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Track Structure Code for Low-Energy Protons

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INTRODUCTION

Computer simulation of charged particle tracks has contributed significantly to our understanding of the micro- and nanodosimetry of radiations in tissue-like matter (1). Current models of the structure of ion tracks are limited to energies above the Bragg peak because there is a lack of cross sections for many of the important interaction processes. Accurate treatment of all interactions, including excitation and ionization by dressed ions and neutrals, and charge exchange processes which play an important role in the energy degradation of ions at these energies, is needed. In this paper we briefly discuss a new model for the development and extension of the ion track-segment simulation to lower energies below 0.3 MeV/u.

CROSS SECTIONS

The reliability of basic cross-section data appropriate to the stopping of low-energy ions in water was examined. These data are needed for the extension of current charged-particle track-simulation codes to heavy ions with energies where electron capture and electron loss by the moving projectile become important. Calculations of electronic stopping cross sections for low-energy protons were performed using available interaction cross sections and mean energy loss per collision data. The electronic stopping cross section for protons is defined by

$$L_e(T) = \sum_j f_p Q_j \sigma_j(T) + \sum_k f_H Q_k \sigma_k(T), \qquad (1)$$

where j represents interactions leading to ionization, excitation and electron capture by proton impact, and k represents ionization, excitation and electron loss by neutral hydrogen impact; $\sigma(T)$ represents total cross sections for processes k and j at kinetic energy T for proton and atomic hydrogen interactions, respectively; Q is the mean energy transfer in each interaction; and f_p and f_H are the equilibrium charge fractions for protons and atomic hydrogen, respectively. Total ionization cross sections and the mean energies of secondary electrons ejected by proton and hydrogen impact were obtained from experimental data for water vapor, which are available over most of the energy range of interest. In the region where data were lacking the existing data were fitted and extrapolated. The electron capture and loss cross sections were obtained using previously published models (2). The mean energy loss by the proton in an electron capture process was taken as the energy necessary to provide translational energy, for the electron to move at the proton velocity, plus the energy difference between the initial and final bound states of the electron. For electron loss the mean energy loss by the hydrogen atom was assumed to be the binding energy of the ground state of the hydrogen.

Elastic scattering cross sections needed for the proton track code were evaluated using procedures given by Everhart et al. (3) and assuming Coulomb potentials with screening functions. The deflection angle θ is obtained as a function of the impact parameter, p:

$$\theta = \pi - 2\int_{r_{min}}^{\infty} \frac{p}{r^2\sqrt{1 - V(r)/T_{cm} - p^2/r^2}}\, dr \qquad (2)$$

where r_{min} is the distance of closest approach, T_{cm} is the particle energy in the center-of-mass system. The differential cross section is evaluated by

$$\sigma(\theta) = -\frac{p}{\sin\theta}\frac{\mathrm{d}p}{\mathrm{d}\theta}. \tag{3}$$

θ and $\sigma(\theta)$ are functions of the impact parameter and the particle energy. In order to reduce the divergence of the total cross section, the cutoff angles, θ_{cut}, were set such as to limit the increase in the scattering probability (4). The nuclear stopping cross section is given by

$$L_n(T) = 2\pi\int_{\theta_{cut}}^{\pi} \sigma(\theta)W(\theta,T)\sin\theta \ \mathrm{d}\theta \tag{4}$$

where the energy transfer to the recoiling atom, $W(\theta,T)$, is given by

$$W(\theta,T) = 4T\frac{M_t M}{(M_t + M)^2}\sin^2\frac{\theta}{2}. \tag{5}$$

RESULTS AND DISCUSSION

Figure 1 shows the calculated electronic and nuclear stopping cross sections of water vapor in comparison with the published data. The electronic stopping cross sections for protons in water vapor are in agreement with the ICRU49 data (5) to app. 20% for proton energies less than 300 keV. The nuclear stopping cross sections agreed well with the ICRU data.

