Investigating the Effect of H^+-ion Irradiation on Layered α-MoO_3 Flakes by Defect Engineering

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ABSTRACT

Layered transition metal dichalcogenides (TMDs) with a band gap in the range 1-2 eV is the emerging new class of two-dimensional (2D) materials that can interact with light to convert the photons to electrical signals for its attractive applications in photonics, electronics, and optoelectronics [1]. However, there is the presence of uncontrollable defects, which degrades the functionalities of TMDs at higher temperatures. To overcome the aforementioned limitations of TMDs, there is a need for a new material. α-MoO_3 is a promising 2D oxide material that possesses a high charge carrier mobility of approximately 1100 $cm^2\ V^{-1}s^{-1}$ [2] and a high k-dielectric value of over 200 [3]. Additionally, it exhibits good transparency to visible light and can be used to control semiconducting properties [4]. In this study, we first demonstrate the growth of cm-sized α-MoO_3 crystals using physical vapor deposition, followed by reducing their thickness through mechanical exfoliation. We then carry out H^+-ion irradiation on the exfoliated α-MoO_3 flakes using a 30 keV source with a fluence of 1×10^{16} ions/cm^2. Interestingly, a new broad photoluminescence peak induced by defects is observed in the visible range (~570 nm) of the electromagnetic spectrum. To determine the origin of this peak, we performed HSE calculations by considering the oxygen vacancy in α-MoO_3. We found that the additional peak appears in the theoretical simulated absorption spectra and the total density of state calculation near the same position as the experimental defect-induced PL peak, confirming the defect-induced emission in the H^+-ion irradiated α-MoO_3 flake. This study highlights the potential of α-MoO_3 in tunable optoelectronics applications.

Keywords: *α-MoO_3 crystals; Optoelectronics; Physical Vapor Deposition (PVD); Photoluminescence (PL); Transition metal dichalcogenides (TMDs).*

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