A refined Monte Carlo code for low-energy electron emission from gold material irradiated with sub-keV electrons (Postprint)

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Abstract

Considering the importance of low-energy electrons (LEEs; 0–20 eV) in radiobiology, the radiosensitization potential of gold nanoparticles (AuNPs) as high-flux LEE emitters under sub-keV electron irradiation has been proposed. In this study, a track-structure Monte Carlo simulation program was developed based on dielectric function theory to simulate the transport of electrons below 50 keV in gold materials. In this program, to more accurately describe LEE emission in secondary electron emission, the theories for inelastic scattering, elastic scattering, and electron-acoustic phonon scattering were improved, and the program was further validated using secondary electron yield and backscattering coefficients. A dose calculation module was also developed in this program. To ensure dosimetric accuracy, we used the Monte Carlo toolkit Geant4 to further validate the energy deposition calculations through comparative analysis. The development of this optimized Monte Carlo program lays the foundation for future studies on the impact of AuNPs in targeted radionuclide therapy.

Full Text

A Refined Monte Carlo Code for Low-Energy Electron Emission from Gold Irradiated with Sub-keV Electrons

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Abstract

Given the significance of low-energy electrons (LEEs; 0–20 eV) in radiobiology, gold nanoparticles (AuNPs) have been proposed as high-flux LEE emitters when irradiated with sub-keV electrons. In this study, we developed a track-structure Monte Carlo simulation code based on dielectric theory to simulate electron transport below 50 keV in gold. The code incorporates several modifications, particularly for elastic scattering, to achieve a more precise description of LEE emission in secondary electron emission processes. We validated the code using secondary electron yield and backscattering coefficient data, and further verified its dosimetric accuracy through comparison with the Geant4 Monte Carlo toolkit. This development provides a foundation for future investigations into the role of AuNPs in targeted radionuclide radiotherapy.

Keywords: Monte Carlo code, Secondary electron emission, Low-energy electrons

1 Introduction

The radiobiological importance of medium-energy (< 100 keV) and low-energy (< 20 eV) electrons (LEEs) in radiotherapy has recently been emphasized, particularly relative to conventional high-energy (> 100 keV) electrons. Medium-energy electrons, especially sub-keV Auger electrons (20–500 eV), deposit energy across subcellular dimensions (< 0.5 m) in tissue and exhibit higher linear energy transfer (LET: 4–26 keV/ m) and greater relative biological effectiveness (RBE: 1–20) compared to conventional ~MeV X/γ-rays (LET: 0.2–2 keV/ m, RBE: 1). Consequently, like heavy-charged particles, these electrons can induce extreme toxicity in small tumors, cell clusters, or micrometastases, showing significant potential for highly targeted implant radiation therapy. However, this potential can only be realized if the radiation source is located sufficiently close to the cell nucleus or membrane.

More importantly, these nearly non-ionizing LEEs have traditionally been considered less significant in radiology due to the ionization potential of liquid water (11.7 eV). Following pioneering work by Sanche et al., several studies have demonstrated that ultralow-energy electrons (LEEs or quasi-free electrons: 0–20 eV) can increase DNA strand break yields. Although some LEEs cannot directly ionize molecules, they can still induce DNA cleavage—including single-strand breaks (SSBs) and double-strand breaks (DSBs)—with high cross sections via dissociative electron attachment. Therefore, accurate modeling of medium-energy electron and LEE transport in biological systems is critical.

In targeted radionuclide therapy, radiolabeled high-Z nanoparticles, particularly

gold nanoparticles (AuNPs), increase absorbed dose in the immediate vicinity and enhance LEE emission through interactions with 10–200 keV photons and ~MeV electrons. Unfortunately, external beams used in radiotherapy, such as photons and electrons, penetrate biological tissues only on the millimeter and centimeter scales, respectively, limiting the applicability of AuNPs in localized nanoscale radiotherapy. To address this limitation, an Auger electron source attached to AuNPs has been proposed to generate larger quantities of secondary LEEs through interactions with gold. These secondary LEEs have shorter ranges than the primary Auger electrons and further localize radiation energy within approximately 1–10 nm. Nevertheless, the effects of AuNPs irradiated with medium- and low-energy Auger electrons remain poorly studied, and the accuracy of such studies cannot be guaranteed.

