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A new method for the determination of the optical mass of electrons in metals

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Abstract. Generalizing the Drude conductivity and using experimental data for the complex refractive index or for the complex dielectric function an expression is derived for the determination of the frequency-dependent electron mass, defined as the optical mass. Values for the optical mass are calculated for 27 metals, including in a few both the solid phase and the liquid phase. Additionally, a new formula for the estimation of the polarizability of metals is given and evaluated for 15 metals. Good agreement between existing published literature values and our calculation is found for the optical mass in the zero-frequency limit as well as for the polarizability.

1. Introduction

Although the effective mass is an important quantity in solid state physics in many aspects, there is no stringent rule in the literature for the use of the terms ‘effective mass’ or ‘optical mass’. Sometimes this leads to confusion, especially among non-experts in this field of solid state physics. The well known formula

$$\frac{1}{m^*} = \frac{1}{\hbar^2} \sum_{ij} \frac{\partial^2 E_n(k)}{\partial k_i \partial k_j} \quad (1)$$

is used by some workers as the definition of the effective mass (see, e.g., Ashcroft and Mermin (1976)) and by others for the optical mass (see, e.g., Brust (1970)). Both definitions can be, of course, correct if one clearly distinguishes m^* as a measure of the deviations of the true band structure from the free-electron model at zero temperature or as including the influence of phonons at higher temperatures or as incorporating the interaction with photons. Obviously, for a clear distinction between the several possibilities it would be desirable that m^* be labelled accordingly or written explicitly as a function of the respective variables such as $m^*(T)$ or $m^*(T, \omega)$.

For clarity, we propose the expression ‘optical mass’ for the third version and shall use it in what follows. The ‘optical mass’ depends on the photon frequency ω and on the temperature T and can be determined, as we shall show below, from optical data. The ‘effective mass’ is then defined and measured in the frequency-independent case. In the limit $\omega \rightarrow 0$ both should, of course, converge to the same value.

It should be stressed at this point that the goal of the paper is the derivation of a simple expression for the calculation of the optical mass from tabulated data and not an *ab-initio*

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determination of it within the framework of band-structure theory. Our approach, therefore, is guided more by an experimental than by a theoretical point of view.

Since the optical mass is not only an interesting quantity in itself but also an important input parameter for theoretical calculations (e.g. the optical properties (Hüttner 1994, 1995a)) or evaluations from experimental data (e.g. the intraband plasma frequency Ω_p (Smith and Segall 1986)), we shall present values of m^* later in the paper in table 1.

2. Theoretical model

The key quantity for the calculation of the optical properties of solids is the complex dielectric function

$$\varepsilon(\omega, T) = \varepsilon_0(\omega, T) + i \frac{4\pi}{\omega} \sigma(\omega, T). \quad (2)$$

The conductivity can be expressed in first-order-time-dependent perturbation theory by (Ashcroft and Mermin 1976)

$$\sigma(\omega) = \frac{e^2\tau}{1 - i\omega\tau} \int dk \frac{f(E(k))}{4\pi^3} \left[\frac{1}{m} - \frac{\hbar^2}{m^2} \sum_{n'} \left(\frac{\langle nk | \nabla | n'k \rangle \langle n'k | \nabla | nk \rangle}{\hbar\omega + E_n(k) - E_{n'}(k)} + \frac{\langle nk | \nabla | n'k \rangle \langle n'k | \nabla | nk \rangle}{-\hbar\omega + E_n(k) - E_{n'}(k)} \right) \right] \quad (3)$$

where for simplification we have omitted the indices and assumed a common scattering time for all bands. (For the full expression in the absence of collisions refer to Ashcroft and Mermin (1976, p 252).)

Interpreting the expression in square brackets as a temperature- and frequency-dependent effective mass, we can define a generalized complex Drude conductivity by

$$\sigma(\omega, T) = \frac{\sigma_D(\omega, T)}{1 - i\omega\tau} \quad (4)$$

with the real part given by

$$\sigma_D(\omega, T) = \frac{\omega_p^2(T)\tau(T)}{4\pi M(\omega, T)} = \frac{\Omega_p^2(\omega, T)\tau(T)}{4\pi} \quad (5)$$

where ω_p is the plasma frequency, Ω_p corresponds to the intraband plasma frequency, $\tau(T)$ is the Drude scattering time and M is the ratio of the optical electron mass to the bare electron mass.

