OPTICAL PROPERTIES OF YTTERBIUM TRIANTIMONIDE THIN FILMS

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Rare-earth anthimonides represent interesting objects for researches owing to their exclusive properties. For the first time, we have studied the reflection and absorption spectra of α-Yb_5Sb_3 (the Mn_5Si_3-type hexagonal lattice with parameters a = 8.97 Å and c = 6.90 Å) thin films prepared by vacuum-thermal deposition. Based on the analysis of the obtained results, the energy band structures near the extrema of the valency and conduction bands are suggested.

The analysis of experimental data testifies that the trivial (from the position of simple semimetals, as well as from the view of narrow-band semiconductors) approach to the interpretation of electrophysical properties of rare earth (RE) pnictides is inapplicable. The variable polarity of the Hall constant, temperature dependence of the differential thermoelectromotive force, values of these parameters [1–3], intermediate valency of RE ions [1, 4], phenomenon of intermediate valency observed under different external impacts [5–7], and complex band structure conditioned by the $f - d$ and $p - f$ hybridizations [5, 8] observed in a sufficiently large number of compounds of this group require the involvement of numerous mechanisms and processes into the explanation of the physical characteristics of these materials.

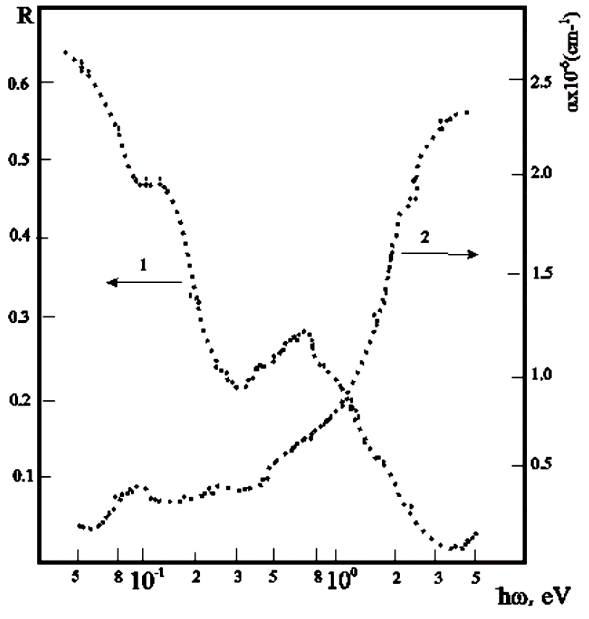

Fig. 1. Typical reflection (*1*) and absorption (*2*) spectra of α-Yb_5Sb_3 thin films

In respect to the above-mentioned, the present work deals with the optical properties of ytterbium triantimonide – α-Yb_5Sb_3 (the Mn_5Si_3-type hexagonal lattice, parameters a=8.97 Å, c=6.90 Å) thin films prepared by a technology described in [9]. The typical reflection spectra presented in Fig. 1 show some peculiarities of the rare earth pnictides, in particular, two clear minima in the visible part of the spectrum with a well-shaped reflection band between them. The reflection coefficient in the long-wave part of the spectrum ($h\omega$<0.2 eV) increases rapidly, and its highest value (∼70%) suggests metal-like properties of the alloys. The reflection minimum E_0=0.35 eV separates the plasma area from that part of the spectrum, where optical peculiarities are conditioned by inter-band electronic transitions. The presence of the second antiresonance structure with the energy $E_0^I = 3.5 \div 4.5$ eV points to a possibility of the carrier distribution throughout the several bands. A sizable variation of the energy of the maxima in different films is to be pointed out. This is due to the variation of the number of electrons participating in E_0 frequency oscillations and is typical of the RE compounds in the course of the RE ion valency change [1].

In all of considered films, the reflection band (whose center of gravity is at $E \approx 0.7$ eV) and the minima of the relevant energies E_0^I represent a thin structure (consists of a number of weak maxima) which points to the complex composition of initial and final electron states. In spite of the fact that α-Yb_5Sb_3 thin films are characterized by strong absorption practically in all investigated area of spectrum, the use of thin films with thickness 0.2 μm applied on sapphire and silicon substrates has allowed us to measure the spectra of reflection and transparency in all the range and, on this

