Effects of controlled cooling rates on $Cs_2AgBiBr_6$ single crystal growth

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Photovoltaic (PV) technologies are currently one of the most widely deployed and cost-effective renewable energy technologies. However, solar cells based on silicon are currently reaching their limit in terms of efficiency. Therefore, the search for new materials has been one of the critical challenges and halide perovskite solar cells have made rapid progress within the last 10 years [1]. Their power conversion efficiency (PCE) has been improved from 3.8% to over 25.2% [1]. The upcoming challenge can be seen in the conservation of such high PCE in lead-free materials. Compared to their counterparts, double perovskites have a much higher temperature resistance and are much more stable. As one of the most promising lead-free halide double perovskites, $Cs_2AgBiBr_6$ has received increasing attentions, due to its high stability and nontoxicity. Nevertheless, it still suffers from a low PCE [2]. To further understand the nature of defects in $Cs_2AgBiBr_6$ and to improve the PCE, the effects of different cooling rates on the solution-based synthesis are investigated. $Cs_2AgBiBr_6$ single crystals were synthesized in various timeframes and analyzed by UV-Vis and Raman spectroscopies in order to determine the optical bandgaps and degree of defect formation. By comparison of the peak broadening of Raman spectra and estimated optical bandgap values from UV-Vis spectra, it is concluded that there is a correlation between the indirect bandgap value and defect formation with the controlled cooling rate applied during synthesis. Contrary to our general understanding in single crystal growth, for $Cs_2AgBiBr_6$ a slow-cooling process is found to result in more defects and disorder with a lower indirect optical bandgap.

References

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