Inserting equation (4) and the first expression in equation (5) into equation (2) and taking the square of the absolute value of the dielectric function, we find a quadratic equation for M :

$$M^2 \{ |\varepsilon|^2 - \varepsilon_0^2 \} + \frac{2\varepsilon_0\omega_p^2\tau^2}{1 + \omega^2\tau^2} M - \frac{\omega_p^4\tau^2}{\omega^2(1 + \omega^2\tau^2)} = 0 \quad (6)$$

where we have suppressed the dependence on ω and T in this formula and we shall continue to do so. The physical solution of equation (6) is

$$M = \frac{\varepsilon_0\omega_p^2}{\omega^2[(n^2 + k^2)^2 - \varepsilon_0^2][1 + (\omega\tau)^{-2}]} \left\{ \left[1 + \frac{[(n^2 + k^2)^2 - \varepsilon_0^2](1 + \omega^2\tau^2)}{\varepsilon_0^2\omega^2\tau^2} \right]^{1/2} - 1 \right\} \quad (7)$$

where the dielectric function is expressed through the components of the complex refractive index. Although equation (7) is the main result, we shall give two simpler expressions which are more suitable for a quick estimate. For photon frequencies well below the plasma frequency the absolute value of the complex refractive index is usually much larger

than unity for metals. Thus neglecting unity in the expression in curly brackets we get as an approximate formula

$$M_{app} = \frac{\omega_p^2}{\omega^2[(n^2 + k^2)^2 - \varepsilon_0^2]^{1/2}} \frac{1}{(1 + [\omega\tau]^{-2})^{1/2}}. \quad (7a)$$

Taking into account the condition $\omega\tau \gg 1$, which is mostly fulfilled in the optical range, and neglecting ε_0 , equation (7a) reduces to a very simple formula suitable for a quick estimate

$$M_{fast} = \frac{\omega_p^2}{\omega^2(n^2 + k^2)}. \quad (7b)$$

3. Discussion

3.1. Case $\omega\tau \gg 1$

Equation (7b) holds in this limit. For an evaluation, one needs only the plasma frequency ω_p (see, e.g., Ashcroft and Mermin (1976)) and the tabulated values of the components n and k of the complex refractive index (e.g. from compilations edited by Palik (1985, 1991)). The other two equations additionally require the Drude scattering time τ and the dielectric constant ε at $\omega = 0$. Usually the scattering time can be obtained from the second expression in equation (5). However, this is not allowed here because we have already used this equation for the derivation of M . On the other hand, for some metals the Drude plasma frequency Ω_p is known and, in these cases, one can use the last term of equation (5). A mass-independent term for τ can also be found within the framework of Drude's theory utilizing the real and imaginary parts of the dielectric function:

$$\tau = \frac{\varepsilon_0 - \varepsilon_1}{\omega\varepsilon_2} = \frac{\varepsilon_0 - n^2 + k^2}{\omega 2nk}. \quad (8)$$

Although for frequencies below the interband transitions both possibilities should lead to the same value for M , our experience is that τ obtained from equation (5) leads to better results especially at these low frequencies. Apparently, the influence of experimental uncertainties may be reduced by employing an independently measured quantity. There are still other possibilities, especially suitable for the low-frequency range. Allen *et al* (1986) published a simple formula for the calculation of the electron-phonon scattering rate $1/\tau$ from a solution of the Bloch-Boltzmann equation in lowest order which, however, depends on the transport electron-phonon coupling-constant λ_{tr} . Unfortunately, this quantity is known only for a few metals. Another simple method would be to evaluate Ω_p by means of a value for $M(\omega = 0)$ determined, for example, by specific heat or T_c measurements. Indeed, this method has been used in the most cases.

Some remarks must be made about the contribution of the interband terms which usually appear in the discussed range of frequencies. Although we designated equation (4) as a generalized Drude expression, it contains, owing to equation (3), also the interband conductivity. In the vicinity of the interband frequencies we shall find, for this reason, marked deviations in the values of $M(\omega, T)$ in comparison with the constant value of the effective mass determined, for example, by specific heat measurements or from the relation between the electron-phonon coupling parameter λ and the effective mass $M = 1 + \lambda$ (Allen 1987). Between and below these frequencies we expect an almost flat behaviour of M as a function of ω . Its value may differ from region to region since different parts of the band structure contribute and a changed effective number of electrons may be involved.

