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Raman study of the as-prepared and flash-lamp annealed thin films of Cu_2ZnSnS_4 nanocrystals mixed with PEDOT:PSS

New materials for future of renewable energy, especially photovoltaics, should be cheap, environmentally friendly and have a direct bandgap, which ensures sufficient absorption in the entire solar spectrum. However, absorption of light is usually also accompanied by additional heating of the device. This heat can be either wasted or transformed into extra electrical energy. That is why materials that allow photovoltaics to be combined with thermoelectrics are gaining popularity. One of the materials that are attracting the attention of researchers in this respect is Cu_2ZnSnS_4 (CZTS). It has nontoxic and relatively cheap constituents as well as promising photovoltaic and thermoelectrical properties. CZTS can be produced by a variety of techniques, including low-temperature colloidal synthesis in aqueous solutions. This “green” chemistry approach makes it an even more attractive candidate for future applications in novel renewable energy devices. However, due to the complex structure of CZTS, there are several structural modifications, and a high probability of the formation of antisite Cu_{Zn} and Zn_{Cu} defects as well as secondary phases in the form of binary and ternary compounds from constituent elements. By varying the nanocrystal (NC) synthesis parameters and the conditions of NC film deposition, the formation of secondary phases and antisite defects can be suppressed. Another widely used material in both photovoltaic and thermoelectrical applications is the p-type conductive polymer PEDOT:PSS. In some works CZTS NCs and PEDOT:PSS were used as parts of the same device structure but as separate layers with different functional roles in the device. On the other hand, incorporation of CZTS NCs into a PEDOT:PSS matrix can be a promising approach, since as shown in the literature [1–3] for other nanoparticles adding them to PEDOT:PSS may improve its thermoelectric properties. Another perspective of the CZTS NC-PEDOT:PSS composite is the combination of the excellent properties of CZTS as an absorber of solar radiation and the high electrical conductivity of PEDOT:PSS. This approach could solve the problem of poor electrical transport between NCs, which is the main obstacle on the way towards potential applications of any kind of NC thin film. Not only the NC synthesis and the thin film preparation conditions but also post-synthesis processing of the NC films is important to improve the functional properties of the NC films. In terms of scalability and processing time, flash lamp annealing (FLA) technique (also known as intense pulse light (IPL) annealing) is an interesting alternative to furnace annealing. This technique is known for over 50 years, but began to gain popularity just for the last few years with the technology transition towards thin-film roll-to-roll manufacturing. Raman spectroscopy is a very powerful tool for CZTS NCs characterization. It allows not only the presence of possible secondary phases to be determined, but also structural modification of CZTS NCs to be identified. Here we present results of a Raman spectroscopy study of CZTS/PEDOT:PSS composite films, prepared from aqueous colloidal solution of CZTS NCs mixed in different proportions with PEDOT:PSS solution and deposited onto glass substrates. The parameters of the film deposition were optimized to avoid aggregation of the NCs and formation of secondary phases in them. Subsequently, the composite films were subjected to FLA treatment. To the best of the authors’ knowledge, this is the first study of FLA treatment of PEDOT:PSS and CZTS NCs in PEDOT:PSS matrix. It was revealed, that even small concentrations of PEDOT:PSS in mixed composites lead to the formation of optically more homogeneous films. Moreover, the FLA treatment increases the stability and improves the crystallinity of CZTS NCs with simultaneous decomposition of PEDOT:PSS.

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