A recent study found that a stable monolayer film of ^{125}I on gold-coated mica substrates amplifies LEE emission by sixfold. This enhancement was attributed to secondary electron emission (SEE) from the metal surface, driven by abundant Auger electrons emitted during ^{125}I decay (23.0 Auger electrons per decay with an average energy of 0.5 keV). Previous SEE experiments with gold foils have shown that primary electrons of 500–750 eV produce the highest secondary electron yield (SEY; the number of true secondary electrons (0–50 eV) emitted per incident electron) of approximately 1.2–1.7. Based on these findings, the potential of LEE therapy combining Auger electron emitters with AuNPs has been suggested. Therefore, the primary objective of this study is to develop a Monte Carlo simulation code for sub-keV electron and LEE transport in gold.

In conventional Monte Carlo simulations, electron transport is typically handled through condensed history methods, including multiple scattering, single scattering, and continuous slowing down approximation (CSDA) strategies. While effective and computationally efficient for macroscopic scenarios, these approaches fail to provide detailed descriptions of low-energy electrons because they neglect the actual energy loss in individual inelastic collisions. More accurate techniques, such as energy straggling strategies in materials science or track-structure strategies for microdosimetry, have been developed to address this limitation. These methods require detailed descriptions of each electron interaction and consider discrete energy losses during transport.

Various well-established general-purpose Monte Carlo toolkits exist, including Geant4, MCNP, JMCT, SuperMC, and EGSnrc, which are suitable for simulating diverse particles. However, most generic Monte Carlo codes employ condensed history methods rather than track-structure approaches. Recently, track-structure tools such as Geant4-DNA, NOREC, KURBUC, and PARTRAC have been implemented to simulate discrete electron transport in liquid water down to several eV. Sakata et al. developed two discrete models, Geant4_{{{DNA}}*{{Au}}}{2016} and Geant4_{{{DNA}}*{{Au}}}{2018}, for electron transport in gold down to 10 eV. An extension of Geant4 MicroElec has also been developed for microdosimetry and SEE simulations in various materials. He et al. developed a Monte Carlo code for low-energy incident

electron transport (down to 50 eV) in Al, Ti, Pt, and Au using both CSDA and track-structure strategies. Nevertheless, Monte Carlo codes that consider both LEE emission from gold surfaces and dosimetric accuracy within gold material remain lacking.

Accordingly, we have developed a refined Monte Carlo simulation code for sub-keV electron transport in nanoscale gold material. This study aims to simulate LEE emission from gold irradiated with sub-keV electrons, which will benefit future research on AuNPs in targeted radionuclide therapy. We demonstrate the simulation structure and discuss the physical mechanisms and refinements in detail. A truncation method for elastic cross sections was implemented by considering Mott theory and electron-acoustic phonon scattering theory. In the inelastic calculations, exchange effects, Born corrections, and relativistic effects were simultaneously considered. The initial energy of Fermi electrons in conduction band excitations was refined from the Fermi energy to values sampled from the joint density of states. The simulated SEE and calculated energy deposition were used to evaluate the reliability of the developed code for low-energy applications and the accuracy of LEE emission and dosimetry calculations for future studies.

2 Experimental

The present Monte Carlo code was developed for low-energy electron simulations in gold using the energy straggling strategy. A comprehensive description of this approach is provided by Tang et al. This method considers specific electron interactions and individual energy losses in each inelastic event, thereby improving the accuracy of secondary electron yield and energy distribution calculations.

