Electronic stopping power of slow ions in solids from first principles

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Coupled electron-ion dynamics, at the Ehrenfest dynamics level, using the time dependent density functional theory with the SIESTA pseudopotential code is used to simulate strongly non-adiabatic process of the passage of slow ions through solids. It is an improvement over a previous method that considers only the electron dynamics, describes the moving ion with its screened Coulomb potential, and places a chain of atomic orbital bases along its trajectory. We consider the projectile and the atoms of the target material on equal footing. That is, just like the target atoms, the projectile is described with its pseudo-potentials and atomic orbital basis is attached to it. This improved description of the process and the projectile leads to a much better agreement with the experiments.

We calculate the electronic stopping power of slow ions with velocity $v \sim 0.05-0.50$ a.u. in various crystalline metals and ceramics. Non-linearities in the velocity dependence of the stopping and the threshold effect are discussed. We find reasonably good qualitative and quantitative agreement with the available experimental data. For H and He ions moving in gold, we also calculate the electron-hole pair spectrum around the fermi level by projecting the time evolved electronic state onto the ground state for the instantaneous nuclear configuration. We find that there is a significant contribution to the stopping from the deep lying d-band states even for a slow projectile. For the series of insulators explored, the material dependence of the threshold and other electronic stopping features are presented. Interesting results are found for the variation with the impact parameter and projectile dependence, especially when comparing sparsely packed with densely packed systems.

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