Although the correct value of the zero-frequency dielectric constant ε_0 is not very well known for metals, a few calculated by Sturm *et al* (1990) indicate values between one and three. Therefore, one can take the free-electron value $\varepsilon_0 = 1$ as long as $n^2 + k^2$ is much larger than unity. A method for the evaluation of ε_0 from the optical data, needed when $n^2 + k^2$ becomes of the order of unity, is described in the next section and an example is given in the appendix.

3.2. Case $\omega\tau \ll 1$

On the one hand this range has the advantage that interband transitions usually do not occur but on the other hand it needs, despite the smallness of the scattering time τ of the order of femtoseconds, frequencies deep in the infrared. Therefore only a few measurements have been reported. Probably the most extensive compilation of data has been provided by Ordal *et al* (1983, 1985, 1987). Unfortunately, the scatter between different measurements is large and may have been caused by different methods of sample preparation and also by the use of the Kramers–Kronig relation with an assumed high-frequency behaviour. Figure 3 given later, which displays the optical mass of gold, may serve as an example for it.

4. Determination of the polarizability ε_0

In general, the real part $\varepsilon_0(\omega)$ is not a constant and represents the polarization of the rest of the crystal generated by the core and d electrons if $\varepsilon'(\omega)$ is considered to be the contribution from the conduction electrons. Yet it is expected that $\varepsilon_0(\omega)$ has a low dispersion because the d-electrons and the core electrons are lying sufficiently deeply below the Fermi energy in most cases. This means that we can put $\varepsilon_0(\omega) = \varepsilon_0 = \text{constant}$ for $\omega \ll E_d$ and E_{core} . Although $\varepsilon_0(\omega)$ is usually not very much larger than unity, the correct value can be important since, for example, it enters the sum rule for the oscillator strengths and, here more significantly, it can become comparable with $n^2 + k^2$ at high frequencies.

Describing the contributions from the interband transitions by an oscillator-like model (see, e.g. Ehrenreich and Phillip (1962) and Hüttner (1994)) the real part of the dielectric function can be written as

$$\varepsilon'(\omega) = \varepsilon_0(\omega) - \frac{4\pi}{\omega} \left(\frac{\sigma_D \omega \tau}{1 + \omega^2 \tau^2} - \frac{\omega_p^2 \omega}{4\pi} \sum_n \frac{A_n [\omega_n^2 + v_n^2 - \omega^2]}{[\omega_n^2 + v_n^2 - \omega^2]^2 + 4\omega^2 v_n^2} \right). \quad (9)$$

Here A_n is the oscillator strength of the n th interband transition and v_n is the scattering frequency belonging to it. Assuming ω to be much larger than v_n and ω_n , equation (9) can be simplified to

$$-\varepsilon'(\omega) = -\varepsilon_0 + \frac{1}{\omega^2} \left(\frac{4\pi\sigma_D}{\tau} + \omega_p^2 \left[\varepsilon_0 - \frac{1}{M} \right] \right) \quad (10)$$

where we have replaced the sum over the oscillator strengths by the f -sum rule $\sum_n A_n = \varepsilon_0 - M^{-1}$ (Sturm and Ashcroft 1974). Plotting the experimental values of $-\varepsilon'(\omega)$ as a function of ω^{-2} , we obtain $-\varepsilon_0$ as the intersection with the $-\varepsilon'$ axis and the terms in large parentheses as the slope of this function. The latter is not only a byproduct but it can be used to check whether the conditions for the derivation of equation (10) are met for the metal investigated.

To this end, one substitutes M by means of equation (5) and finds by cancelling the σ_D -terms that the large parentheses in equation (10) are equal to the product of the square of the plasma frequency times ε_0 . Since the plasma frequencies are known for most metals,

one has, apart from the straightness of the plot, a second proof. The square root of the slope divided by ε_0 should correspond to the plasma frequency. Examples are listed in table 2 below.