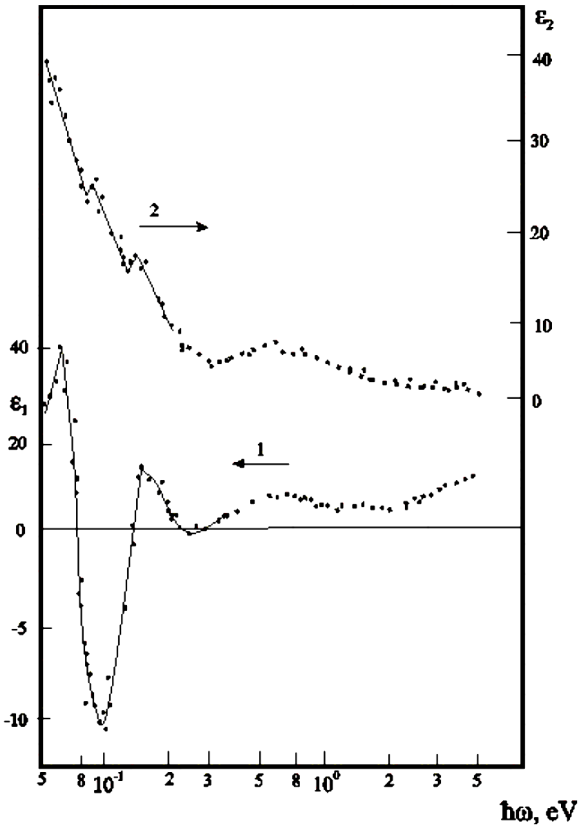

Fig. 2. Spectra of the imaginary (*1*) and real (*2*) parts of the dielectric permittivity in α-Yb_5Sb_3 thin films

basis, to calculate the spectrum of absorption. The absorption spectrum of ytterbium triantimonide (Fig. 1) can conventionally be split into two parts. The first includes the spectral interval from 0.05 to 0.5 eV. In this area, against the background of a weak alternation of the absorption factor, two maxima at E_1=0.1 eV and E_I^I=0.28 eV are observed. For the second part of the spectrum ($h\omega$>0.5 eV), the monotonous growth of the absorption factor is typical. However, the presence of two different tilting angles in the $\alpha(h\omega)$ dependence (for the energies of 0.5–1.0 eV and $h\omega$>1.0 eV) is also detected. This points to the contribution of several inter-band electronic transitions in the formation of the absorption edge. On the basis of the measured reflection and transparency spectra, the spectral dependences of the major optical parameters have been calculated. The minimum of the imaginary part of the dielectric permittivity at about 0.3 eV (Fig. 2) corresponds to a comparatively wide area of electron transitions between the valence and conduction bands from the part of the spectrum, where optical properties are greatly influenced by transitions from the strongly localized f-band. For

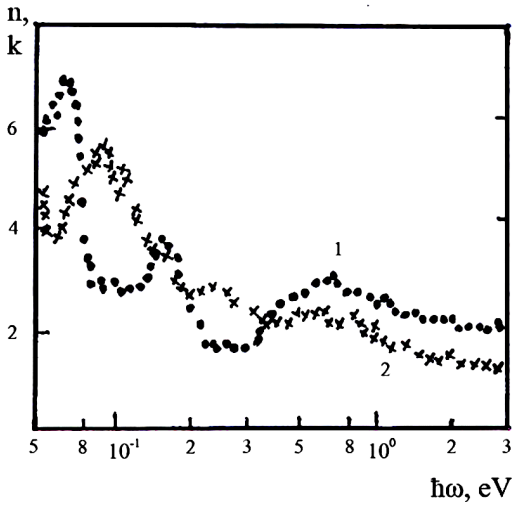

Fig. 3. Spectral dependences of the refraction (n, 1) and absorption (k, 2) indices of α-Yb_5Sb_3 thin films

energies $h\omega$<0.3 eV, the mentioned mechanism must call forth the presence of maxima with a small half-width within the ε_2 and ε_1 spectra, as well as in the spectra of the absorption (k) and refraction (n) indices for energy $h\omega$<0.3 eV (Fig. 3).

As follows from the spectral peculiarities of the real part of the dielectric permittivity (Fig. 2), free carriers are distributed between several bands. Changing the polarity of the $\varepsilon(h\omega)$ curve (with negative angle) at 0.07 and 0.25 eV energies can be attributed to inter-band and sub-band electron transitions. Moreover, the crossing of the zero value with positive angle at energies of 0.125 and 0.3 eV points to oscillatory processes corresponding to the characteristic frequencies, which is confirmed by the location of maxima of the loss function at 0.3 and 0.32 eV. As for the rapid growth of $\mathrm{Im}\varepsilon^{-1}$ (Fig. 4) in the ultraviolet area, the latter is due to plasma oscillations of valence electrons. However, the intensity of inter-band electronic transitions in this area does not enable a reliable evaluation of the plasma frequency.

Based on the obtained experimental data and the consideration of peculiarities of the band structure of the RE pnictides [8], certain assumptions can be made regarding the energy band structure of Yb_5Sb_3 near the extremum of the valence and conduction bands (Fig. 5).

