}{\sinh\left[\dfrac{\hbar\beta}{2}\left[\omega+\dfrac{\Omega}{2}\right]\right]\sinh\left[\dfrac{\hbar\beta}{2}\left[\omega-\dfrac{\Omega}{2}\right]\right]}\\&\times\int d\mathbf{q}\frac{1}{(2\pi)^3}g(\mathbf{q})^2q^2\sum_i Z_i^2\left[\frac{Z_i}{m_i(\mathbf{q})}\right]^2\\&\times\left[\operatorname{Im}\chi_i\left[\mathbf{q},\omega+\frac{\Omega}{2}\right]\operatorname{Im}D\left[\mathbf{q},\omega-\frac{\Omega}{2}\right]+\operatorname{Im}\chi_i\left[\mathbf{q},\omega-\frac{\Omega}{2}\right]\operatorname{Im}D\left[\mathbf{q},\omega+\frac{\Omega}{2}\right]\right] ,\end{aligned} \tag{2.5}$$

where we have averaged over the direction of the polarization vector for the light. The anisotropic energy dispersions for the conduction bands are taken into account. The warping of the valence bands is neglected as is usually done.[15,16] In doing so we get four pairwise-degenerate hole bands: two heavy-hole bands and two light-hole bands. The electron-phonon coupling constant has the following angular dependence for the conduction-band valleys:

$$g^2(\mathbf{q})=\frac{\hbar q}{2\rho c_s}\{(E_1-\tfrac{1}{3}E_2)^2 - \cos^2\theta[(E_1-\tfrac{1}{3}E_2)^2-(E_1+\tfrac{2}{3}E_2)^2]\} , \tag{2.6}$$

where the angle θ is defined with respect to each conduction-band ellipsoid according to Fig. 1. The parameters E_1 and E_2 are elastic constants with the room-temperature values[17] -5.6 and 9.23 eV, respectively. The two remaining parameters ρ and c_s are the density of the material and the speed of sound with the values[17] 2.33 g/cm^3 and 8.47×10^5 cm/s, respectively. For the valence bands we use the coupling valid for isotropic bands, i.e., the curly brackets in Eq. (2.6) are replaced there by E_1^2.

Our obtained numerical results are displayed in Figs. 2–5. The first two figures show the absorption as a function of plasma density for the two wavelengths 10.6 and 2.5 μm, respectively, which are the wavelengths used in the experiments in Refs. 3 and 2, respectively. Curves a, b, and c represent the total result, the contribution from particle scattering, and the phonon contribution, respectively. It is found that the particle scattering gives a non-negligible contribution for both wavelengths and even dominates for the longer of the two. In Figs. 4 and 5 we have plotted the absorption as a function of photon energy for two plasma densities. Here, curves a, b, and c denote the phonon contribution, the full result, and the particle-scattering contribution, respectively. The particle scattering dominates for lower photon energies.

Just to get a crude check of our results we applied them to the experimental situation in Ref. 1. We determined the scattering rate for the case when the plasmon energy coincides with the photon energy, which in the experiments had the value 1.99 eV. The plasma density equals 5×10^{21} cm^{-3} at this point. This is the density at which interesting things happen in the experiments. Our expressions are certainly outside the limits of their validity in this situation, but we proceeded nevertheless. For this plasma density the scattering rate $\tau=1/c\alpha$ if $\omega\tau\gg1$. Using our obtained value for α we found τ to be 9×10^{-16} s, which is in fair agreement with what was deduced from the experiments, viz., 3×10^{-16} s. We refrain from presenting a detailed comparison with the results from Refs. 2 and 3. Both sets of experiments show a higher absorption than what we obtain. It is difficult to pinpoint the cause of this discrepancy. Possible explanations are that the plasma densities were higher than anticipated in the experiments or that the plasmas were inhomogeneous. Another possibility is that extra absorption processes contributed, such as processes induced by the surface. In the theory we have assumed the carriers to be thermalized and located in the states near the band edges. This assumption may not be valid in the experimental situation. If not, this probably results in a much higher absorption. At this point it is not possible to discriminate between the given explanations for the deviation between the theoretical and experimental results. More work is needed on both the experimental and theoretical side. We plan to put some effort into investigating the last in the list of possible explanations, given above.