It is worthwhile noting that equation (10) contains more information than an expression derived many years ago by Cohen (1958). In his paper he showed that $n^2 - k^2$ could be fitted by $A - B/\omega^2$ in the range $\omega\tau \gg 1$. Our experience, however, tells us that data for many metals can be plotted in such a straight line for different intervals especially if these are fairly short. From the work of Cohen (1958), one can also derive a formula for the optical mass in the same limit, $\omega\tau \gg 1$. In our notation it is

$$M = \frac{\omega_p^2 \tau^2}{(\varepsilon_0 - n^2 + k^2)(1 + \omega^2 \tau^2)}. \quad (11)$$

In some cases we find good agreement with the values evaluated from equation (7) or (7a) in this limit (e.g. for Al) and in other cases not (e.g. for Li). Typical for all is a larger standard deviation in comparison with our results.

5. Results and discussion

In this section we present table 1 with the optical mass calculated by means of equation (7) together with the frequency range $\Delta\omega$ belonging to it. The necessary input parameter plasma frequency ω_p , intraband plasma frequency Ω_p , DC conductivity ρ_{dc} and polarizability ε_0 are also listed. The intraband plasma frequency has been calculated in most cases using a literature value for the effective mass as discussed above. We have favoured this method at the expense of equation (8) because it usually leads to a smaller standard deviation even if the mean values are similar for most metals. For many systems we use the free-electron value for ε_0 because we were not able to calculate the right value from the available experimental data. Fortunately, the error is negligible for these results of $M(\omega)$ since in all these cases $n^2 + k^2$ is clearly greater than unity. An extrapolation of the optical mass to zero frequency can be performed if the course of $M(\omega)$ versus frequency justifies this, as is the case, for example, for Al. Physically this is realized if the complex dielectric function or the complex refractive index was measured at sufficiently low frequencies, at least below the essential interband transitions.

For a better comparison, we have tried to collect from the literature in the last column of table 1 the most accepted values for the effective mass.

Some remarks should be made about the table. The standard deviations given do not result from strong fluctuations between neighbouring $M(\omega)$ -values (these are in all cases very small), but from the slope of the curve in the investigated frequency interval. The number of points used in the statistical calculation exceed ten even for very short intervals.

The interpolated values of the effective mass $M(\omega \rightarrow 0)$, for the metals in the liquid state are similar to the results found in the solid state with one remarkable exception, bismuth. Ashcroft and Mermin (1976) reported for this semimetal the very small value $M_{eff} = 0.047$. The reason for this can be traced back to the relatively complicated Fermi surface caused by a slight distortion of the crystal structure from the simple cubic monatomic Bravais lattice. From this point of view the dramatic change in the value of the effective mass during the phase transition must follow from a rearrangement in the proximity order of the atoms in the liquid state. Justification for this conclusion is obtained from the known behaviour of the optical properties of the liquid polyvalent metals. For aluminium (Hüttner 1994), lead (Hüttner 1995a), and tin (Hüttner 1995b) we have revealed that the optical properties in the

Table 1.