The low-energy limit of the developed code was set to 0.5 eV above the Fermi level (5.53 eV) of gold. Bremsstrahlung was not considered, and the reasonable high-energy limit of the code is 100 keV. The basic simulation structure is illustrated in Fig. 1a [Figure 1: see original paper]. All formulae below are expressed in atomic units.

2.1 Elastic Scattering

Elastic scattering between incident electrons and the strong nuclear Coulomb field represents the primary cause of angular deflection in electron trajectories. Due to the large nuclear mass relative to electrons, energy transfer during elastic scattering is negligible. In this study, electron elastic total cross sections and differential cross sections were calculated based on Mott theory using the ELSEPA code developed by Salvat et al. The muffin-tin radius (1.44 Å) of gold was also considered for solid-state calculations. In the latest version of ELSEPA, this low-energy limit was extended down to 5 eV. The modification of elastic scattering was introduced through electron-acoustic phonon scattering.

Fig. 1a shows a schematic diagram of the simulation structure. Fig. 1b presents

phonon dispersion relations (longitudinal and transverse modes) for Au, where circles represent experimental data [Figure 1: see original paper]. Fig. 1c displays the new elastic mean free path (Mott-eph) interpolated from Mott cross sections and electron-phonon cross sections.

At very low energies, electrons tend to behave as Bloch waves rather than particles. Thus, they can interact with the collective movement of atoms in a solid—phonons. We applied the theory for electron-acoustic phonon scattering described by Fitting et al. and modified by Verduin and Theulings. The electron-acoustic phonon scattering rate is given by:

$$P_{ac}(E) = D(E), 2k_BTA{+}E4\pi(2N_{BZ}{+}1)m_D\epsilon_{ac}\hbar\omega_{BZ}\hbar\rho_m[\ln(A{+}EA{+}EE \geq E_{BZ}$$

where ϵ_{ac} is the acoustic deformation potential, k_B is the Boltzmann constant, T is temperature, c_s is sound velocity, ρ_m is mass density, and $A = 5E_{BZ}$ is the screening factor adopted by Bradford and Woolf. The variable E_{BZ} is the Brillouin zone energy given by $E_{BZ} = (\hbar k_{BZ})^2$, where the boundary wave vector is found at $k_{BZ} = 2\pi/a$ if the first Brillouin zone is assumed spherical. Here, a is the lattice constant, and $D(E)$ is the density of states (DOS), typically assumed to have a parabolic dispersion relation. In this case, $D(E)$ is expressed as:

$$D(E) = 3(E - E_{CB})$$

where m_D is the effective DOS mass and E_{CB} is the energy at the bottom of the conduction band (equal to 0 for metals). N_{BZ} is the acoustic phonon population $N(k,T)$ at the Brillouin zone boundary ($k = k_{BZ}$). The acoustic phonon population follows the Bose-Einstein distribution:

$$N(k,T) = \hbar\omega_{ac}(k)) - 1\exp($$

where ω_{BZ} is the acoustic phonon energy $\omega_{ac}(k)$ at the Brillouin-zone boundary. The acoustic phonon energy follows a dispersion relation modified to fit experimental data:

$$\omega_{ac}(k) = c_sk - \alpha k^2 - \beta k^3$$

where α and β are fitting parameters. There are three acoustic phonon modes: one longitudinal and two transverse. For the longitudinal mode, the parameters are $c_s = 3240$ m/s, $\alpha = 3.5 \times 10^{-8}$ m^2/s, and $\beta = 3.5 \times 10^{-18}$ m^3/s. For the transverse modes, the parameters are $c_s = 1200$ m/s, $\alpha = -7.6 \times 10^{-8}$ m^2/s, and $\beta = 5.3 \times 10^{-18}$ m^3/s. The fitted phonon dispersion relations are shown in Fig. 1b.