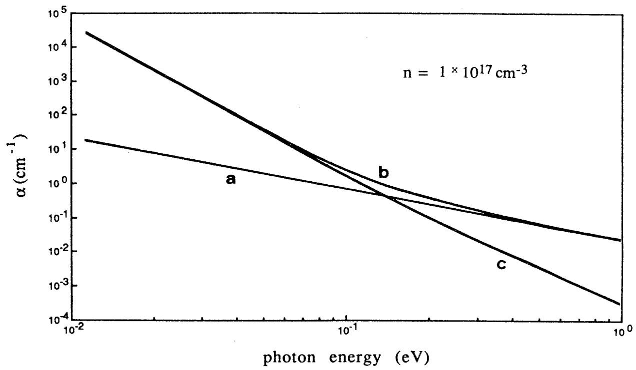

FIG. 5. The same as Fig. 4 but now for the density 1×10^{17} cm^{-3}.

III. SUMMARY AND CONCLUSIONS

We have presented the results for the free-carrier absorption in a multicomponent plasma, including the contributions from carrier scattering, impurity scattering, and phonon absorption and emission. Numerical results have been produced for an electron-hole plasma in silicon. We found that the particle scattering gave important contributions and even dominated for high plasma densities and/or low photon energies.

ACKNOWLEDGMENTS

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APPENDIX

The final result for the absorption in a multicomponent plasma, in the presence of impurities and with phonon coupling included, is