Metal	ω_p (eV)	Ω_p (eV)	ϵ_0	ρ ($\mu\Omega$ cm)	$\Delta\omega$ (eV)	$M(\omega)$	$M(\omega \rightarrow 0)$	M_{eff}
Ag	8.9	8.9	3.23	1.68	0.04–0.62	0.98 ± 0.01	0.98	$0.99\text{--}1.04^a$
Al	15.0	12.5	1.05	2.65	0.006–1.0	1.46 ± 0.18	1.53	1.52^b
Al, liquid	14.0	13.2	1.0	32.5	1.28–3.0	1.08 ± 0.10		1.19^c
Au	9.0	8.4	2.94	2.26	0.1–1.0	1.17 ± 0.02	1.14	1.1^d
Be	18.4	28.4	1.0	4.0	0.02–0.4	3.24 ± 2.32	0.84	0.46^a
Bi, liquid	14.0	14.0	1.0	131	0.62–2.14	0.99 ± 0.01	0.99	
Ca	8.0	8.0	1.0	3.85	0.75–1.5	1.77 ± 0.05		1.8^e
Co, fcc	10.3	7.9	1.0	6.24	0.09–0.11	11.22 ± 0.49		
Co, hex	10.3	7.9	1.17	6.24	0.07–0.10	7.52 ± 1.51		1.71^f
Cr	13.2	10.1	1.17	12.9	0.04–0.50	7.52 ± 1.51		1.72^f
Cu	10.8	8.8	1.46	1.72	0.02–0.74	1.94 ± 0.07		1.45 ± 0.06^g
Fe	15.3	11.1	2.24	9.7	0.02–0.07	2.30 ± 0.72	2.01	1.9^h
Hg, liquid	7.7	5.4	2.94	98.4	0.2–1.4	1.00 ± 0.40	1.69	2.0^i
Ir	16.5	13.9	2.05	5.07	0.1–1.0	4.56 ± 0.43	3.06	1.41^h
K	4.3	4.1	1.27	6.15	1.76–2.61	1.10 ± 0.07	1.07	1.08 ± 0.02^j
Li	7.1	5.4	1.0	10.0	0.15–6.45	1.26 ± 0.19	1.44	1.45^d
Mo	10.5	8.8	3.71	5.33	0.1–0.2	1.96 ± 0.03	1.83	$1.43^h\text{--}2.00^f$
Na	5.9	5.6	1.3	4.2	0.55–1.05	1.17 ± 0.02	1.13	$0.98^d\text{--}1.25^k$
Nb	8.7	5.8	1.0	16.0	0.12–0.45	1.46 ± 0.01	1.45	1.86^f
Ni	7.7	7.1	1.0	7.04	0.004–0.025	1.69 ± 0.29		1.7^h
Pb	13.0	8.8	1.0	21.0	0.002–0.31	2.80 ± 0.16	2.70	$2.12\text{--}2.71^l$
Pb, liquid	12.7	11.6	1.0	96.0	0.62–3.7	1.00 ± 0.11	1.24	1.2^m
Pd	6.8	5.2	1.0	10.55	0.1–0.14	1.59 ± 0.14		1.66^f
Rh	18.6	13.2	2.1	4.78	0.1–1.0	4.32 ± 0.92		1.87^f
Sn, liquid	13.8	13.8	1.0	48.7	0.62–2.14	0.99 ± 0.04	1.05	0.98 ± 0.05^o
Ta	10.1	7.4	1.0	12.45	0.01–0.12	1.61 ± 0.17	1.61	1.65^l
Ti	17.8	15.0	1.0	42.7	0.006–1.51	1.22 ± 0.11		1.39^f
V	12.5	8.5	1.0	24.8	0.1–0.32	4.02 ± 0.91	1.61	1.63^f
W	11.7	10.2	1.0	5.33	0.06–0.3		1.56	1.31^h

^a From Parkins *et al* (1981).

^b From Sturm *et al* (1990).

^c From Hüttner (1994), $T = 1550$ K.

^d From Pines (1963).

^e From Ashcroft and Mermin (1976).

^f From Perrot and Rassolt (1994).

^g From Cohen (1958).

^h From Allen (1987).

ⁱ From Pines (1963), solid Hg.

^j From Palmer and Schnatterly (1971).

^k From Ashcroft and Lawrence (1968).

^l From Grimvall (1976).

^m From Inagaki *et al* (1982).

^o From Petrakian *et al* (1980).

liquid state can only be explained under the assumption of band structures which are, by and large, similar in both states.

Inspection of the curves of $M(\omega)$ versus ω shows that the optical mass contains more information than only the bending of the electron energy. Prominent interband transitions produce structures, similar to the typical behaviour of the frequency-dependent dielectric function in ionic crystals, caused by the change in the sign of the energy denominator equation (3). For frequencies above the interband transitions but below the plasma frequency, $M(\omega)$ approaches $1/\epsilon_0$. Since the metal attains a dielectric behaviour for even

larger energies, $\omega > \omega_p$, the optical mass disappears proportionally to ω^{-2} in this range. Figure 1 displays a plot over four decades of the frequency dependence of $M(\omega)$ for Al. There are two prominent interband transitions due to parallel bands at about $\omega = 0.5$ eV and $\omega = 1.5$ eV. Additional structures below 0.5 eV may result, as suggested by Brust (1970) and Szmulowicz and Segall (1981), from lower-lying transitions. However, the flat behaviour at very low energies does not support their assumption that transitions exist down to zero frequency. More recently, Lee and Chang (1994) deduced from an *ab-initio* pseudopotential calculation that $\omega = 0.1$ eV for the onset of the interband conductivity, in fairly good agreement with figure 1. This conclusion is also confirmed by the good agreement of the value of $M(\omega \rightarrow 0)$ with the theoretically calculated value $M_{eff} = 1.49$ (Perrot and Rasolt 1994).

