Optical properties of copper iodide

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Copper iodide is an optically isotropic wide band gap semiconductor with a band gap and exciton binding energy of about 3.1 eV and 62 meV, respectively [1, 2]. Although the first optical characterization of copper halides started in the 60s of the last century, e.g., by Cardona [3] and Suga [4], these materials came into the focus of research especially in the last years, due to their transparency in the visible spectral range and intrinsic p-type conductivity [1].

Here we report on the emission properties and the dielectric function of CuI. Using femtosecond pump-probe spectroscopic ellipsometry, the time-resolved dielectric function of PLD-grown CuI thin films was measured. We show the change of the dielectric function as a result of laser-pulse induced excess carrier dynamics. Beside screening effects of the excitonic contribution, we observe a small increase in the absorption below the band gap after a delay time between the pump and probe pulse of about 400 fs. Responsible for this enhancement might be valence- to valence-band transitions resulting from the laser-induced increased carrier density in the order of 10^{19} cm^{-3}.

In order to investigate the bulk properties, we excited CuI crystals with photon energies below the band gap energy. The obtained photoluminescence (PL) spectra exhibit a redshift compared to the conventional PL emission. This can be attributed to self-absorption and is in agreement with simulation which takes into account the internal emission spectrum at a given focal point, the propagation of the emitted photons inside the crystal and the absorption coefficient of CuI. For an excitation energy of about 2.74 eV, we determine a change of the expected power law for two-photon PL of the entire intensity given by $I \propto P^2$ [5] and the exponent decreases down to 1.5, which might be attributed to the presence of real states within the band gap. A comparison with DFT calculations indicates that a substitution of copper by iodine in Cu-rich crystals can lead to such real states within the band gap [6].

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