$$
\begin{aligned}
\alpha(\Omega)=&-\frac{2\pi e^2\hbar}{c\sqrt{\kappa(\Omega)}\Omega^3}\sum_{i,j}Z_i^2Z_j^2\left(\frac{Z_i}{m_i}-\frac{Z_j}{m_j}\right)^2\\
&\times\int_0^\infty d\omega\frac{1}{2\pi}\frac{\sinh\left(\frac{\hbar\beta\Omega}{2}\right)}{\sinh\left[\frac{\hbar\beta}{2}\left(\omega+\frac{\Omega}{2}\right)\right]\sinh\left[\frac{\hbar\beta}{2}\left(\omega-\frac{\Omega}{2}\right)\right]}\\
&\times\int d\mathbf{q}\frac{1}{(2\pi)^3}q_\mu^2\\
&\times\left\{\mathrm{Im}\left[\Gamma\left(\mathbf{q},\omega+\frac{\Omega}{2}\right)\right]\mathrm{Im}\left[\Gamma\left(\mathbf{q},\omega-\frac{\Omega}{2}\right)\chi_i\left(\mathbf{q},\omega-\frac{\Omega}{2}\right)\chi_j\left(\mathbf{q},\omega-\frac{\Omega}{2}\right)\right]\right.\\
&\quad+\mathrm{Im}\left[\Gamma\left(\mathbf{q},\omega-\frac{\Omega}{2}\right)\right]\mathrm{Im}\left[\Gamma\left(\mathbf{q},\omega+\frac{\Omega}{2}\right)\chi_i\left(\mathbf{q},\omega+\frac{\Omega}{2}\right)\chi_j\left(\mathbf{q},\omega+\frac{\Omega}{2}\right)\right]\\
&\quad-\mathrm{Im}\left[\Gamma\left(\mathbf{q},\omega+\frac{\Omega}{2}\right)\chi_i\left(\mathbf{q},\omega+\frac{\Omega}{2}\right)\right]\mathrm{Im}\left[\Gamma\left(\mathbf{q},\omega-\frac{\Omega}{2}\right)\chi_j\left(\mathbf{q},\omega-\frac{\Omega}{2}\right)\right]\\
&\quad\left.-\mathrm{Im}\left[\Gamma\left(\mathbf{q},\omega+\frac{\Omega}{2}\right)\chi_j\left(\mathbf{q},\omega+\frac{\Omega}{2}\right)\right]\mathrm{Im}\left[\Gamma\left(\mathbf{q},\omega-\frac{\Omega}{2}\right)\chi_i\left(\mathbf{q},\omega-\frac{\Omega}{2}\right)\right]\right\}\\
&-\frac{4\pi e^2\hbar}{c\sqrt{\kappa(\Omega)}\Omega^3}\sum_i Z_i^2\left(\frac{Z_i}{m_i}\right)^2\\
&\times\int_0^\infty d\omega\frac{1}{2\pi}\frac{\sinh\left(\frac{\hbar\beta\Omega}{2}\right)}{\sinh\left[\frac{\hbar\beta}{2}\left(\omega+\frac{\Omega}{2}\right)\right]\sinh\left[\frac{\hbar\beta}{2}\left(\omega-\frac{\Omega}{2}\right)\right]}\\
&\times\int d\mathbf{q}\frac{1}{(2\pi)^3}q_\mu^2g^2(\mathbf{q})\\
&\times\left\{\mathrm{Im}\left[\Lambda\left(\mathbf{q},\omega+\frac{\Omega}{2}\right)\right]\mathrm{Im}\left[\Lambda\left(\mathbf{q},\omega-\frac{\Omega}{2}\right)\chi_i\left(\mathbf{q},\omega-\frac{\Omega}{2}\right)D\left(\mathbf{q},\omega-\frac{\Omega}{2}\right)\right]\right.\\
&\quad+\mathrm{Im}\left[\Lambda\left(\mathbf{q},\omega-\frac{\Omega}{2}\right)\right]\mathrm{Im}\left[\Lambda\left(\mathbf{q},\omega+\frac{\Omega}{2}\right)\chi_i\left(\mathbf{q},\omega+\frac{\Omega}{2}\right)D\left(\mathbf{q},\omega+\frac{\Omega}{2}\right)\right]\\
&\quad-\mathrm{Im}\left[\Lambda\left(\mathbf{q},\omega+\frac{\Omega}{2}\right)\chi_i\left(\mathbf{q},\omega+\frac{\Omega}{2}\right)\right]\mathrm{Im}\left[\Lambda\left(\mathbf{q},\omega-\frac{\Omega}{2}\right)D\left(\mathbf{q},\omega-\frac{\Omega}{2}\right)\right]\\
&\quad\left.-\mathrm{Im}\left[\Lambda\left(\mathbf{q},\omega+\frac{\Omega}{2}\right)D\left(\mathbf{q},\omega+\frac{\Omega}{2}\right)\right]\mathrm{Im}\left[\Lambda\left(\mathbf{q},\omega-\frac{\Omega}{2}\right)\chi_i\left(\mathbf{q},\omega-\frac{\Omega}{2}\right)\right]\right\}\\
&-\frac{2\pi e^2\mathbf{n}_{\mathrm{imp}}}{c\sqrt{\kappa(\Omega)}\Omega^3}\sum_{i,j}Z_i^2Z_j^2\left(\frac{Z_i}{m_i}-\frac{Z_j}{m_j}\right)^2\int d\mathbf{q}\frac{1}{(2\pi)^3}q_\mu^2S(q)\left|\frac{\omega_0(q)}{\epsilon_T(\mathbf{q},0)}\right|^2\\
&\qquad\times v(q)\,\mathrm{Im}\left(\frac{[\chi_i(\mathbf{q},0)-\chi_i(\mathbf{q},\Omega)][\chi_j(\mathbf{q},0)-\chi_j(\mathbf{q},\Omega)]}{\epsilon_T(\mathbf{q},\Omega)}\right)\\
&-\frac{4\pi e^2\mathbf{n}_{\mathrm{imp}}}{c\sqrt{\kappa(\Omega)}\Omega^3}\sum_i Z_i^2\left(\frac{Z_i}{m_i}\right)^2\int d\mathbf{q}\frac{1}{(2\pi)^3}q_\mu^2S(q)\left|\frac{\omega_0(q)}{\epsilon_T(\mathbf{q},0)}\right|^2\frac{\mathrm{Im}\{\Lambda(\mathbf{q},\Omega)[\chi_i(\mathbf{q},0)-\chi_i(\mathbf{q},\Omega)]\}}{\Lambda(\mathbf{q},0)}\\
&-\frac{4\pi e^2\mathbf{n}_{\mathrm{imp}}}{c\sqrt{\kappa(\Omega)}\Omega^3}\sum_{i,j}Z_i^2Z_j^2\left(\frac{Z_i}{m_i}\right)^2\int d\mathbf{q}\frac{1}{(2\pi)^3}q_\mu^2S(q)\left|\frac{\omega_0(q)}{\epsilon_T(\mathbf{q},0)}\right|^2\chi_j(\mathbf{q},0)\\
&\qquad\times\mathrm{Im}\{\Lambda(\mathbf{q},\Omega)[\chi_i(\mathbf{q},0)-\chi_i(\mathbf{q},\Omega)]g(\mathbf{q})^2[D(\mathbf{q},0)-D(\mathbf{q},\Omega)]\}\ .
\end{aligned}
\tag{A1}
$$

