Phonon and electron excitations in diatom abstraction via Eley-Rideal mechanism from metal surfaces

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Quasiclassical molecular dynamics simulations are performed to study the influence of the two main energy loss channels on Eley-Rideal recombination of H_2 and N_2 on two crystallographic planes of tungsten, (100) and (110). Calculations are carried out within the single adsorbate limit under normal incidence. A Generalized Langevin Surface Oscillator (GLO) scheme [1,2,3] is used to simulate the energy transfer due phonon excitations, whereas the electron hole (e-h) pair excitations are implemented using the Local Density Friction Approximation (LDFA) [4]. Phonon excitations are found to reduce reactivity for N_2 recombination, but do not affect H_2 abstraction. The effect of electronic friction on reactivity is small for both chemical species and is directly related to the reduction of the collision energy of the projectile. In the case of nitrogen, smaller friction mediated energy losses are found when surface motion is implemented. This coupling is explained by the reduced velocity of the outgoing molecule. Finally, the internal energies of the formed molecules are analyzed: Dissipation to e-h pairs, similar for both species, is shown to take energy from the translation of the formed molecules, whereas dissipation to phonons, only significant for N_2, also affects vibration.

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