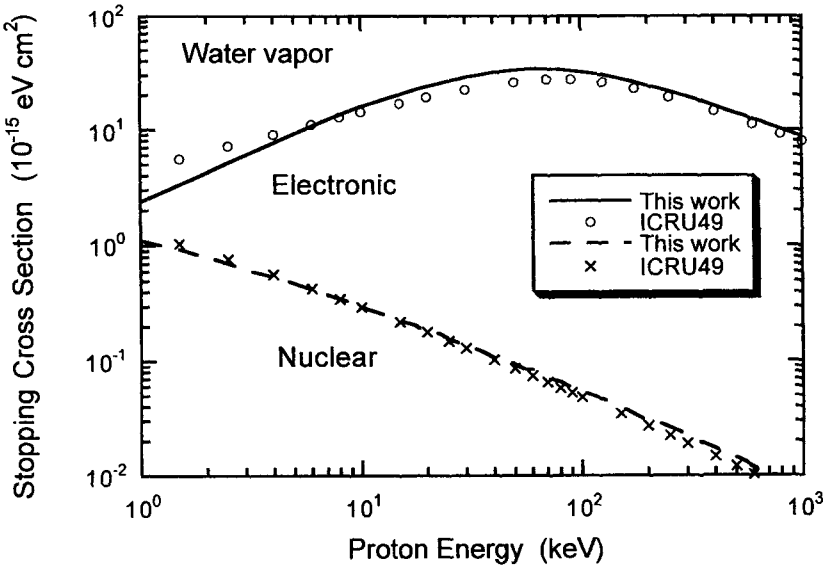

Figure 1 *Comparison of the electronic and the nuclear stopping cross sections of water vapor.*

It is concluded that the evaluated cross-section data is usable as the input data for a Monte Carlo track structure code for low-energy protons. Track data of secondary electrons generated during the slowing down of protons and hydrogen atoms were stored and were used as the input data for the electron track code *kurbuc* (6). The calculated proton ranges agreed well with the tabulated data (5). The W-values were derived from scoring the number of electron-H_2O^+ pairs due to ionization and charge exchange cycle by taking into account the ionization events by the energetic secondary electrons. Figure 2 shows the calculated W-values in comparison with

various published data. Energy dependence of the W-values shows a flat minimum around 10 keV which is similar to the experimental data for protons in CO_2 and N_2 (7). The W-value of 31.2 eV at 1 MeV was close to the experimentally determined asymptotic limit, 30.5 eV (8).

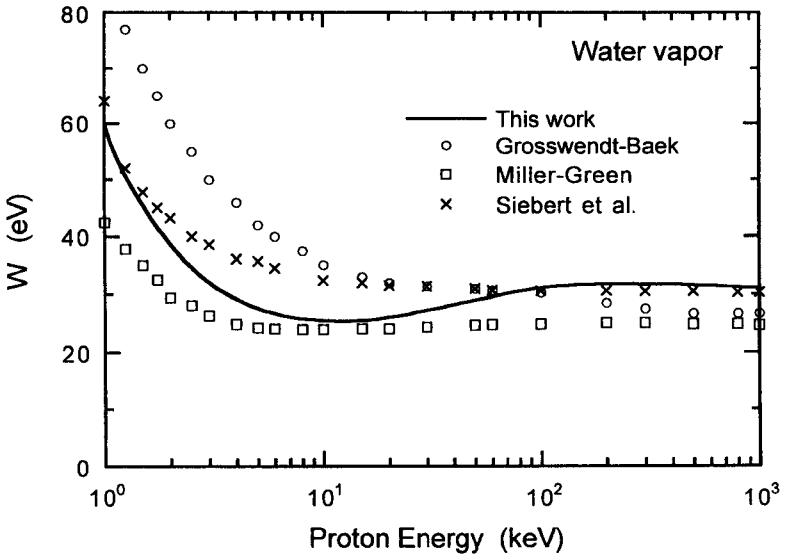

Figure 2 *Mean energy W required to produce an ion pair for protons slowed down in water vapor.*

CONCLUSIONS

A new model for the development and extension of the ion track-segment simulation to lower energies below 0.3 MeV/u was proposed. The preliminary calculations gave the plausible results for the basic physical data accompanying proton slowing-down in water vapor, such as stopping cross sections, ranges and W-values. We suggest developments are needed to extend track simulations to other particles and energies such as for slow ions (to include for example charge exchange and full slowing down) and for very high-energy ions (including nuclear fragmentation), to allow description of effects from practical radiations such as radon, neutrons and in space flight.

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