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OPTICAL PROPERTIES OF SCANDIUM THIN FILMS

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The optical properties of transition metals have received considerable attention in the last decade[1]. In the case of scandium, only the optical measurement by Weaver and Olson[1,2] between 0.2 and 5 eV are available. In this communication we present a new investigation on the optical properties of Sc. We measured the reflectivity of polycrystalline thin films grown in ultrahigh vacuum from 0.22 to 5.5 eV before air exposure and from 0.22 to 35 eV after air exposure. We noticed remarkable effects of surface contamination on the reflectivity and, consequently, on the dielectric function for the samples exposed to air.

Sc films, 150 nm thick, were prepared at the Department de Physique du Solide, Université de Provence, Marseille, by electron gun evaporation of pure scandium onto optically flat substrates. During deposition, the pressure was in the low 10^{-7} Pa range and the substrate temperature was kept at 350 C. The films were polycrystalline and the crystallites had h.c.p. structure and were preferentially oriented with the $\hat{c}$ axis perpendicular to the substrate surface.

Normal incidence reflectivity measurements were performed between 0.22 eV and 5.5 eV without removing the samples from the ultrahigh vacuum evaporation chamber (vacuum-measured reflectivity) using the reflectivity set-up available at the Department de Physique du Solide[3]. The samples were then moved to the reflectivity set-up available on the vacuum ultraviolet beam line of PULS for the measurements above 5 eV[4]. We extended the reflectivity measurements performed at PULS on the air exposed samples to the low energy range 0.22-5.5 eV in order to check the differences with respect to the vacuum-measured spectrum. The reflectivity spectra are shown in Fig. 1.

The reflectivity of the sample exposed to air is lower than the vacuum measured reflectivity in the common spectral region. In the vacuum ultraviolet several structures are present, namely one shoulder around 5.6 eV, two peaks at 7.6 eV and 10.3 eV and a broad band with the maximum at 21 eV. Both reflectivity spectra are in good agreement with the reflectivity reported by Weaver and Olson(1) (shown in Fig. 1 for comparison) for E⊥$\hat{c}$ for a single crystal at 4.2 K except that the latter shows weak structures in corrispondence of our plateau between 0.6 and 2.5 eV.

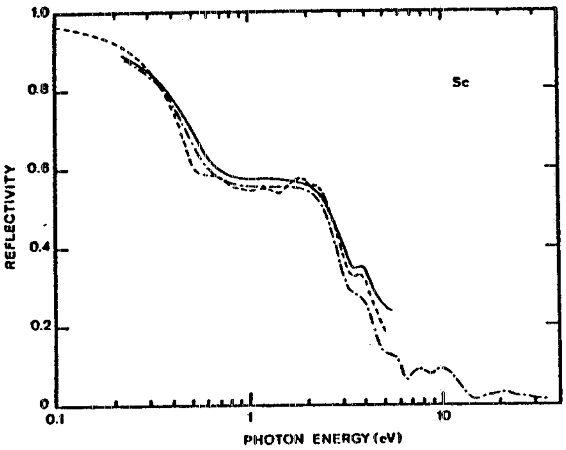

Fig. 1 - Reflectivity of different Sc samples:

————	vacuum-measured one;
—·—·—·—	air exposed film;
— — — —	single crystal(1).

The effects due to air contamination become evident in the Im(-1/ε) function, Fig. 2, that we calculated from the reflectivity with the Kramers Krönig relations. The sharp peak at 13 eV is present also in the experimental Im(-1/ε) obtained from electron energy loss experiments in both pure Sc metal and Sc_2O_3 and attributed to a collective excitation of the conduction electrons (ref.5,6). Instead, the broad band peaking at 23.5 eV is present only in the Sc_2O_3 spectrum(5,6), indicating the presence of a thick oxyde layer on the surface of our air-contamined samples.Thus we assign the 21 eV reflectivity peak to electronic transitions in the surface oxyde layer, possibly between the oxygen 2p states and empty conduction bands. Below 6 eVthe oxyde layer is transparent and the reflectivity structures can be assigned to Sc metal interband transitions. The assignment of the two peaks at 7.6 and 10.3 eV to either Sc metal or to the surface oxyde layer is not yet possible.

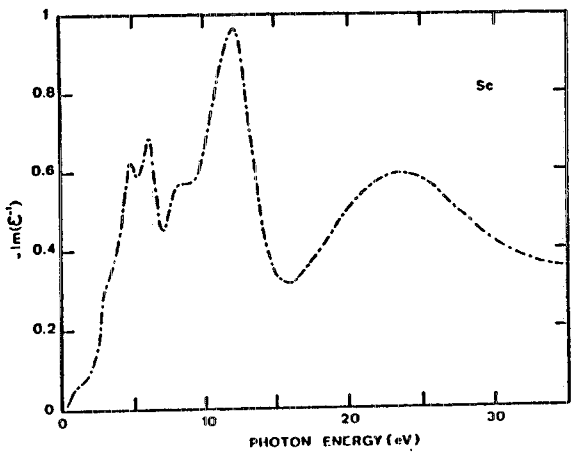

Fig. 2 - Im(-1/ε) function of Sc derived from the reflectivity of the air exposed film.

In order to interpret the optical properties of Sc below 6 eV, we have calculated the interband part $\varepsilon_{2b}^{\parallel,\perp}$ of the imaginary part of the dielectric tensor from the nonrelativistic Sc energy,bands calculated by

Das[7]. In Table I we compare the energies of the structures in the theoretical $\varepsilon_{2b}^{\parallel,\perp}$ with those obtained from the experimental curves[2] (the symbols $\parallel$ and $\perp$ refer to the polarization of the incident radiation parallel and perpendicular to the crystal $\hat{c}$ axis).

TABLE I - Energies (eV) of the features observed in the calculated and experimental[2] $\varepsilon_2^{\parallel}$ and $\varepsilon_2^{\perp}$ spectra.

$\varepsilon_{2b}^{\parallel}$ calculated		0.7	1.47	2.0	3.6	5.1
$\varepsilon_2^{\parallel}$ experimental		1.0	1.8	2.2	3.4	
$\varepsilon_{2b}^{\perp}$ calculated	0.27	0.68	0.93	1.31	1.9	4.1
$\varepsilon_2^{\perp}$ experimental		0.65	1.1	1.4	2.1	3.5

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