Monte Carlo simulations of 1keV to 100keV electron trajectories from vacuum through solids into air and resulting current density and energy profiles.

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ABSTRACT

Design and optimization of systems which perform electron beam irradiation under atmospheric conditions requires both the modeling of pure electron optics inside electron beam guns as well as the treatment of electrons passing through solid films and the adjacent gas.
It is shown that in order to simulate trajectories of electrons from an emitting metal cathode, through high vacuum (with effectively no electron-gas collisions), through a solid object (typically a thin foil acting as wall), into air and onto a target a combination of different modeling approaches for the various domains is required.

1. INTRODCTION

Increased awareness to use environmentally friendly methods for surface sterilization, i.e. without the use of chemicals, has rejuvenated interest in methods based on electron beam irradiation. Secondly, electron beam irradiation enables a very high degree of control of the sterilization process and can be employed in cases where other (e.g. heat based) methods are not applicable. This is particularly important in applications such as preparation of spacecraft for life detection missions [1], [2].
While sterilization of bulk material, such as food, with high energy electrons (several MeV) has been used for many decades, surface treatment with medium energy electrons in the presence of gas is only recently gaining attention.

2. METHODS

Design and optimization of systems which perform electron irradiation under atmospheric conditions requires both the modeling of pure electron optics inside electron beam guns as well as the treatment of electrons passing through solid films and the adjacent gas. Thus far, Monte Carlo electron beam simulations have been described either as typical electron optics simulations (i.e. collision free in vacuum), or exclusively in solids [3]-[6] or gases (plasmas) [7]-[9] with emphasis on the electron matter interaction.
By combining different modeling approaches for the various domains a more complex simulation system can be created which permits to model the entire path of electrons from an emitting metal cathode, through high vacuum (with effectively no electron-gas collisions), through a solid object (typically a thin foil acting as wall), into air and onto a target.

3. RESULTS

The discussed method builds partially on [5], although comparison with other sources (NIST) revealed that some of the material data in [5] appear to be erroneous. Fig. 1 shows the energy loss per distance traveled for electrons in three different solids as function electron energy. Effects due to crystallographic structure are neglected. Typical values are on the order dE_{kin}/dr = 1 eV/nm …100 eV/nm for usually encountered electron beam energies (i.e. acceleration potentials).

Very recently, highly accurate solutions for differential and total elastic scattering cross sections of electrons with $E_{kin} \geq$ 1keV on various neutral atoms have been published which are based on Dirac partial-wave calculation using the ELSEPA code [10] which have also been published in comprehensive form by ICRU in [11]. These data are of critical importance and are being incorporated in the presented simulation system.

Fig. 2 shows as an example of such result as provided in [11] the total cross-section σ for elastic scattering of electrons by aluminum.

Of further importance it the mean free path between elastic scattering events and typical values will range from λ=1nm…100nm dependent on the material and electron energy (Fig. 2). For 100keV electrons in Titanium this value is about 50nm and the previously mentioned energy loss per distance traveled is on the order of 1.3eV/nm.

Fig 4 shows an example of a simulation of a generic electron beam gun producing an electron beam with E_{kin} =20keV. The yellow base represents foil through which electron beam will penetrate.

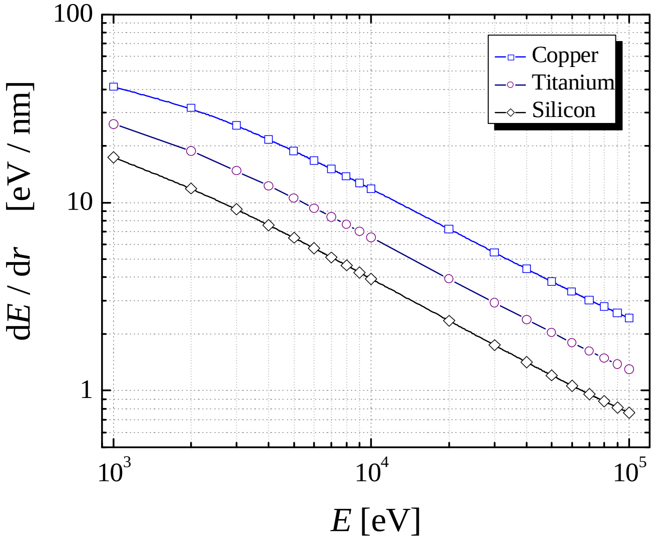

Fig. 2 Energy loss per distance traveled for electrons in three different solids as function electron energy. (Crystallographic structure neglected); based on NIST data

