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Study of electronic and thermal properties of $CH_3NH_3PbX_3$ (X = Br, I) single crystals using photoacoustic methods

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Introduction

Metal halide perovskite (PVK) based solar cell has drawn much attention recently due to its outstanding optoelectronic characteristics. PVK is also attracting attention as a thermoelectric material. It is important to investigate the fundamental properties of PVK material such as electronic and thermal properties such as photoexcited carrier lifetime, carrier diffusivity, surface recombination velocity, and thermal diffusivity for implementing greater performance for solar cell and pyroelectric devices. In this direction, PVK single crystal is chosen as our research subject thanks to it being free of boundary and low density of trap states properties which indicates a proper platform to research the intrinsic properties. On the other hand, the photoacoustic (PA) method is a non-contact and non-destructive measurement method that utilizes the photothermal conversion phenomenon, which has been applied to the evaluation of the thermal and electronic properties of various semiconductor materials [1]. In this work, the reflection detection configuration (RDC) and transmission detection configuration (TDC) of the PA technique [2] was used to simultaneously measure the optical, electronic, and thermal properties of $CH_3NH_3PbBr_3$ and $CH_3NH_3PbI_3$ single crystals.

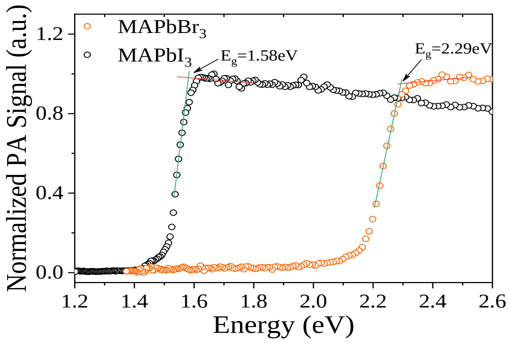

Figure 1. PA spectrum measured under RDC mode of $MAPbBr_3$ (orange circle) and $MAPbI_3$ (black circle) single crystal

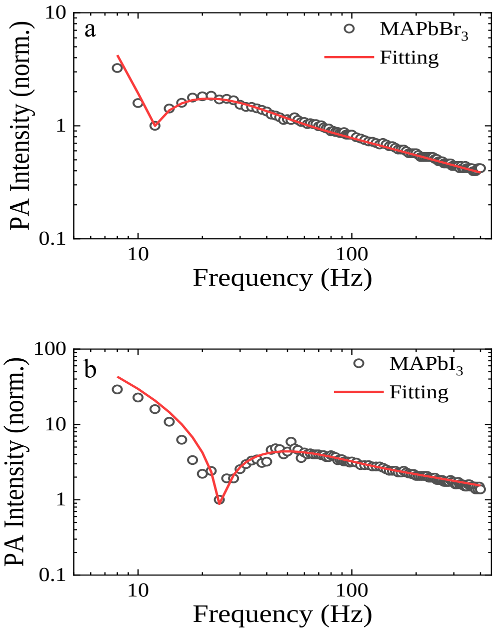

Figure 2. Dependence of the PA signal intensity of (a). $MAPbBr_3$ and (b). $MAPbI_3$ single crystal on modulation frequency measured under TDC mode.

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Experiment

The space-confined inverse temperature crystallization method was used to grow $CH_3NH_3PbBr_3$ and $CH_3NH_3PbI_3$ single crystal thin films with a thickness of approximately 200μm. Under RDC mode, the PA signal was measured from 400nm to 1200nm keeping the frequency of excitation light fixed at 33Hz. While in TDC, 450nm and 775nm excitation light was used for $CH_3NH_3PbBr_3$ and $CH_3NH_3PbI_3$ single crystals respectively to measure the modulation frequency dependence PA signal intensity from 10Hz to 400Hz.

Results and Discussion

In **Fig.1** the PA spectra of $CH3NH3PbBr_3$ and $CH3NH3PbI_3$ single crystal thin film under RDC mode were shown. The frequency dependence of PA signal intensity of $CH_3NH_3PbBr_3$ and $CH_3NH_3PbI_3$ crystals were shown in **Fig.2a**, and **Fig.2b** respectively. Based on previous research and theoretical equation, we obtained surface recombination velocity (S), carrier diffusivity (D), excess carrier lifetime (τ), and thermal diffusivity (D_{th}) with the developed program. Further, the τ, D, and D_{th} gained from impedance spectroscopy (IS), space charge limited current (SCLC), and the Flash method were consistent with that fitted from the PA technique. The corresponding data were summarized in **Table 1**.

$CH_3NH_3PbBr_3$	PA	Other technique
D(cm^2/s)	8	7.3
τ(μs)	50	70
D_{th}(cm^2/s)	0.003	0.0036
$CH_3NH_3PbI_3$	PA	Other technique
D(cm^2/s)	7	8.4
τ(μs)	100	133
D_{th}(cm^2/s)	0.0018	0.0021

Table 1. Comparison of D, τ, D_{th} fitted from the PA technique with other characterizations (SCLC, Impedance Spectroscopy, the Flash method).

Conclusion

The PA technique has been demonstrated to be a powerful method that can simultaneously and non-destructively evaluate the optical, thermal, and electronic properties of perovskite materials. It will be applied to the evaluation of such properties of different kinds of perovskite materials and provide important information for achieving the high performance of solar cells.

Reference

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