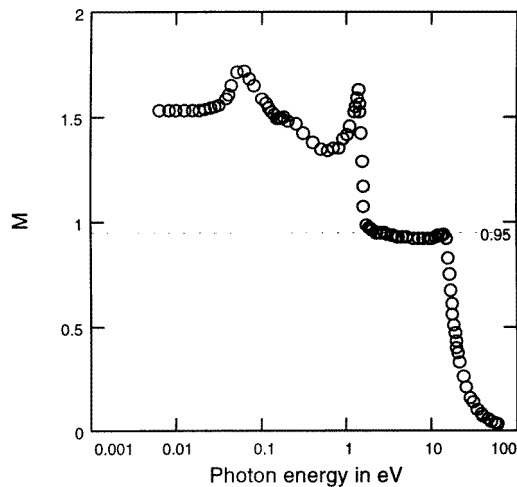


Figure 1. Optical mass of Al calculated from the data of Smith *et al* (1985).

Silver, as depicted in figure 2, has no interband transitions below 3.9 eV. This results in a constant value for $M(\omega)$ in this region. The slight difference at low energies between the data taken from the paper of Winsemius *et al* (1976) and those of Bennett and Bennett (1966) are due to different types of sample preparation. Although being masked by the semilogarithmic plot, $M(\omega)$ possesses a short constant behaviour around $1/\epsilon_0$ below the plasma frequency where ϵ_0 equals 3.23 (see table A1 in the appendix). Since gold has a similar band structure we expect a comparable behaviour as for silver. This conjecture is confirmed by the measurement of Weaver *et al* (1981) between 0.1 and 1.0 eV but not by the data of Ordal *et al* (1987) at lower energies which were determined from a Kramers–Kronig analysis (figure 3).

Figure 4 contains a comparison between the values of the optical mass of Li calculated by means of equation (7) and equation (11) given by Cohen (1958). Although the product $\omega\tau$ complies with the necessary condition for the validity of equation (11), it always improves as the frequency increases, i.e. it increases from about 3 for the lowest photon frequency to 230 for the highest photon frequency; the agreement between the results of both approaches becomes worse as $\omega\tau$ increases. The reason for this is in the different ways in which the real and imaginary parts of the refractive index enter the equations. For some metals, it should be mentioned, we find closer agreement between the calculated values. The last

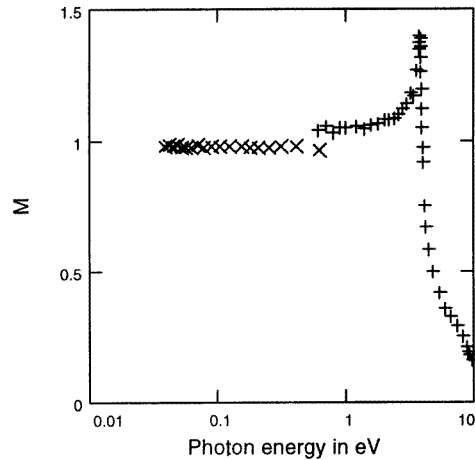


Figure 2. Optical mass of Ag calculated from the data of Bennett and Bennett (1966) (\times) and Winsemius *et al* (1976) (+).

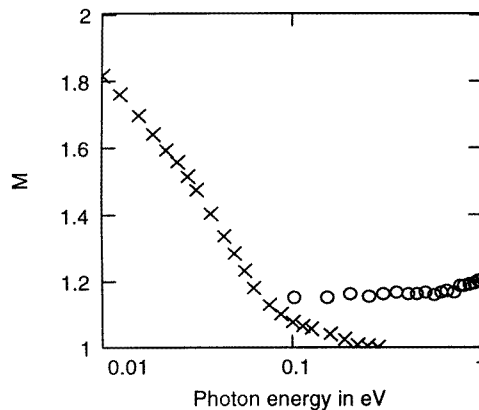


Figure 3. Optical mass of Au calculated from the data of Ordal *et al* (1987) (\times) and Weaver *et al* (1981) (\circ).

two figures are devoted to liquid metals. In figure 5 we present the optical mass of liquid aluminium calculated from the data of Krishnan and Nordine (1993) taken at $T = 1550$ K. Despite the existing scatter between the few values the overall trend is reminiscent of the behaviour of $M(\omega)$ of solid Al (figure 1). There is an increase in $M(\omega)$ just below the interband transition at about 1.4 eV and a decrease to a fairly flat behaviour above 1.4 eV. This conclusion is supported by the solid-like shape of the absorption of liquid Al with a peak at $\omega = 1.4$ eV (Krishnan and Nordine 1993) and by theoretical calculations which predict for $T = 1550$ K a peak at $\omega = 1.45$ eV and $M(\omega \rightarrow 0) = 1.19$ (Hüttner 1994).

