

MASnI₃ペロブスカイト格子欠陥の電子顕微鏡観察

Electron microscopy of Lattice Defects in MASnI₃ Perovskite

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Lead (Pb)-based perovskite materials have gained significant attention in the photovoltaic field in recent years. However, the toxicity of lead has raised widespread concerns. Tin (Sn)-based perovskites as one of the most promising alternatives, not only address the toxicity issues associated with lead but also retain optoelectronic properties. But the power conversion efficiency (PCE) of Sn-based perovskite solar cells has only reached around 15%^[1], significantly lower than the record efficiency of 25.47% achieved by Pb-based perovskite solar cells^[2]. The performance of Sn-based perovskites is primarily influenced by the oxidation of Sn²⁺ to Sn⁴⁺ and the formation of lattice defects, particularly those involving iodine (I) and Sn, which critically degrade the material's optoelectronic properties and long-term stability.

To investigate the impact of crystal structure and defects in MASnI₃, we prepared MASnI₃ precursor solutions using one-step method, and fabricated thin films using spin coating followed by short-time heating, as well as powders through drop casting followed by prolonged heating. Transmission electron microscopy (TEM) was used to observe the lattice structure of MASnI₃, and potential structural defects were suggested based on the analysis of inverse fast

Fourier transform (IFFT) images (Fig. 1a). To further explore the potential presence of the defects, the image simulation of perfect structure and defect models (Fig. 1b) in different MASnI₃ supercells were conducted by TEMPAS. In the 3×3×3 supercell (Fig. 1d), the atomic brightness contrast of the simulated TEM image at defect sites is nearly indistinguishable from defect-free regions, whereas in the 2×2×2 supercell (Fig. 1c), defects are more apparent. This difference may be due to defect concentration, which is approximately 4.17% in the 2×2×2 supercell compared to 1.23% in the 3×3×3 supercell. Higher defect concentrations seem to make defects more readily observable. The characteristics and distribution of vacancy defects in MASnI₃ crystals

are tentatively explored through a combination of experimental observations and image simulations. These findings may offer theoretical insights and technical guidance for improving the stability of Pb-free perovskite solar cells.

[1] Wang L, Bi H, Liu J, et al. ACS Energy Letters, 2024, 9 (12): 6238-6244.

[2] Liu K, Hu T, Cai Z, et al. Energy & Environmental Science, 2024, 17(15): 5576-5587.

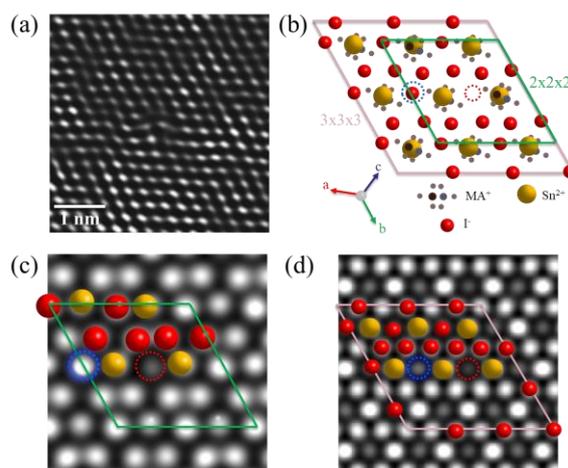


Fig. 1 (a) The IFFT image of MASnI₃ with a possible vacancy defect. (b) Crystal structures of MASnI₃ with I vacancy in different sizes from [111] direction. Simulated TEM images of MASnI₃ with I vacancy in (c) 2×2×2 supercell (Defocus: 600Å, thickness: 106Å) and (d) 3×3×3 supercell (Defocus: -300Å, thickness: 33Å). The red dashed circle: I vacancy; the blue dashed circle: normal I site.