THE OPTICAL CONSTANTS OF ZINC

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The optical constants n and κ ($n - i\kappa$ is the complex refractive index) of zinc are measured in the spectral range from 1.2 to 10 microns at room temperature. The following microcharacteristics of zinc are obtained from n and κ: the concentration of conduction electrons $N = 3.38 \times 10^{22}$ cm^{-3}, the mean electron velocity on the Fermi surface $\langle v_F \rangle = 0.92 \times 10^8$ cm/sec, the total area of the Fermi surface $S_F = 1.8 \times 10^{-37}$ g^2-cm^2/sec^2, and the effective electron collision frequency $\nu = 1.08 \times 10^{14}$ sec^{-1}. The following absolute values of the Fourier components of the pseudopotential were determined using data on the optical conductivity in the visible and near-infrared region cited in the literature: $|V_{\{1\bar{1}0,1\}}| = 0.74$ eV and $|V_{\{000,2\}}| = 0.50$ eV. The value of N calculated from the Fourier components of the pseudopotential is in good agreement with the value obtained from measurements in the infrared region.

1. A relation has recently been established between the Fourier components of the pseudopotential and the optical properties of metals in the long-wave spectral range where they are determined by the conduction electrons;[1] it has also been shown that these Fourier components can be determined from optical measurements in the short-wave region for which the interband transitions are important.[2-5] Thus, measurements in the long-wave and short-wave range turn out to be related to one another. The conclusions of the theory have been compared with experimental results for indium, aluminum, lead, and tin,[2,6,7] i.e., for group III and group IV nontransition metals. It is of interest to compare theory and experiment for group II metals.

In this paper we present previously carried out measurements of the optical constants of zinc in the infrared region. On the basis of these measurements we have determined the following microcharacteristics of the conduction electrons: the average concentration of the conduction electrons N, the mean velocity of the electrons on the Fermi surface v_F, the total area of the Fermi surface S_F, and the average effective collision frequency of the electrons. We determined the Fourier components of the pseudopotential in accordance with the data in the literature referring to the investigation of the optical properties of zinc in the short-wave region,[8,5] and from these we calculated the concentration of conduction electrons. As will be seen below, the results of the determination of N from the long-wave and short-wave measurements agree with one another.

2. Zinc is a divalent metal which forms a close-packed hexagonal lattice with the ratio c/a = 1.856 (for T = 298°K).[9] In this case the free-electron sphere is intersected by the Bragg planes with nonzero structure factors presented in Table I.

According to [1], using Table I we obtain for the mean concentration of conduction electrons the following relations:

$$\frac{N_{val} - N}{N_{val}} = 1.27 \frac{|V_{\{000,2\}}|}{E_F^0}\left(\frac{1}{2} + \frac{\varphi_{\{000,2\}}}{\pi}\right) + 4.08 \frac{|V_{\{1\bar{1}0,0\}}|}{E_F^0}\left(\frac{1}{2} + \frac{\varphi_{\{1\bar{1}0,0\}}}{\pi}\right) + 9.00 \frac{|V_{\{1\bar{1}0,1\}}|}{E_F^0}\left(\frac{1}{2} + \frac{\varphi_{\{1\bar{1}0,1\}}}{\pi}\right), \quad (1)$$

$$\varphi_{\{000,2\}} = \operatorname{arctg} \frac{0.310}{|V_{\{000,2\}}|/E_F^0}, \qquad \varphi_{\{1\bar{1}0,0\}} = \operatorname{arctg} \frac{0.234}{|V_{\{1\bar{1}0,0\}}|/E_F^0},$$

$$\varphi_{\{1\bar{1}0,1\}} = \operatorname{arctg} \frac{0.086}{|V_{\{1\bar{1}0,1\}}|/E_F^0}, \qquad \frac{N}{m} = \frac{1}{3}\operatorname{Sp}\left(\frac{N}{m}\right)_{ij}.$$

Here N_{val} is the concentration of valence electrons; $V_{\{g\}}$ are the Fourier components of the pseudopotential corresponding to the Bragg planes $\{g\} \equiv \{n_1 n_2 n_3, n_4\}$; E_F^0 is the Fermi energy of the free electrons when their concentration is equal to the valence concentration; m is the mass of the free electron.

