Developments for the TRAX simulation code

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Developments

The TRAX single interaction Monte Carlo (MC) simulation code has substantially been enhanced in the past years [1]. External cross sections, including Auger effect, for a large variety of materials are available, and have been used e.g. in nanoparticle simulations [2].

These developments were streamlined and incorporated into the code's main branch [3]. In addition, cross section handling was overhauled in order to treat target materials as atoms, molecules (compounds) or mixtures, depending on the interaction type. For example, for electronic interactions a water molecule is seen as a molecule, whereas for nuclear interactions it is a mixture.

Applications

A possible application of the new features is the prediction of microscopic dose deposition in solid state dosimeters, e.g. TLDs. These devices are made of LiF, which might be treated as mixture of Li and F. The single interaction cross sections of the constituents for a variety of ionization, excitation and elastic processes were collected [1]. As a first goal, classical radial dose distributions are generated, which are usually required for LEM type microscopic models [4].

Results

Figure 1 shows a comparison with a conventional (condensed random walk) MC calculation [1], [5]. Substantial differences occur in the inner part (<5nm) of the ion track. These might be due to different (low-energy) cross sections being used, as well as due to a different energy cutoff: 50eV vs 2eV used in TRAX. Figure 2 shows a comparison with the analytical formulae used by [4] to calculate TL dosimeter efficiencies. Here, the agreement appears to be better except for the innermost part. It remains to be investigated, whether the higher core dose will lead to a better agreement of measured and calculated TL efficiencies.

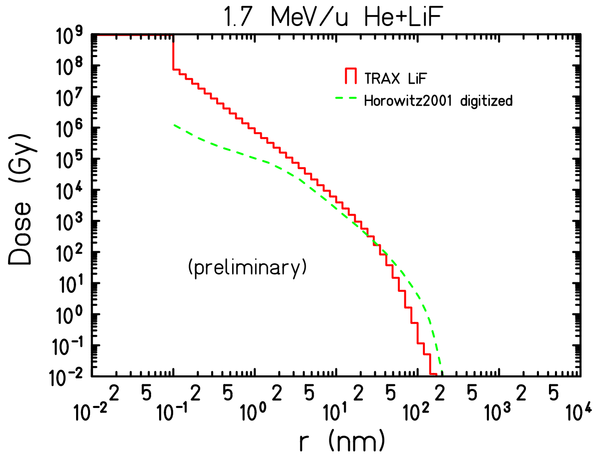

Figure 1: Radial dose profiles for helium ions. Dashed: Reproduced from [5], solid: TRAX calculation.

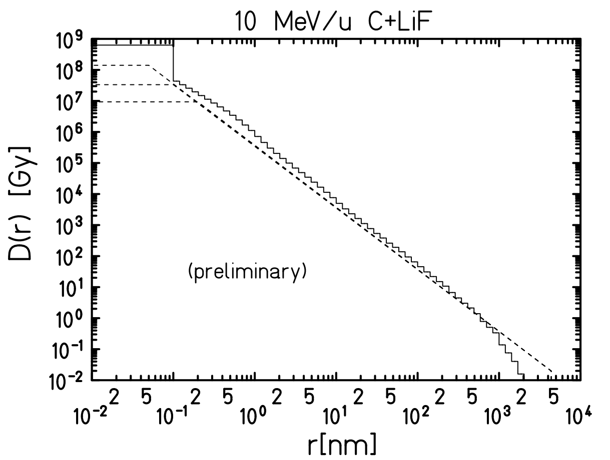

Figure 2: Radial dose profiles for carbon ions. Dashed: analytical formula from [4], solid: TRAX calculation.

References

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