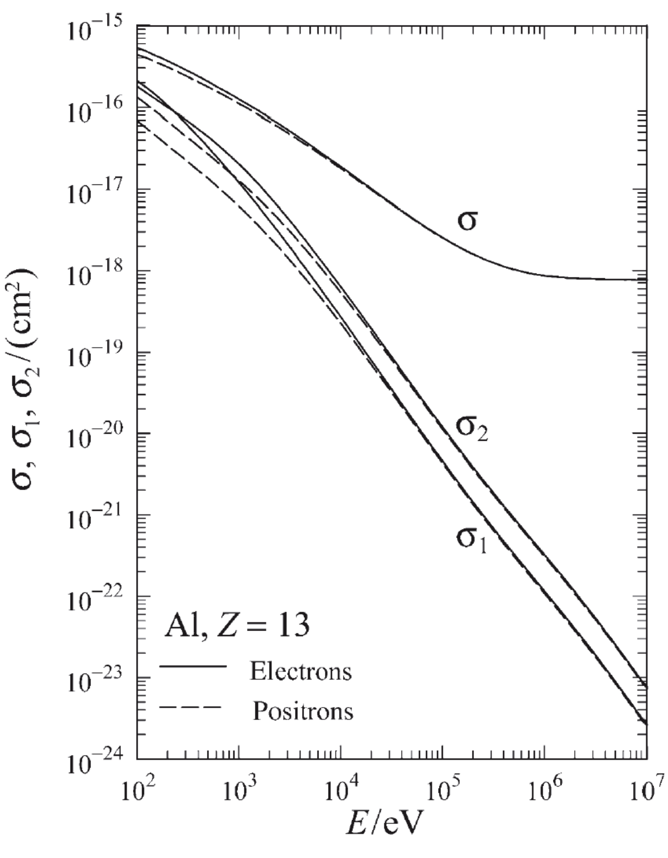

Fig. 3 Total cross-section σ, 1st transport cross-section σ_1, and second transport cross-section σ_2 for elastic scattering of electrons by aluminum. (from [10])

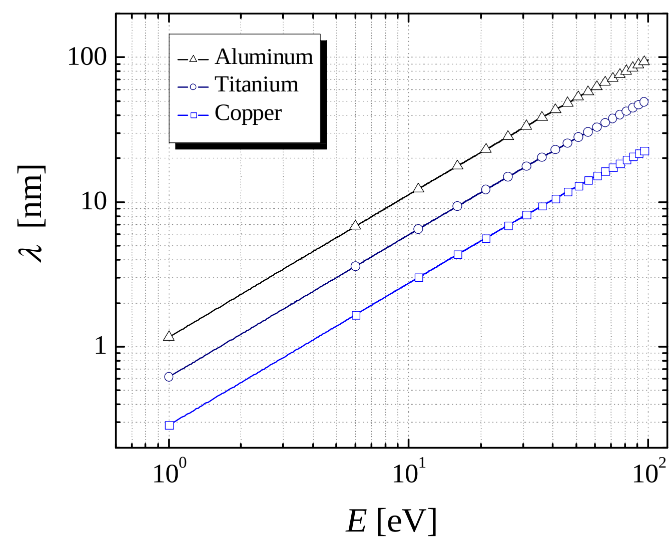

Fig. 1 Mean free path between eleastic scattering events for electrons in three different solids as a function energy. (Crystallographic structure neglected); based on ICRU data

Typically, an electron gun creates an image of its cathode at the surface of a solid foil which acts as transmission window to the atmosphere. The spatial electron current density profile $j(x,y,E)$is modulated during the electron transmission through the solid both spatially and energetically.

The electron trajectory integration regimes are different for vacuum and medium. However, electrons are continuously tracked and scattering events are considered individually, i.e. no averaging or “condensed history” or other simplifying approaches are employed in the simulation.

Fig. 5 and Fig. 6 show examples of trajectories of electrons in Titanium with initial energies of 20keV and 100keV. Notice the distinctly different appearance.

When exiting the solid, and dependent on its thickness, the transmitted electrons have a current density profile $j'(x,y,E)$ with a lower, but typically much wider energy distribution than the original distribution which is almost exclusively determined by the thermal emission process. These distributions constitute then the input for the electron tracing in air. Current density profiles (translating into dose profiles) have been obtained at different planes of models.

Such simulations permit the optimization of electron beam shapes, foil thickness and structure, as well as spatial dose profiles.

