

Contribution ID : **68** Type : **Poster**

Monte Carlo simulation of carbon-ion energy deposition in tissue modeled with nanoparticles

Thursday, 22 October 2026 17:00 (2:00)

Abstract

A Monte Carlo simulation of ^{12}C ion transport at 225˜MeV/u in an idealized tissue medium incorporating nanoparticle-enriched regions is presented. The ion–atom interaction is described by a Yukawa-type screened potential within the first Born approximation, from which differential and total cross sections, mean free path, and collision probabilities are calculated. Energy loss is modeled using the Bethe–Bloch formula, extended to mixtures via Bragg additivity. The spatial heterogeneity of the tissue is represented by a periodic distribution of spherical regions controlled by a geometric parameter adjusted to the cellular scale (∼50˜μm), within which variable nanoparticle concentrations are assigned. The model was validated by reproducing Bragg curves in pure water, obtaining a peak at ∼10.15˜cm depth and ∼202˜MeV/mm in height, consistent with reported clinical values. Eleven compounds (Ag, Au, Bi, Fe$*{3}O{4}, Pb, Pt, SiO{2}, Ta, TiO{2}$, W, and ZnO) were analyzed at concentrations of 1–10\%, identifying Pt, W, and Au as the materials with the largest increase in energy deposition within the doped regions, reaching values of 180–200˜MeV/mm near the Bragg peak. The code was developed entirely in Python, implementing parallel execution through process distribution and intermediate storage in SQLite databases, which allows scaling the number of simulated trajectories according to available computational resources. The software is open access and designed to be reproducible and adaptable.

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Session Classification : Poster Session