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Role of electronic excitations in ion collisions with carbon nanostructures.[1] DAVID TOMANEK, Michigan State University, YOSHIYUKI MIYAMOTO, NEC Corporation, ARKADY KRASHENINNIKOV, Helsinki University of Technology — We study the effect of electronic excitations during collisions of protons with sp^2 bonded carbon nanostructures by performing molecular dynamics simulations. To obtain microscopic insight into the collision process in real time, we combine time-dependent density functional calculations for electrons with molecular dynamics simulations for ions, and compare the results to molecular dynamics simulations in the electronic ground state. The simulations for protons colliding with carbon nanotubes and graphite are performed in the interesting range of impact energies of tens to hundreds of eV, corresponding to ion velocities covering a broad range around the Fermi velocity of the target, v_F=8×10^5 m/s. In agreement with the binary collision approximation, we find only negligible deviations from Born-Oppenheimer dynamics for projectile velocities well below the Fermi velocity. Our results establish validity limits for the Born-Oppenheimer approximation, and also the threshold energy for sputtering of carbon nanotubes and graphite.

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