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Electronic characteristics of chromium layers on the basis of two-band conductivity model

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Two-band conductivity model has been used to interpret the optical properties of chromium layers obtained by thermal evaporation in vacuum onto the substrates of different temperatures. On the basis of this model, the basic kinetic characteristics such as collision frequency of electrons and their concentrations have been calculated. The values of electric conductivity at the temperature of 35 °C measured experimentally appeared to be highly consistent with those calculated theoretically on the basis of the two-band model.

1. Introduction

The optical measurements carried out within a broad spectral range are the source of data referring to the electron structure of the layer examined. In order to explain the behaviour of the layer immerged in an electromagnetic field, the dependence of the electric permittivity $\varepsilon = \varepsilon_1 - i\varepsilon_2$ on the field frequency ω must be examined. Therefore, the near infrared region seems to be convenient enough since the experimental difficulties are not great, while the collisions of the conductivity electrons are still completely perceptable.

The two-band model of conductivity [1] has been applied to the calculation of the electron characteristics of the chromium layers based on optical measurements in the broad (1–25 μm) spectral range. Also the concentrations (N_k, N_l) as well as the relaxation frequencies (γ_k, γ_l) of the basic two groups of conductivity electrons have been calculated for the chromium layers examined. The optical measurements have been completed by the measurements of specific conductivity of those layers at the temperature of 35 °C. The obtained experimental values appeared to be of very high consistence with the values calculated on the basis of the two-band model of conductivity.

2. Experimental part

The chromium layers were produced by thermal evaporation performed in the NA–500 vacuum unit (made by the Vacuum Equipment Works in Bolesławiec,

Poland). The substrate material was spectrally pure JMC–703 chromium. The chromium layers were evaporated from a tungsten boat in the vacuum of order of 1.33×10^{-4} Pa (10^{-6} Pa) onto the polished substrates made of quartz glass. The substrates were heated from the temperature 35 °C to 600 °C during the evaporation process. The substrate temperature T_s was measured by a thermocouple in vacuum. The evaporation rate was of order of 5 Å/s, while the thickness of the layers obtained was of order of 160–200 nm.

For the layers obtained in this way, the reflection coefficient $R(\omega)$ was measured within the 0.2–25 μm wavelength range for normal incidence [2].

Additionally, in the visible (0.4–0.65 μm) spectral range ellipsometric measurements in the air have been carried out for the incidence angles 65° and 70° from which the optical constants (n, k) have been calculated in the visible spectral range. The ellipsometric examinations as well as the Kronig–Kramers relations allowed us to calculate the optical constants for the chromium layers in the whole (0.2–25 μm) spectral range. The structure, the phase composition and the texture were examined using both electron microscopy and X-ray techniques [3].

3. Results of measurements

The spectral dependences of the optical constants (n, k) within the 1–25 μm spectral range for chromium layers evaporated onto a heated substrate of different temperatures T_s (35, 200, 400, 600 °C) have been presented in Fig. 1. A distinct

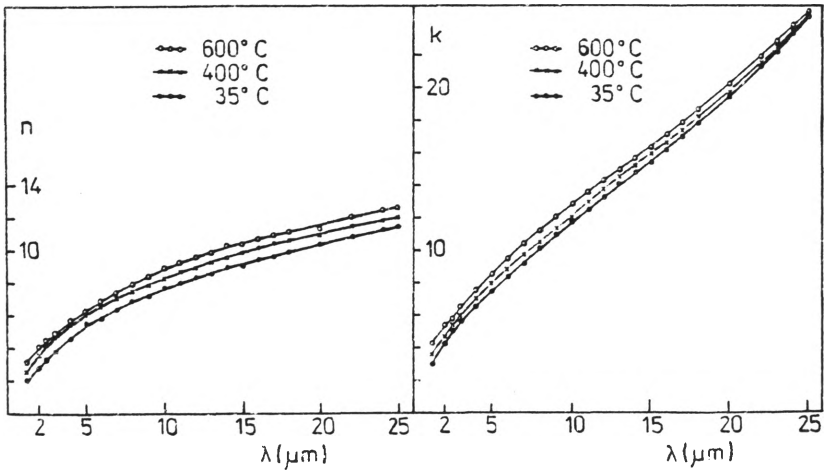

Fig. 1. Spectral dependences of the optical constants (n, k) for the chromium layers evaporated on the substrates of different temperatures T_s

dependence of the optical constants in layers on the substrate temperature T_s has been observed. The values of both the refraction coefficient n and the absorption coefficient k increase with the increase of substrate temperature T_s during the layer condensation.