Figure 6 shows the optical mass of liquid Pb at $T = 614$ K. A linear extrapolation to zero frequency gives $M(0) = 1.24$, close to $M = 1.2$ found from the experimental data of Inagaki *et al* (1982) if we invert their effective number of electrons N^* into M_{eff} .

At this point, it should be emphasized once more that the peak in $M(\omega)$ as well as in the absorption clearly indicates the existence of a band structure in liquid Al which therefore

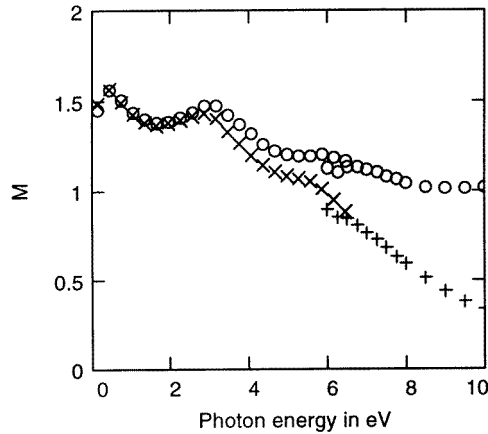


Figure 4. Optical mass of Li calculated from the data of Rasigni and Rasigni (1976) (\times) and Callcott and Arakawa (1974) ($+$); the values (\circ) are calculated from the expression given by Cohen (1958), equation (11).

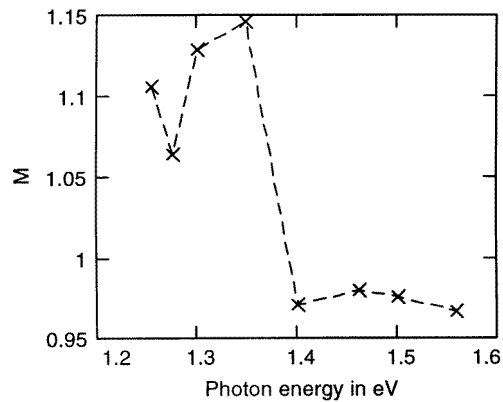


Figure 5. Optical mass of liquid Al calculated from the data of Krishnan and Nordine (1993); guide for the eye.

cannot be described by a Drude model alone. Being determined by the proximity order there is no plausible reason why this behaviour should not hold true for any liquid metal.

6. Conclusions

By newly interpreting a standard formula for the frequency-dependent conductivity we have introduced a generalized Drude conductivity and derived from this an expression for the frequency-dependent effective mass of the electrons, called the optical mass. Additionally we give a new expression for the determination of the polarizability ϵ_0 of metals and their plasma frequency from measured values of the real part of the dielectric function. We find good agreement with data given in the literature for both the polarizability and the optical mass in the zero-frequency limit. For some metals we have obtained for the first time, to

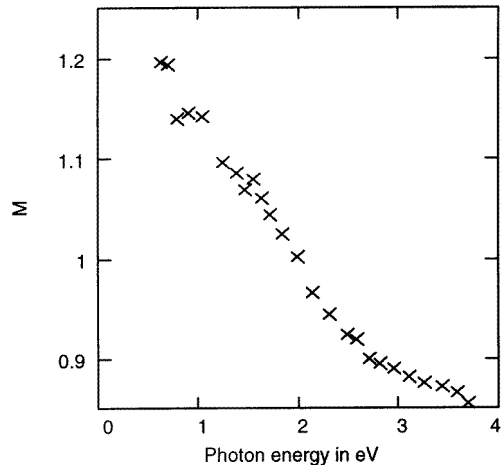


Figure 6. Optical mass of liquid Pb calculated from the data of Inagaki *et al* (1982).

the best of our knowledge, estimates for the polarizability. The shape of the optical mass as a function of frequency shows pronounced peaks which are related to the band structure of the metal. Moreover, one seems to be able to decide from the calculation of the optical mass whether a low-frequency cut-off for interband transitions exists or not, provided that measurements of the refractive index or the dielectric function were made to sufficiently low frequencies. As an example this is demonstrated for aluminium. Since the method holds for both the solid and the liquid state we were able to determine also some values for the optical mass of liquid metals. Stressing this point again, we have to conclude from the shape of the curves and from the values found that the properties of liquid metals result from a still existing band structure and that they cannot be described by the free-electron model.

