Electron Energy Deposition in Molecular Hydrogen: A Monte Carlo Simulation Using Accurate Cross Sections

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A simulation of the process of electron energy deposition in molecular hydrogen in the energy range 0–500 eV is reviewed. The simulation employs the accurate Molecular Convergent Close-Coupling (MCCC) cross section data set [1]. A new method for sampling continuum excitations of a given target in Monte Carlo simulations is presented and explicitly compared with the use of single differential ionisation cross sections in a simulation of H_2. The results of a benchmark calculation of the mean energy per ion pair in H_2 are presented, yielding excellent agreement with experiment and the previous simulation of Dalgarno et al [2]. Finally, a generalisation of the simulation to explicitly include vibrational excitation and dissociation is used to examine dissociative effects in the electron energy deposition process.

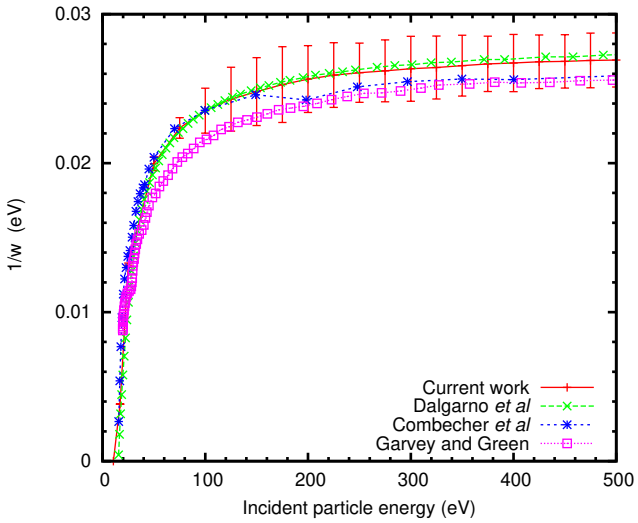

Figure 1: The mean energy per ion pair (w) calculated using the present simulation. The present results [1] are compared with Dalgarno et al [2], Combecher et al [3] and Garvey and Green [4]

[1] R. K. Horton et al *Plasma Sources Sci. Technol.* **30**, 115004 (2021).

[2] A. Dalgarno, M. Yan and W. Liu *The Astrophysical Journal Supplement Series* **125**, 237-256 (1999).

[3] D. Combecher *Radiation Research* **84**, 189-218 (1980).

[4] R. H. Garvey and A. E. S. Green *Phys. Rev. A* **14**, 946-953 (1976).