The quantity q_μ is the projection of the vector $\mathbf{q}$ on the polarization vector of the light and $\chi_i(\mathbf{q},\omega)$ is the polarizability for component i. The function $\Gamma(\mathbf{q},\omega)$ is defined as

$$\Gamma(\mathbf{q},\omega)=\frac{v(q)}{\epsilon_L(\mathbf{q},\omega)-v(q)\sum_l Z_l^2\chi_l(\mathbf{q},\omega)}=\frac{v(q)}{\epsilon_T(\mathbf{q},\omega)}\ , \tag{A2}$$

where $\epsilon_L(\mathbf{q},\omega)$ is the lattice dielectric function, i.e., the dielectric function for the system in absence of the carriers in the plasma. If the plasma is an electron-hole plasma in a semiconductor, the lattice dielectric function has its contributions from the phonons and from valence-electron excitations across the band gap. The function $\Lambda(\mathbf{q},\omega)$ is defined as $\Lambda(\mathbf{q},\omega)=\epsilon_L(\mathbf{q},\omega)/\epsilon_T(\mathbf{q},\omega)$. The phonons enter the expressions, apart from through the contribution to the lattice dielectric function, through $g(\mathbf{q})$ and $D(\mathbf{q},\omega)$, the electron-phonon coupling constant and phonon Green's function, respectively. In Ref. 4, dispersionless optical phonons were considered. Here we have generalized the expressions slightly to make them valid for all types of phonons, hence the wave-vector-dependent phonon Green's functions. In the general case, the electron-phonon coupling is not identical for the different plasma components. We have refrained from taking that into account in Eq. (A1) since the expressions are already rather complicated. However, in Sec. II, when we treat a specific situation, we take this into account after having performed simplifications motivated by the situation at hand. If the reader needs a more general expression, Ref. 18 might come handy. The last three contributions in Eq. (A1) come from the impurity scattering. We have assumed the impurity concentration to be $\mathbf{n}_{\mathrm{imp}}$, the distribution of impurities to be given by the structure factor $S(q)$, and each impurity potential is denoted by $\omega_0(q)$.

We note that the first and third contributions in Eq. (A1) disappear in a one-component plasma. The last three contributions are only present in the presence of impurities. The second and fifth terms give contributions only if phonon coupling is included. The phonons, however, also modify the rest of the terms.

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