Atomic-scale description of electron beam effects in nanotubes and two-dimensional materials

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Recent developments in transmission electron microscopy (TEM) and computational resources have allowed quantitative atomic-level analysis of irradiation damage. We combine state-of-the-art TEM experiments with dynamical ab initio simulations to establish a detailed understanding of knock-on events in carbon nanotubes and two-dimensional materials under an electron beam. Irradiation-induced structural changes will be discussed in the context of pristine and doped carbon nanotubes and graphene, hexagonal boron nitride and transition metal dichalcogenide mono-layers, and in two-dimensional silica glass. The presented results have important implications for characterization methods involving energetic electrons, and provide basis for future advances in atomic-level engineering.

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