The Fourier components V_g can be determined from the position of the maximum of the main bands of the interband conductivity, connected with transitions near Bragg planes.[3,4] As follows from [4],

$$|V_g| = \hbar(\omega_g)_{max} / 2t. \quad (2)$$

Here $(\omega_g)_{max}$ is the frequency which corresponds to the maximum of the interband conductivity; t is a factor which depends on the band width whose magnitude lies between 1 and 1.06. In most cases one can assume that $t \approx 1.05 \pm 0.01$.

The magnitude of the interband conductivity $\tilde{\sigma}$ is proportional to $(\mathbf{e} \cdot \mathbf{p}_g)^2$ [see, for example, (11) in [4]]

Table I. Characteristics of the Bragg planes intersecting the free-electron sphere of zinc.

Indices of the Bragg planes $\{n_1, n_2, n_3, n_4\}$	Number of planes	$\frac{p_{\{n_1 n_2 n_3, n_4\}}}{p_F^0}$	Structural factors $F_{\{n_1, n_2, n_3, n_4\}}$
{000.2}	2	0.808	2
{110.0}	6	0.865	1
{110.1}	12	0.955	$\sqrt{3}$

Note. Here the indices of the Bragg planes refer to the four hexagonal axes; $p_{\{n_1, n_2, n_3, n_4\}}$ is the distance of the Bragg plane from the center of the zone Γ, and p_F^0 is the radius of the free-electron sphere in momentum space.

where $\mathbf{e} = \mathbf{E}/|\mathbf{E}|$, $\mathbf{E}$ is the electric vector of the light wave, and $\mathbf{p}_g$ is a vector directed along the normal to the Bragg plane whose magnitude in momentum space is equal to the distance from the center of the zone Γ to this plane. Therefore for anisotropic crystals $\tilde{\sigma}$ depends on the orientation of $\mathbf{E}$. In order to describe $\tilde{\sigma}$ of zinc, let us consider the polarizations $\mathbf{E}_\parallel$ and $\mathbf{E}_\perp$ parallel and perpendicular to the C axis. The $\{000,2\}$ band of the interband conductivity should only be observed for $\mathbf{E}_\parallel$; the $\{1\bar{1}0,0\}$ band should only be observed for $\mathbf{E}_\perp$, and the $\{110,1\}$ band for both polarizations with the ratio $\tilde{\sigma}_\perp/\tilde{\sigma}_\parallel = 2.3$.

The investigation of the interband conductivity of single crystals using polarized light facilitates the identification of the observed bands.[1)]

3. We measured the optical constants of zinc in the infrared region by the polarization method with fourfold reflection of the light from the investigated mirrors on a setup described in [10]. The samples were prepared by vacuum evaporation of zinc and deposition on polished glass substrates. In order to obtain good samples a very thin layer of zinc and lead was initially simultaneously deposited from two different evaporators. The lead heater was then turned off and a thick layer of zinc only deposited. The purity of the starting material was 99.99%.

Several series of measurements were carried out. Each series of measurements was performed on newly prepared samples. The final results were obtained by averaging over all series. The error in determining the optical constants amounted to 1–3% for κ and 2–5% for n.

The results of the measurements are presented in Table II and in Figs. 1 and 2. The figures also show the values of the optical constants of zinc calculated in accordance with the graphs of [11, 12].[2)] The optical constants obtained in [11] refer to mechanically polished

Table II. Optical constants of polycrystalline zinc.

λ, μ	n	κ	λ, μ	n	κ
10.0	15.3	47.6	3.19	1.86	16.6
8.0	9.05	40.7	2.68	1.26	13.3
7.0	7.6	36.1	2.14	1.01	10.65
6.0	5.8	31.6	1.55	0.95	7.28
5.0	3.77	26.2	1.23	1.17	4.92
4.0	2.58	21.3			

Note. Here $n - i\kappa$ is the complex refractive index.

single crystals of zinc and light polarized parallel and perpendicular to the C axis. It is seen from the figures that the average values of the optical constants obtained in [11] are close to those obtained in our work, although they are slightly lower. In [12] use was made of films obtained by vacuum deposition. The results of that paper differ considerably both from our results and from those of [11]. In our opinion this is connected with the poor quality of the samples used in [12].