The structural examinations showed that the layers obtained under these conditions are built of $\alpha-Cr$ chromium of regular spatially centred lattice (b.c.c.). A change of layer texture with the change of the substrate temperature T_s has been stated. For the layers evaporated at low temperatures, the crystallite orientation (texture) {110} is prevailing, while for the layers deposited on the substrates of temperature about 600 °C, the texture {200} occurs. The layers obtained at the substrate temperature of 35 °C have a fine crystalline structure of crystal sizes of order of 20 Å, while the layers obtained at the high substrate temperature (600 °C) are built of crystallites of sizes ranging from 700 to 1700 Å closely adjacent to each other.

When the optical constants of the examined layers are known, spectral dependences of the real (ε_1) and imaginary (ε_2) parts of the electric permittivity may be calculated (Fig. 2). The imaginary part of the electric permittivity increases with the increase of the substrate temperature T_s during condensation. On the other hand, the substrate temperature T_s has no practical influence on the real part of the electric permittivity of the layer. Both ε_1 and ε_2 increase monotonically with the increase

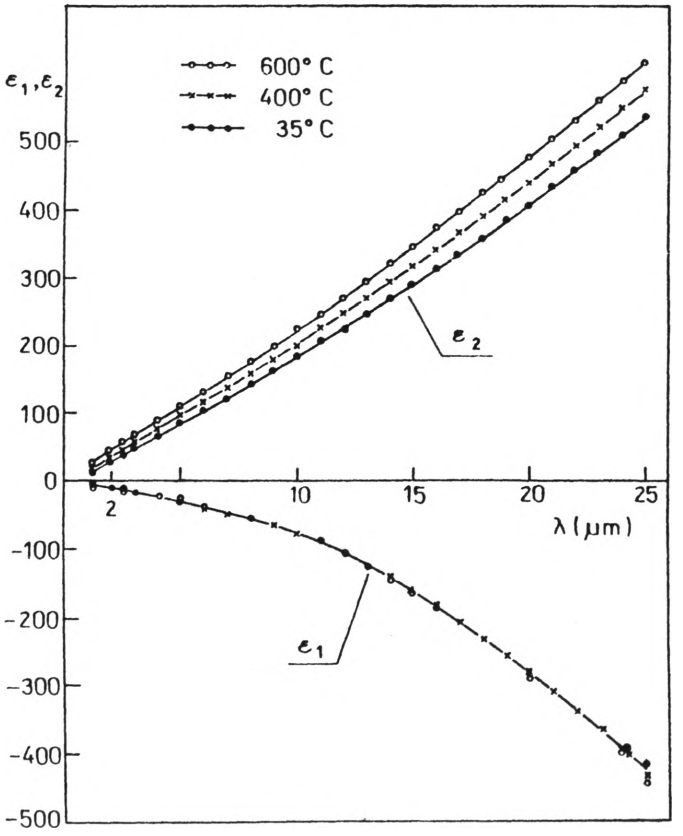

Fig. 2. Spectral dependences of the real ε_1 and imaginary ε_2 parts of the electric permittivity for the chromium layers deposited on the substrates of different temperature T_s

of the wavelength (Fig. 2). The monotonic character of the changes of the electric permittivity, which is dependent on the frequency, indicates that in this region intraband transitions of the conductivity electrons are of a crucial importance.

4. Discussion of the results

The spectral dependences of the real ε_1 and imaginary ε_2 parts of the electric permittivity of the nontransparent layers are described (according to the two-band conductivity model) by the following formulae:

$$\varepsilon_1(\omega) = n^2(\omega) - k^2(\omega) = P - \frac{\Omega_k^2}{\omega^2+\gamma_k^2} - \frac{\Omega_l^2}{\omega^2+\gamma_l^2}, \tag{1}$$

$$\varepsilon_2(\omega) = 2n(\omega)k(\omega) = \frac{\Omega_k^2\,\gamma_k}{(\omega^2+\gamma_k^2)\,\omega} + \frac{\Omega_l^2\,\gamma_l}{(\omega^2+\gamma_l^2)\,\omega} \tag{2}$$

where: $\Omega_{k(l)}^2 = Ne^2/m$ — squared frequency of the plasma vibrations,
$N_{k(l)}$ — concentration of the conductivity electrons,
$\gamma_{k(l)}$ — effective relaxation frequency described by collisions of electron with: lattice ions, dopings and among each other,
P — constant owing to which the values of $\varepsilon_1(\omega)$ and $\varepsilon_2(\omega)$, calculated from the formulae (1) and (2), can be matched to the values measured experimentally for the whole spectral range $(\omega_1 - \omega_2)$.

The index $k(l)$ refers to the considered groups of electrons (k and l).

