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Updating the GOS for ionisation and excitation of liquid water: new proton impact cross section dataset relevant for Geant4-DNA

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The processes involved in the passage of radiation through matter is of great interest in medical radiation physics among other areas. Monte Carlo codes are widely used in research fields such as micro/nanodosimetry and computational radiobiology, which demand an accurate modelling of the interaction cross sections in liquid water and other materials of interest. In Geant4-DNA, the physical processes are simulated together with the radiation-induced physico-chemistry and chemistry processes for water radiolysis at sub-cellular scale, all of which contributes to the later damage caused to DNA. At present, no cross sections for the interaction of ions in liquid water have been experimentally determined. Up to our knowledge, the only data available are for the impact of ions in water vapour and these are scarce. Because of this, great efforts have been made to model interactions of radiation with liquid water.

In particular, the extension of the ionisation and excitation models for proton above 100 MeV was performed by the authors of this work [1], using the Relativistic Plane Wave Born Approximation (RPWBA) [2]. This theory separates the contribution to the DDCS of the projectile and the medium, being the last one represented by the generalized oscillator strength (GOS). The latter plays a key role on the determination of the cross section. For a condensed medium, its computation by means of first quantum principles become unfeasible because it is necessary to deal with a many-particle system. Fortunately, the GOS can be computed from the dielectric function (DF) of the medium. The implemented cross section datasets were computed used a GOS model for liquid water based on ideas developed in previous works [3,4].

Here, a new extended optical-data GOS based on Drude functions is presented and used to characterize the most recent available data for the liquid water DF [4], which has not been done previously. This update allows to compute a new dataset of cross sections, which is in good agreement with the experimental data available in water vapour as a reference. Furthermore, the stopping power computed with this model for relativistic proton energies are in excellent agreement with the ICRU report 90 within 1%, validating the dataset also for the higher energy regime.

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