Quantum theory of sputtering rates in 2D materials by transmission electron microscopy

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Abstract

Many computational models have been developed to predict the rates of atomic displacements in two-dimensional (2D) materials under electron beam irradiation. However, these models often drastically underestimate the displacement rates in 2D insulators, in which beam-induced electronic excitations can reduce the binding energies of the irradiated atoms. This bond softening leads to a qualitative disagreement between theory and experiment, in that substantial sputtering is experimentally observed at beam energies deemed far too small to drive atomic dislocation by many current models. To address these theoretical shortcomings, we developed a first-principles method to calculate the probability of beam-induced electronic excitations by coupling quantum electrodynamics (QED) scattering amplitudes to density functional theory (DFT) single-particle orbitals. The presented theory then explicitly considers the effect of these electronic excitations on the sputtering cross section. Applying this method to 2D hexagonal BN and MoS_2 significantly increases their calculated sputtering cross sections and correctly yields appreciable sputtering rates at beam energies previously predicted to leave the crystals intact. The proposed QED-DFT approach can be easily extended to describe a rich variety of beam-driven phenomena in any crystalline material.

Reference: A. Yoshimura, et al, Nanoscale **15**, 1053-1067 (2023)


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