Acknowledgments

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Appendix

For aluminium, we demonstrate in this appendix the method for the determination of the polarizability, ε_0 . The data for the real part of the dielectric function are taken from Palik (1985) for photon frequencies between 7 and 15 eV. Plotting the data as a function of ω^{-2} we get the straight line shown in figure A1.

A linear regression fit yields for the intersection the value $\varepsilon_0 = 1.05$ and for the slope 243.7. The plasma frequency is obtained from $(243.7/1.05)^{0.5}$ as $\omega_p = 15.2$ eV. Both values are in good agreement with values reported in the literature. The polarizability is in the range between the experimental values of Smith *et al* (in Palik (1985)), $\varepsilon_0 = 1.03$ – 1.04 , and the theoretical value of Sturm *et al* (1990), $\varepsilon_0 = 1.08$. The plasma frequency was measured by Raether (1980) as $\omega_p = 15.3$ eV.

Table A1.

Metal	ϵ_0 (from equation (10))	ω_p (eV) (from equation (10))	ϵ_0 (from the literature)	ω_p (eV) (from the literature)
Ag	3.23	7.45		8.98 ^a
Al	1.05	15.02	1.08 ^b , 1.04 ^c	15.3 ^d
Au	2.94	5.62		9.02 ^a
Be	0.99	17.31		17.04 ^a
Co	1.17	7.68		10.3 ^e
Cu	1.46	8.45	6.0 ^f	8.5 ^e
Fe	2.24	10.19		15.27 ^a
Hg	2.94	7.26	2.76 ^b	7.5 ^d
Ir	2.05	12.6		
K	1.27	3.84	1.25 \pm 0.05 ^g	4.29 ^d
Li	1.00	7.04	1.00 ^h	7.12 ⁱ
Mo	3.71	10.5		10.1 ^j
Na	1.30	5.27	1.34 ^d	5.95 ^d
Pt	2.84	6.08		6.2 ^k

^a From Ashcroft and Mermin (1976).

^b From Sturm *et al* (1990).

^c From Smith *et al* (1985).

^d From Raether (1980).

^e From Missell and Atkins (1973).

^f From Roberts (1960).

^g From Palmer and Schnatterly (1971).

^h From Rasigni and Rasigni (1977).

ⁱ From Kunz (1966).

^j From Apholte and Ulmer (1966).

^k From Klemperer and Shepperd (1963).

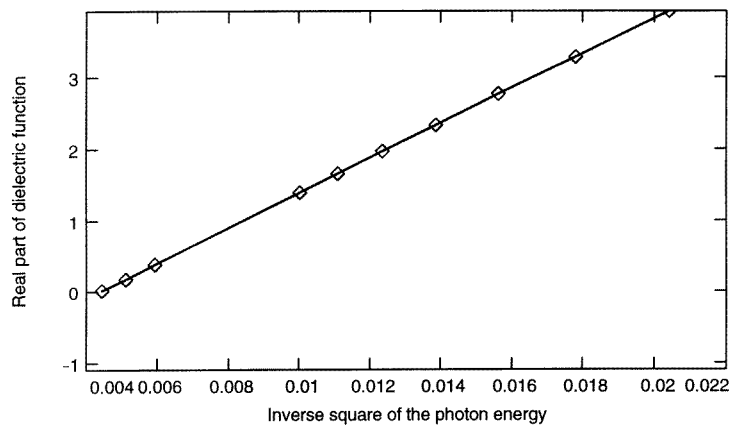


Figure A1. Determination of the polarizability by linear regression fit of the data taken from the work of Smith *et al* (1985).

Table A1 contains a compilation of the values for ϵ_0 and ω_p calculated from equation (10) together with data from the literature for comparison.

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