NSTI-Nanotech 2008, www.nsti.org, ISBN 978-1-4200-8505-1 Vol. 3

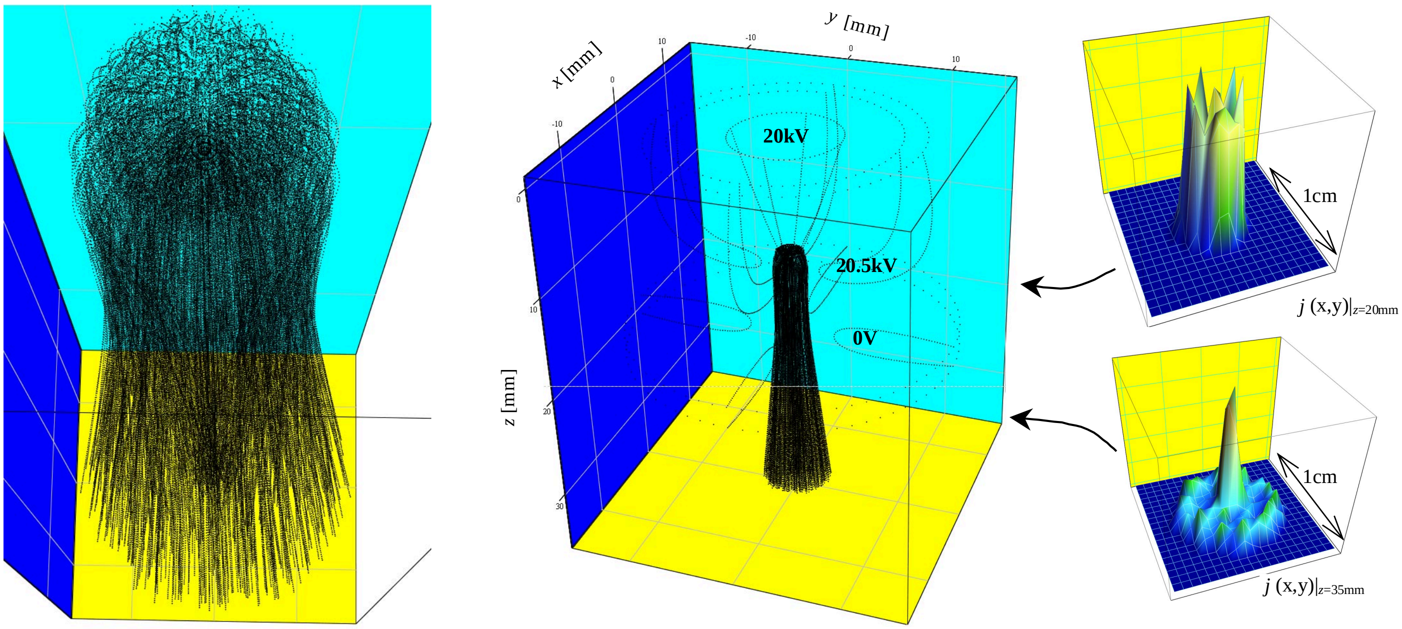

Fig. 4 Monte Carlo simulation of an electron gun; electron energy E_{kin}=20keV; Left and center: trajectories of 10^4 electrons, dotted shapes indicate electrodes, yellow base represents foil through which electron beam will penetrate; right: current densities $j(x,y)$ in planes at z=20mm and z=35mm, current densities plots based on 10^6 electron trajectories

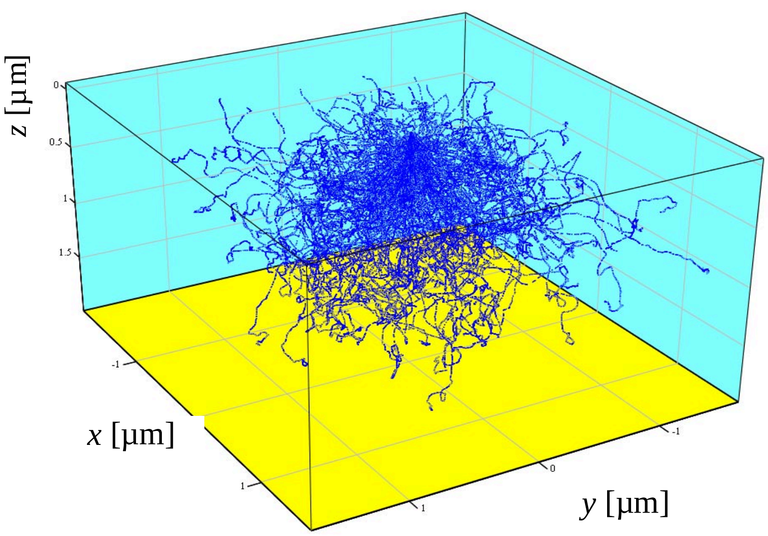

Fig. 5 Monte Carlo simulation of 500 electrons with an initial energy of ${}_iE_{kin}$=20keV in a 5μm thick Titanium foil. 0% transmission, 25% backscattered, average energy of backscattered electrons: ${}_bE_{kin}$=13.3keV

