A far UV spectroscopy study of $SrMgF_4$ single crystals

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In this work we have studied experimentally the properties of the electronic structure of $SrMgF_4$ single crystals based on optical and luminescence spectroscopy. Two spectroscopic methods were used: a low-temperature (7-293K) luminescence spectroscopy upon selective photo excitation by synchrotron radiation at SUPERLUMI station. Figures 1-3 show the main essentially results.

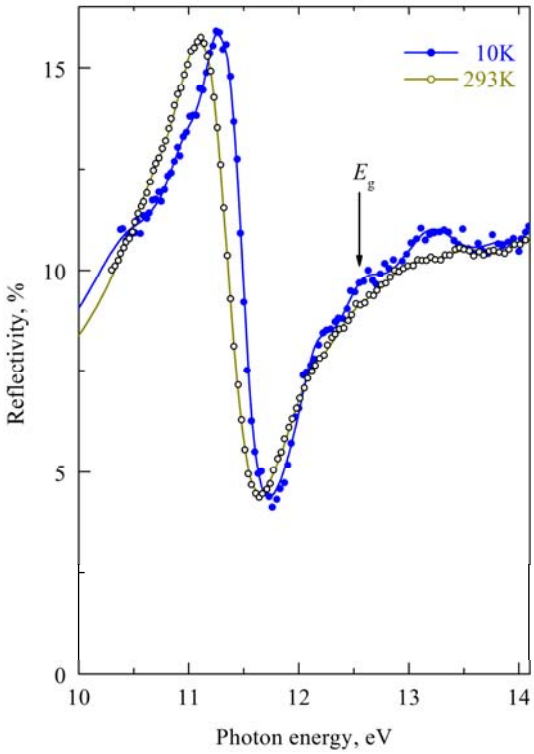

Figure 1: Fragment of the reflection spectra of $SrMgF_4$ crystal at T= 10 and 293 K. The points correspond to the experimental data, the solid lines are the result of the approximation. The vertical arrow indicates the band gap E_g at 10 K.

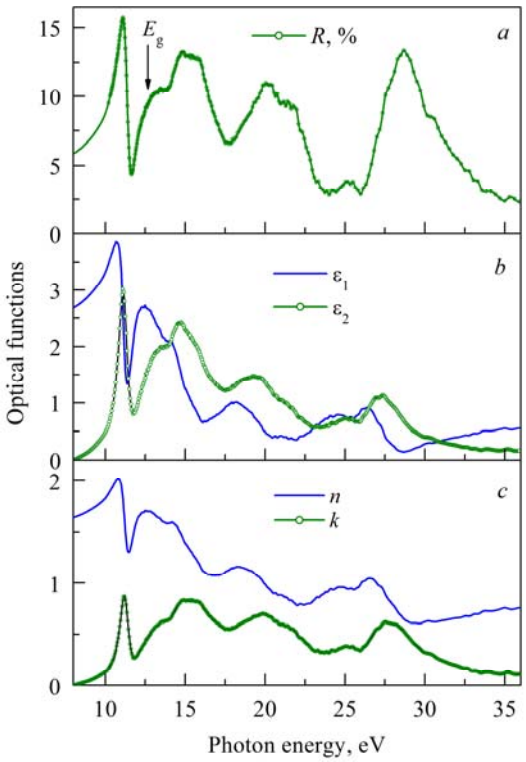

Figure 2: Spectra of $SrMgF_4$ crystal: (*a*) reflection spectrum recorded at T= 293 K, (*b*, *c*) spectra of the optical functions calculated by Kramers-Krönig transform.

Various electronic structure properties of undoped single crystals of $SrMgF_4$ have been determined for the first time. This result is based on the experimental data on the low-temperature (10-293 K) time-resolved vacuum ultraviolet synchrotron spectroscopy, far ultraviolet (3.7-36 eV) reflectance spectra and calculations for optical functions spectra. The band gap of investigated compound was found at E_g= 12.55 eV, the energy threshold for creation of the unrelaxed excitons at $E_{n=1}$= 11.38 eV, and the low-energy fundamental absorption edge at 10.3 eV. Two groups of photoluminescence (PL) bands have been identified: the exciton-type emissions at 2.6-3.3 and 3.3-4.2 eV and defect-related emissions at 1.8-2.6 and 4.2-5.5 eV. It was shown that PL excitation (PLE) for the exciton-type emission bands occurs mainly at the low-energy tail of the fundamental absorption of the crystal with a maximum at 10.7 eV. At excitation energies above E_g, the energy transfer from the host lattice to the PL emission centers is inefficient. The paper discusses the origin of the excitonic-type PLE spectra taking into account the results of modeling the PLE spectra shape in the framework of a simple diffusion theory and surface energy losses.