The best fitting of the values of $\varepsilon_1(\omega)$ and $\varepsilon_2(\omega)$ calculated on the basis of Eqs. (1) and (2) to the measured values ε_1 and ε_2 for the examined chromium layers within the whole wavelength range (1 – 25 μm) was achieved for the values of P gathered in Table 1. In the same table, there are also collected the critical values of P_0 from which the calculations of ε_1 and ε_2 according to formulae (1) and (2) may be started.

Table 1. Temperature dependence of P parameter

T_s	35 °C	200 °C	400 °C	600 °C
P_0	−3.43	−4.71	−5.65	−6.27
P	7.45	6.20	4.99	−1.10

Basing on the known value of P it is possible to calculate the kinetic characteristics of the conductivity electrons for the examined chromium layers produced by thermal evaporating onto substrates of different temperatures T_s. The obtained values have been collected in Table 2.

Formula (2) allows us to determine the limiting value ($\omega \to 0$) of the electric permittivity of the examined layers

$$\sigma_0 = \varepsilon_2 \omega \varepsilon_0 = \varepsilon_0 \left(\frac{\Omega_k^2}{\gamma_k} + \frac{\Omega_l^2}{\gamma_l} \right). \tag{3}$$

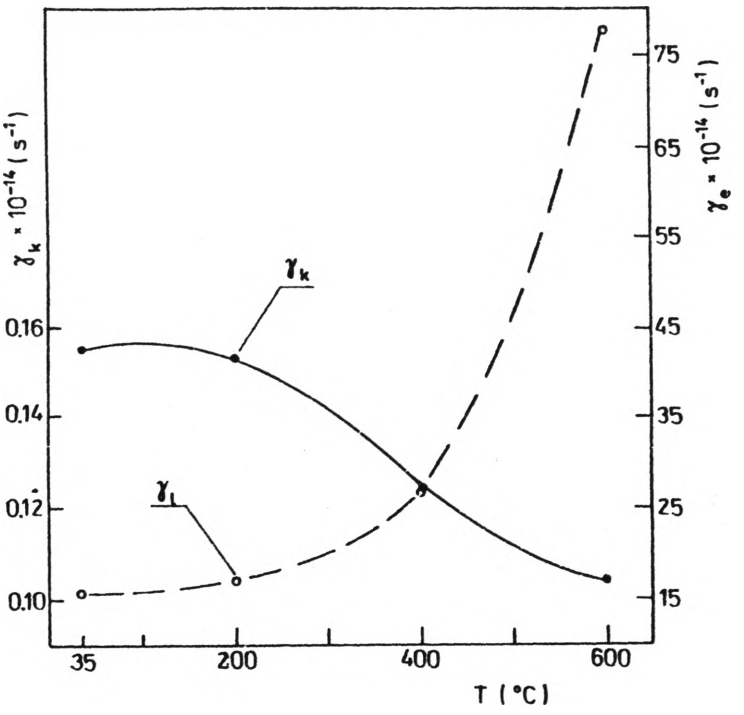

Fig. 3. Dependence of the relaxation frequency $\gamma_{k(l)}$ for k- and l-groups of the conductivity electrons in chromium layers on the substrate temperature T_s (o o o – γ_l, • • • – γ_k)

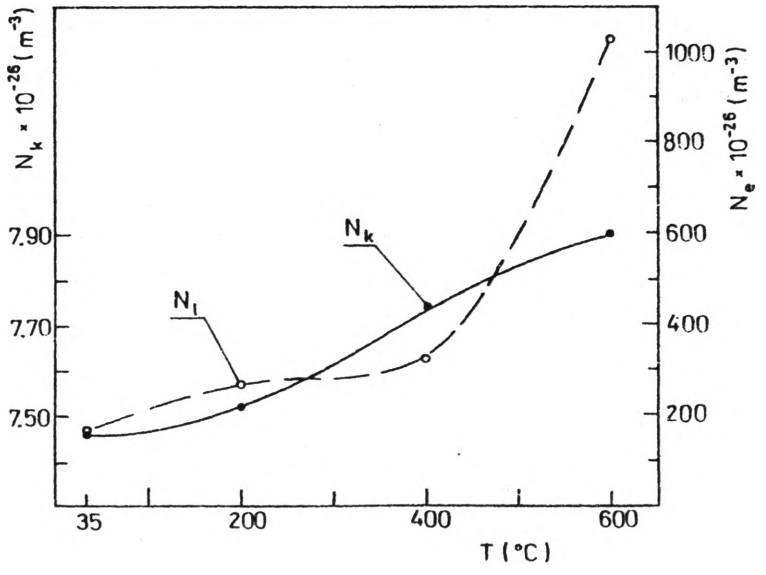

Fig. 4. Dependence of concentration $N_{k(l)}$ for k- and l-groups of the conductivity electrons in chromium layers on the substrate temperature T_s (• • • – N_k, o o o – N_l)

The values $\rho_0 = \sigma_0^{-1}$ calculated according to formula (3) for the examined chromium layers are collected in Table 3 together with the values of the specific resistance $\rho_{0(exp)}$ of the examined layers measured experimentally.

