Swift Chemical Etching of 2D Materials under Electron Beam in Transmission Electron Microscope

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The interaction of energetic electrons with the specimen during imaging in a transmission electron microscope (TEM) can give rise to the formation of defects or even complete destruction of the sample. This is particularly relevant to atomically thin two-dimensional (2D) materials. Depending on electron energy and material type, different mechanisms such as knock-on (ballistic) damage, inelastic interactions including ionization and excitations, as well as beam-mediated chemical etching can govern defect production. Using first-principles calculations combined with the McKinley-Feshbach formalism, we investigate damage creation in two representative 2D materials, MoS2 and hexagonal boron nitride (hBN) with adsorbed single adatoms (H, C, N, O, etc.), which can originate from molecules always present in the TEM column. We assess the ballistic displacement threshold energies T for the host atoms in 2D materials when adatoms are present and demonstrate that T can be reduced, as chemical bonds are locally weakened due to the formation of new bonds with the adatom. We further calculate the partial and total cross sections for atom displacement from MoS2 and hBN, compare our results to the available experimental data, and conclude that adatoms should play a role in damage creation in MoS2 and hBN sheets at electron energies below the knock-on threshold of the pristine system, thus mediating the formation of electron beam-induced damage. As chemical interactions of the host material with adatoms are involved, and because defects form under the beam on a sub-picosecond time scale, we call this channel for defect production swift chemical etching.