New theoretical atomic radiation library for basic science and applications

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Unstable atomic nuclei release excess energy through various radioactive decay processes by emitting neutrons, alpha- and beta-particles or electromagnetic radiation. In some cases, including internal conversion and electron capture, the atom remains ionised after the nuclear decay event. Atomic relaxation occurs rapidly via radiative and non-radiative processes, often referred as atomic radiations. Radiative processes are those involving the emission of characteristic X-rays. Non-radiative processes include emission of Auger, Coster-Kronig and super Coster-Kronig electrons.

While these atomic radiations usually only carry a fraction of the available nuclear decay energy, because of their high cross section to interact with matter, they are important for nuclear dosimetry and a range of applications. Since the early 70s, when the use of Auger electrons for cancer therapy was first suggested by Howell [1], considerable advances have been made in understanding the radiobiological effect of low energy electrons. In contrast to nuclear radiations, the experimental data on low-energy atomic radiations are scarce, therefore in most cases, theoretical transition energies and rates are used to evaluate the absorbed energy dose. Unfortunately, these calculations are based a very different physical assumptions and approximations resulting very different emission rates [2].

Recently, we have proposed an Auger-cascade model [2, 3,4] to provide more realistic theoretical descriptions of atomic radiations. The model based on a full Monte Carlo approach to treat the stochastic nature of the creation of the initial vacancy in the nuclear decay process and the subsequent propagation of vacancies. To achieve reasonable accuracy a large number of decays need to be calculated. While for a simple system, like 40K, it only takes less than 30 minute to simulate 1 M events, the same calculation for 99mTc could take more than 24 hours. To reduce the CPU time drastically we are developing a new data base, which will contain pre-calculated atomic radiation spectra for Z=6 to 100 systems allowing quick (< 1 s) evaluation of the full energy spectrum.

In this talk we will review the recent progress in the development of the Auger-cascade model and its application for basic science.

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