Quantification and Healing of Defective Atomically-thin Molybdenum Disulfide, Beyond Controlled Creation of Atomic Defects

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Atomically thin 2D materials have opened up an opportunity to investigate the atomic scale details of defects introduced by particle irradiation. Once the atomic configuration of defects and these spatial distribution is revealed, fundamental physics behind complex structure can be well understood without any modeling or assumption. In this work, we created atomically small defects by controlled irradiation of gallium (Ga⁺) ion on monolayer MoS₂ crystal. The optical signature of defects, such as the disorder-related bands and broadening of first-order modes are investigated by Raman spectroscopy. Scanning transmission electron microscopy (STEM) analysis revealed that the majority of the defects are vacancies of few-molybdenum atoms with surrounding several sulfur atoms (VₓMoᵧ⁺S) at low ion dose. As the ion dose increases, the atomic vacancies merge and form nm-sized holes. By using finite crystal length in the defective 2D crystal, the quality of crystal and the characteristic length is determined via STEM image analysis, and then the correlation of the optical signature and the defective structure was discussed. Beyond the creation and the quantification, we have also demonstrated a route to heal the ion irradiation caused atomic vacancy by annealing the defective MoS₂ in hydrogen disulfide (H₂S) atmosphere. The H₂S annealing reduced the defect density to 1/5, and 10% of photoluminescence signal is successfully recovered which was completely quenched by ion irradiation with dose of 2.50×10¹³ ion/cm².