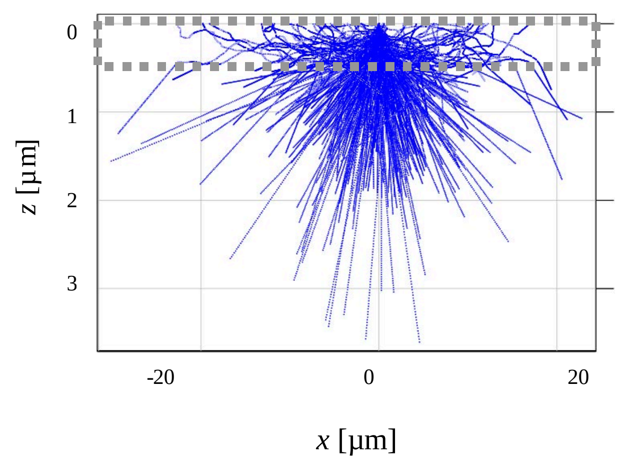

Fig. 6 MC simulation of 500 electrons with an initial energy of ${}_iE_{kin}$=100keV through a 5μm thick Titanium foil. 90% transmission, average energy of transmitted electrons: ${}_tE_{kin}$=90keV; 10% backscattered, average energy of backscattered electrons: ${}_bE_{kin}$=77keV

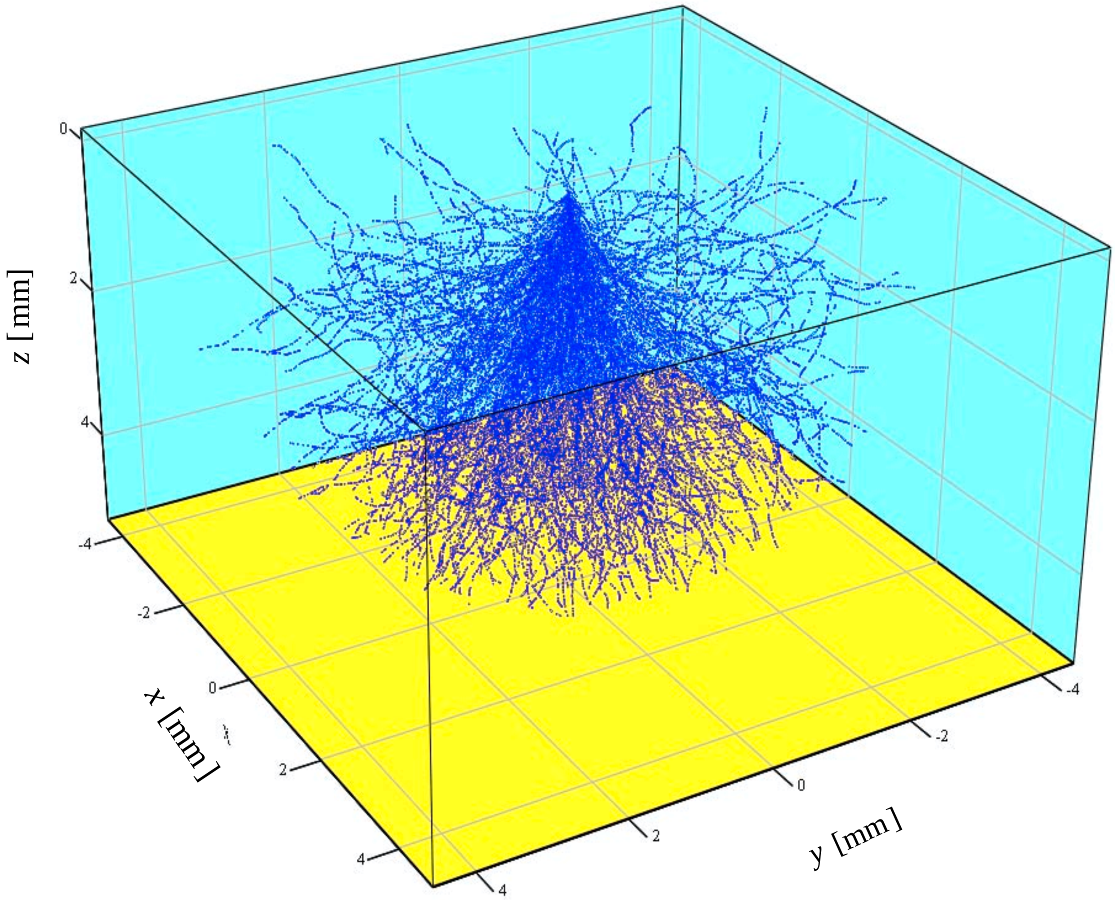

Fig. 7 Monte Carlo simulation of 500 electrons with an initial energy of $_iE_{kin}$=20keV shot into air at p=10^{5}Pa. Simulation terminated at E_{kin}=10keV. Notice the different scale compared to the previous figures.

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