Similar to thulium and samarium mono-antimonides [11, 12], the valence band in ytterbium triantimonides is to consists of several sub-bands. Between the pf and fp hybridized states, produced by the wide valence bands, the narrow f zone (with the width of about several eV),

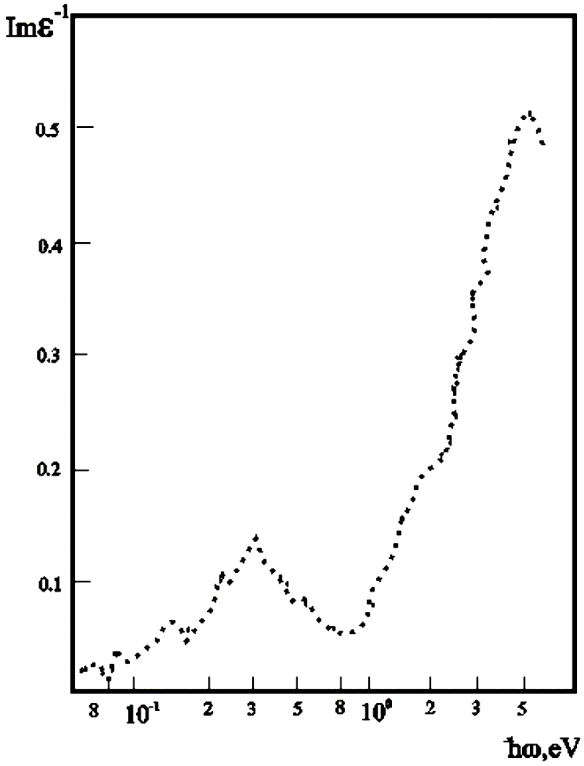

Fig. 4. Loss function spectrum in α-Yb_5Sb_3 thin films

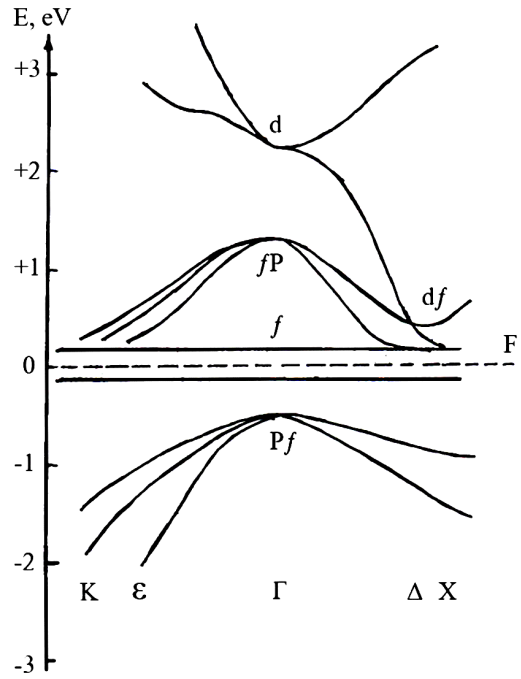

Fig. 5. Scheme of the energetic zones of α-Yb_5Sb_3 thin films

within which the Fermi level is located, must exist. We note that extrema of the pf and fp zones are located at the Γ point. The f band is characterized by a negligible dispersion. The absolute extremum of the conduction band is located at the X point for the majority of similar RE compounds. In the area of deep infrared radiation, high values of the reflection and absorption coefficients, as well as metal-like properties of the material, testify to the hybridization of the conduction band and its overlapping at the X point, with the f-state. At the same time, a positive value of the real part of the dielectric permittivity in the long-wave section of the spectrum enables us to assume the existence of a several-meV gap. Depending on conditions (temperature, deflection from the stoichiometry in specific samples), both the electron and hole priority shares can be observed.

Since the free carriers are distributed over several energy bands, two or more plasma oscillation frequencies may be observed (crossing the zero value of ε_1). The transition of electrons from the f band into the complex conduction band separated from the former by a narrow gap at the X point induces the E^I and E_I^I structures in the optical spectra. At $h\omega$>0.35 eV, the inter-band transitions of electrons from the pf valence band are observed. At the same time, in the range from 0.5 to 1 eV, the indirect Γ-X transitions take place, whereas the direct inter-band $X - X$ transitions are observed at higher energies (the second slope in the spectrum of the absorption coefficient).

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ОПТИЧНІ ВЛАСТИВОСТІ ТОНКИХ ПЛІВОК ТРИАНТИМОНІДУ ІТЕРБІЮ

З.У. Джабуа, А.В. Гігінеішвілі, М.Ю. Стамателі

Р е з ю м е

Антимоніди рідкісноземельних елементів становлять значний науковий інтерес завдяки своїм унікальним властивостям. Вперше досліджено спектри відбиття і поглинання плівок α-Yb_5Sb_3 (гексагональна ґратка типу Mn_5Si_3 з параметрами $a = 8,97$ Å, $c = 6,90$ Å), отриманих методом вакуумно-термічного випаровування. На основі аналізу отриманих результатів запропоновано зонну діаграму для околів екстремумів валентної зони і зони провідності.