The analysis of the contribution of both groups of conductivity electrons (k and l) to the electric permittivity of the examined layers indicates that both these groups k and l contribute to the real part ε_1 of electric permittivity. However, the contribution of the electrons of l-group to ε_1 is practically constant in the whole spectral range (1 – 25 μm) and only slightly depends on the temperature T_s of layer condensation (though a slight decrease with the increase of T_s is observed), Fig. 3. On the other hand, the contribution of the k-group electrons to ε_1 increases rapidly with the increase of wavelengths, practically by two orders of magnitude, but similarly to that of k-group electrons is practically independent of the condensation temperature T_s (Fig. 3). Therefore, no dependence of ε_1 on the substrate temperature T_s is observed in the chromium layers in the temperature range from 35 °C to 600 °C. The imaginary part of the electric permittivity ε_2 in the whole spectral range (1 – 25 μm) is conditioned by the l-group electrons which affect both its value and its dependence on the substrate temperature T_s (Fig. 4).

Table 2. Kinetic characteristics of the electron conductivity

T_s	$\gamma_k \times 10^{14} s^{-1}$	$\gamma_l \times 10^{14} s^{-1}$	$\Omega_k^2 \times 10^{30} s^{-2}$	$\Omega_l^2 \times 10^{30} s^{-2}$	$N_k \times 10^{26} m^{-3}$	$N_l \times 10^{26} m^{-3}$
35 °C	0.155	15.84	2.37	54.54	7.46	171.6
200 °C	0.154	16.93	2.39	86.18	7.52	271.1
400 °C	0.124	26.75	2.46	102.15	7.74	321.3
600 °C	0.104	78.01	2.51	327.75	7.90	1031.1

Table 3. Theoretical and experimental temperature dependences of the specific resistivity ρ_0

	Temperature T_s			
ρ_0 (μΩ cm)	35 °C	200 °C	400 °C	600 °C
$\rho_{0(theor)}$	60.20	54.79	47.75	39.72
$\rho_{0(exp)}$	59.5	54.8	47.8	39.7

As far as the specific conductivity σ_0 of the chromium layers is concerned, its value is practically determined by the k-group of electrons since the contribution of l-electrons is small (Fig. 5). As it follows from Tab. 3, the values of $\rho_{0(theor)}$ and $\rho_{0(exp)}$ are highly consistent.

5. Conclusions

On the basis of the results obtained, the following conclusions may be formulated:

1. The optical properties of the chromium layers may be explained on the basis of

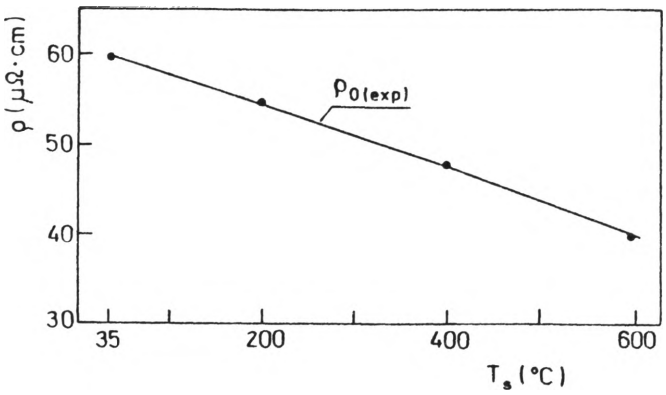

Fig. 5. Dependence of the specific resistance ρ_0 in chromium layers on the substrate temperature T_s • – experimental points, —— – theoretical values)

the two-band model of conductivity, taking into account two groups of conductivity electrons of different relaxation frequency (γ_k, γ_l) and concentration (N_k, N_l), see Figs. 3, 4 and Tab. 2).

2. The substrate temperature T_s in the condensation of chromium layers has no essential influence on kinetic characteristics of electrons in the temperature range from 35 °C to 400 °C. Both γ_k, γ_l and N_k, N_l remain practically the same. In contrast to this, the substrate temperature ($T_s \approx 600$ °C) causes essential changes in both concentration and collision frequency of the two groups of conductivity electrons.

3. The collision frequency of one group (γ_l) increases very distinctly with the increase of the substrate temperature T_s, while that of the other group (γ_k) diminishes only slightly with the increase of the substrate temperature T_s.

4. The concentration of the conductivity electrons for both groups of electrons increases with the increase of the substrate temperature T_s. The changes are very distinct for the *l*-group conductivity electrons.

References

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