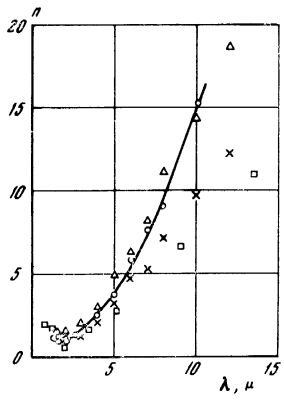

FIG. 1

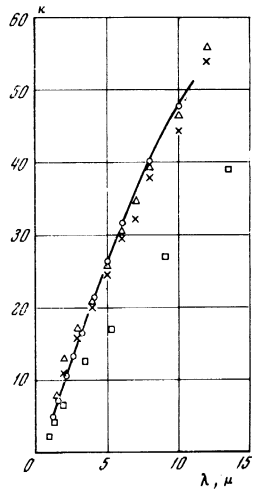

FIG. 2

FIG. 1. The dependence of n of zinc on λ (n is the real part of the complex refractive index): ○ – our work; △ and × for polarization parallel and perpendicular to the C axis from [11]; □ – from [12].

FIG. 2. The dependence of κ of zinc on λ (κ is the imaginary part of the complex refractive index): ○ – our work; △ and × for polarization parallel and perpendicular to the C axis from [11]; □ – from [12].

Experiment has shown that a weakly anomalous skin effect occurs in zinc. The experimental data were therefore processed in accordance with formulas (1)–(4) and (7) of [2]. The results of this processing are presented in Table III. As follows from the table, the corrections β_1 and β_2 connected with the anomalous nature of the skin effect are much smaller than unity; this indicates that the formulas of the weakly anomalous skin effect are applicable. This is also indicated by the value of the ratio $l/\delta \approx 0.3$ where l is the electron mean free path, and δ is the depth of the skin layer.

Furthermore, it is seen from the table that in the 4–10 μ spectral range the values of N, ν, and $\langle v_F \rangle$ do not depend on λ. This means that in this region the effect of the interband transitions can be neglected. The enumerated microcharacteristics were determined as the average values in the indicated spectral range. We present below a summary of the microcharacteristics of zinc.

$$N = (3.38 \pm 0.06) \times 10^{22} \text{ cm}^{-3},$$
$$N/N_{at} = 0.51 \pm 0.01,$$
$$\langle v_F \rangle = (0.92 \pm 0.01) \times 10^8 \text{ cm/sec}$$
$$S_F = 1.8 \cdot 10^{-37} \text{ g}^2\text{-cm}^2/\text{sec}^2,$$
$$\nu = (1.08 \pm 0.06) \times 10^{14} \text{ sec}^{-1},$$

Here N_{at} is the concentration of atoms.

4. Measurements of the optical constants in the visible and near infrared are required in order to determine the Fourier components of the pseudopotential. Such measurements have been carried out in [5, 8, 13, 14]. The most detailed investigations have been carried out in [5, 8] in which use was made of single crystals of zinc and the optical constants were determined for light polarized parallel and perpendicular to the C axis. In [5] the samples were polished mechanically, and in [8] they were electropolished. Since mechanical polishing is

1)For zinc this circumstance was made use of in [5,8].

2)Only small-scale graphs are presented in [11,12]; this makes it extremely difficult to make use of the results of these papers. This refers in particular to [12].

Table III. The results of processing the optical constants of zinc.