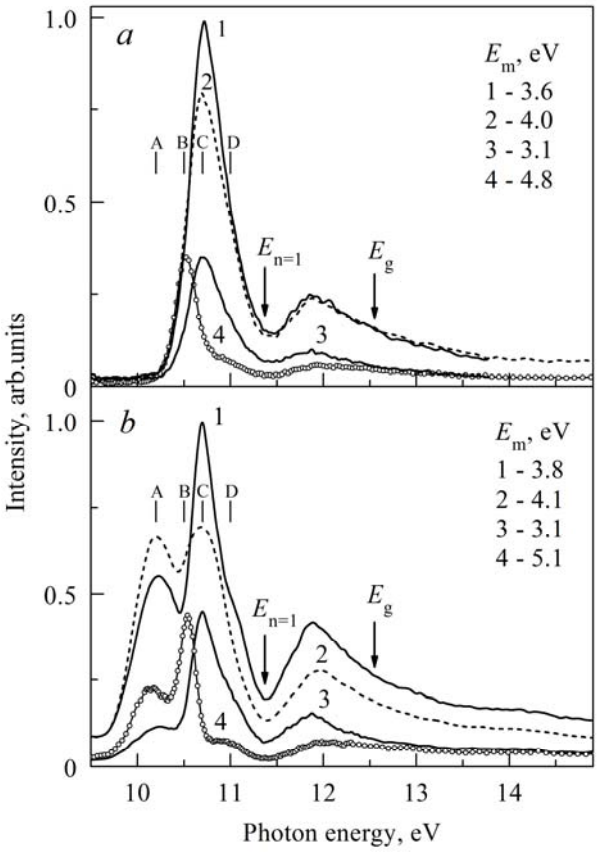

Figure 3: PL excitation spectra of $SrMgF_4$ crystal at T= 10 (1) and 293 K (2, 3) monitoring emission at E_m= 2.2 (1), 2.1 (2), and 2.5 eV (3). Symbols *B*-*D* denote certain PLE bands, the vertical arrows indicate the minimum energy for interband transitions E_g and the position of the first excitonic peak $E_{n=1}$.

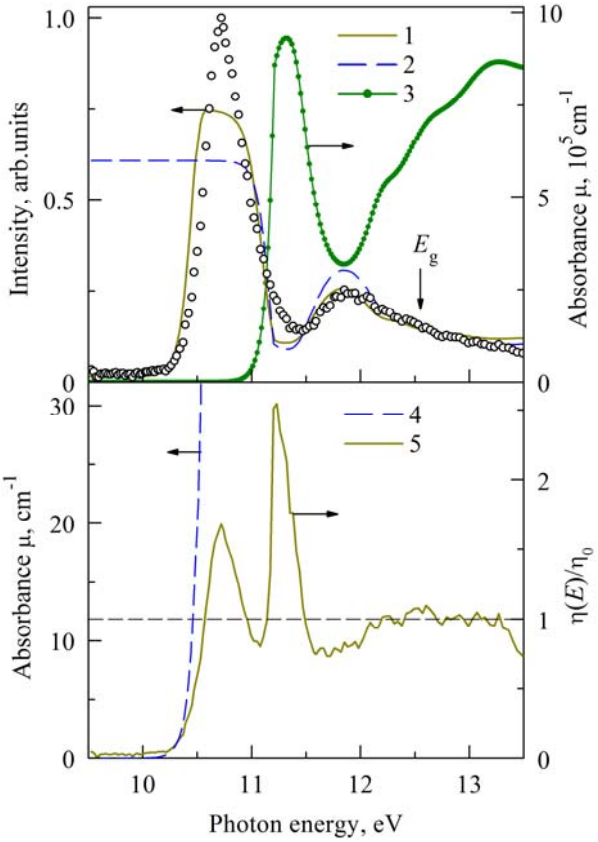

Figure 4: PLE spectra of $SrMgF_4$ crystal at T= 10 K monitoring emission at E_m= 3.64 eV (open circles) and calculated for parameters L= 70 nm and d= 1 mm (1). For comparison, there are shape function $y_0(E)$ (Δ= 20 nm) (2), the calculated optical absorption spectrum μ(E) (3), its zoom for the fundamental absorption edge from 0 to 30 cm^{-1} (4), and the relative quantum yield η(E)/ η$_0$ (5).

The paper presents the results of a study of undoped single crystals $SrMgF_4$, carried out using low-temperature (10-293 K) luminescence-optical VUV spectroscopy with a time resolution upon excitation in the energy range 3.7-36 eV. This optical material shows intense luminescence in wide (from red to ultraviolet) spectral region, which is efficiently excited in the energy range of the low-energy tail of the fundamental absorption. On the basis of the reflection spectra and results of calculation of the optical functions, we have determined for the first time the parameters of the electronic structure of SMF crystals: the value of the minimum energy for interband transitions E_g = 12.55 eV, the position of the energy threshold ($E_{n=1}$) for creation of unrelaxed excitons at 11.38 eV, the position of a dominant peak in PLE spectra of 'excitonic' luminescence at 10.7 eV and the energy position of the fundamental absorption edge at 10.3 eV.

Two groups of PL emission bands: the exciton-type emissions at 2.6-3.3 and 3.3-4.2 eV and defect-related emissions at at 1.8-2.6 and 4.2-5.5 eV, have been identified. It was is shown that PL excitation for the exciton-type emission bands occurs mainly at the low-energy tail of the fundamental absorption of the crystal with a maximum at 10.7 eV, while at energies above E_g the energy transfers from the host lattice to the PL emission centers are inefficient.

Acknowledgments

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