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Optical properties of non-stechiometric Cu_6PS_5I-based thin films deposited by magnetron sputtering

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Cu_6PS_5I superionic conductors belong to the argyrodite family, and are characterized by high ionic conductivity and due to this they are prospective materials for creating renewable energy sources, electrochemical and optical sensors. Cu_6PS_5I-based thin films are deposited onto silicate glass substrates by non-reactive radio frequency magnetron sputtering. Energy-dispersive X-ray spectroscopy was used to ensure the thin films chemical composition.

With Cu content increase, a red shift of the optical transmission spectra is observed. Temperature variations of optical transmission in Cu_6PS_5I-based thin films are similar for all investigated samples, but we illustrate it for $Cu_{5.46}P_{1.68}S_{5.06}I_{0.80}$ thin film. Thus, interferential transmission spectra of $Cu_{5.46}P_{1.68}S_{5.06}I_{0.80}$ thin film were studied at various temperatures within 77–300 K. With temperature increase, a red shift of both the short-wavelength part of the transmission spectrum and the interferential maxima is observed. Besides, a typical decrease of transmission in the interferential maxima with temperature is revealed.

The spectral dependences of the absorption coefficient are derived from the spectrometric studies of interference transmission spectra. A typical Urbach bundle is observed, the temperature behaviour of the Urbach absorption edge in $Cu_{5.46}P_{1.68}S_{5.06}I_{0.80}$ thin film is explained by strong electron-phonon interaction. Temperature dependences of the absorption edge energy position and the Urbach energy for $Cu_{5.46}P_{1.68}S_{5.06}I_{0.80}$ thin film are well described in Einstein model. The influence of different type of disordering on the Urbach tail for $Cu_{5.46}P_{1.68}S_{5.06}I_{0.80}$ thin film is studied.

The dispersion dependences of the refractive index for the $Cu_{5.46}P_{1.68}S_{5.06}I_{0.80}$ thin film was obtained from the interference transmission spectra. With temperature increase the linear increase of refractive index in $Cu_{5.46}P_{1.68}S_{5.06}I_{0.80}$ thin film is revealed.