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Doubly Anisotropic Thermal Oxidation of 2-Dimensional MoS₂ Supported on Silica Substrates

Atomically thin planar crystals may reveal novel knowledge on chemical reactions occurring in a low-dimensional space. Despite the importance of surface chemical reactions, interfacial mass transport between 2-dimensional (2D) materials and supporting substrates is not well understood. In this work, we studied substrate-mediated thermal oxidation of 2D MoS₂ supported on SiO₂/Si wafers. Single and few-layer MoS₂ samples were prepared by mechanically exfoliating bulk MoS₂ crystals onto SiO₂/Si substrates. Oxidation reactions were carried out in a quartz tube furnace for a range of temperatures and partial pressures of oxygen. To characterize the changes in morphology, vibrational and electronic structures, Raman and photoluminescence spectroscopies were employed with atomic force microscopy. We observed anisotropic thermal oxidation reactions which formed triangular oxides (TOs) in the bottommost layer and several times smaller triangular etch pits (TEs) in the topmost layer. The former indicates that oxygen molecules diffuse efficiently through the MoS₂-SiO₂ interface at elevated temperatures. Optical second-harmonic generation spectroscopy verified that the TOs and TEs structures are terminated with zigzag edges. MoS₂ crystals on hexagonal boron nitride and thick graphene did not form TOs, which indicates that the oxidation is greatly enhanced in direct contact with the SiO₂ substrates. We will discuss the possible roles of SiO₂ substrates and other various aspects of the oxidation reaction and oxidized MoS₂ crystals.