λ, μ	$N \cdot 10^{-22}$	$\nu \cdot 10^{-14}$	$\langle v_F \rangle \cdot 10^{-8}$	$\beta_1 \cdot 10^2$	$\beta_2 \cdot 10^2$
10.0	3.49	1.26	0.94	1.7	8.0
8.0	3.37	1.00	0.92	0.9	10.3
7.0	3.40	1.08	0.93	0.8	9.7
6.0	3.44	1.08	0.93	0.6	9.9
5.0	3.27	1.00	0.91	0.4	10.2
4.0	3.31	1.04	0.91	0.2	10.0
3.19	3.14	1.23	0.89	0.2	8.2
2.68	2.82	1.25	0.85	0.1	7.4
2.14	2.84	1.59	0.85	0.1	5.9
1.55	2.59	3.14	0.81	0.1	2.8
1.23	2.11	7.66	0.73	0.1	0.9

Note. β_1 and β_2 are corrections related with the anomalous nature of the skin effect; the formulas for determining these are given in [2].

connected with the production of a cold-hardened layer, we shall in the following give preference to the results of Lettington.[8]

Investigations in the short-wave region showed that there exists a strong band of interband conductivity with a maximum at $\hbar\omega_{max} = 1.54$ eV. This band is observed for both polarizations of the light.[3] The ratio $\tilde{\sigma}_\perp / \tilde{\sigma}_\parallel = 2.5$. According to the theoretical results cited in Sec. 2, this band can be identified with the $\{1\bar{1}0,1\}$ band. The contribution of the conduction elements to σ in this region determined (with the aid of the microcharacteristics obtained in this work) according to formulas (1)–(4) of [7] is negligible (of the order of 4%) and changes neither the position of the maximum nor the width of the band. The relative width of the band determined by the method described in [4] is 0.10. For such a width t = 1.04 (see Fig. 3 in [4]). Using (2), we find that $|V_{\{1\bar{1}0,1\}}| = 0.74$ eV.

Furthermore, it has been shown in [8] that there exists another band, $\tilde{\sigma}$, observed only for light polarized parallel to the C axis. It is considerably weaker than the first band. According to what was stated in Sec. 2, it can be identified with the $\{000,2\}$ band.[4] The contribution of the conduction electrons to σ in the region of this band amounts to about 20%. It does not displace the position of the maximum. For the second band t = 1.05 and according to (2) we find $|V_{\{000,2\}}| = 0.50$ eV.

The third band $\{1\bar{1}0,0\}$ which should only appear for light polarized perpendicular to the C axis was not observed in the indicated publications. This is apparently connected with the fact that it occurs in the region $\lambda > 1.7\,\mu$ for which the appropriate investigations were not carried out.

5. The obtained Fourier components of the pseudopotential allow one to calculate the concentration of conduction electrons N. For zinc the lattice parameters at room temperature are:[9] a = 2.665 Å and c/a = 1.856. This yields $E_F^0 = 9.42$ eV. According to (1), neglecting $V_{\{1\bar{1}0,0\}}$, we obtain $N/N_{at} = 0.79$. The experiment yields $N/N_{at} = 0.51$. It is seen that the fundamental difference between the concentration of conduction electrons and the valence concentration ($N_{val}/N_{at} = 2$) is connected with the Fourier components of the pseudopotential under consideration.

One can estimate $|V_{\{1\bar{1}0,0\}}|$ in accordance with formulas (1) assuming N = 0.51 electron/atom. We find that $|V_{\{1\bar{1}0,0\}}| \approx 0.32$ eV. This means that the maximum should lie in the region $\lambda \sim 1.9\,\mu$. However, at present there are no detailed measurements of the optical constants for light polarized perpendicular to the C axis in the indicated region. The experimental results thus confirm the theoretical conclusions.

The good agreement between the determinations of S_F and $\langle v_F \rangle$ by the optical method and by the anomalous skin-effect method in the microwave region should also be noted. Thus according to Fawcett[15] $S_F/S_F^0 = 0.41$ and $\langle v_F \rangle = 0.87 \times 10^8$ cm/sec. Optical measurements yield $S_F/S_F^0 = 0.50$ and $\langle v_F \rangle = 0.92 \times 10^8$ cm/sec.

[3] The presence of this band was observed in all the indicated papers.

[4] This identification of the bands was carried out in [5]. The positions of the maximum of the first band in [5] and [8] almost coincide. The position of the maximum of the second band in [5] is displaced relative to the position of the maximum of the analogous band in [8]. The ratios of the maxima of σ for the various bands in these papers differ considerably.

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