Subsequently, the inverse mean free path (MFP) or macroscopic cross section can be derived by dividing the scattering rate by electron velocity:

$$\lambda^{-1}(E) = A + E^{-1}(N_{BZ} + 8m_D c_s \hbar\omega_{BZ} k_B T A + EA + EE \geq E_{BZ}$$

where $\lambda_0 \pi \hbar^4 c_s 3\epsilon_{ac}^2 k_B T$. In the region $[E_{BZ}/4, E_{BZ}]$, the inverse MFP is interpolated between values at the upper limit of the top formula and the lower limit of the bottom formula. According to the angular differential scattering rate, the angular differential inverse MFP is:

$$\lambda^{-1}(E)1 - \cos\theta(N_{BZ} + 8m_D c_s \hbar\omega_{BZ} k_B T 1 - \cos\theta 1 - \cos\theta E \geq E_{BZ}$$

The angular distribution of electron-acoustic scattering can be obtained from this equation.

Both acoustic phonon emission and absorption occur in electron-acoustic scattering, though emission probability exceeds absorption probability. Therefore, the weighted average energy loss is primarily considered. Although the energy loss is only a few meV, it cannot be neglected in low-energy regions. The average energy loss E_{ac} during electron-acoustic phonon scattering can be approximated by:

$$E_{ac} = \hbar\omega_{ac}(k)k^2 dk[2N(k,T) + 1]k^2 dk$$

Finally, the acoustic deformation potential of the metal was derived from resistivity based on the Kieft and Bosch model:

$$\epsilon_{ac} = \sqrt{2\hbar e^2 c_s 3\pi m_e k_B T \rho_R \rho_m E_F}$$

where ρ_R is resistivity. Using the parameters above, the acoustic deformation potential of gold was found to be 4.86 eV for the longitudinal mode and 1.80 eV for the transverse mode.

As suggested by Fitting et al., electrons should behave as Bloch waves and interact with phonons at low energies ($<$ 100 eV); however, Mott cross sections become invalid because they produce unrealistically high scattering rates, yielding MFPs shorter than interatomic distances. Therefore, we modified the elastic scattering treatment as follows: Mott cross sections were applied for energies above 100 eV, electron-acoustic phonon cross sections for energies below 50 eV, and interpolation between these regimes. The resulting new elastic MFP is shown in Fig. 1c. While these elastic scattering models may be insufficient for describing the structure of small AuNPs, more accurate atomic potentials for Mott theory will be obtained in future work using advanced techniques such as ab initio and density functional theory (DFT).

2.2 Inelastic Scattering

This study primarily considers electron-electron inelastic scattering. Inelastic cross sections were computed using dielectric theory, which centers on the complex dielectric function $\varepsilon(q,\omega)$, where q is momentum transfer and ω is energy loss. The imaginary part of the inverse dielectric function is the energy loss function (ELF) $\mathrm{Im}[1/\varepsilon(q,\omega)]$, which provides detailed energy loss information for material electrons. From experimental optical data or ab initio and DFT calculations, the dielectric function and ELF can only be obtained at the optical limit ($q \to 0$), known as the optical dielectric function and optical ELF.

To extend the ELF from the optical limit to $q > 0$, we used the extended Drude model and Mermin model. Both models fit the optical ELF using a sum of Drude-type ELFs:

$$\mathrm{Im}\left[\frac{1}{\varepsilon_D(0,\omega)}\right] = \mathrm{Im}\left[\frac{1}{\varepsilon_M(0,\omega)}\right] = \sum A_i \frac{\gamma_i \omega}{(\omega^2 - \omega_{p,i}^2)^2 + \gamma_i^2 \omega^2}$$

where $A_i = a_i \omega_{p,i}^2$ is oscillator intensity, γ_i is damping constant, and $\omega_{p,i}$ is plasma frequency.

The fitting model was built based on several previous studies. In developing Geant4 MicroElec, Valentin and Gibaru et al. used Heaviside step functions to truncate each oscillator in the fitting. Pablo et al. employed an exponential smooth switching function instead of a simple step function for outer-shell electrons. Based on these methodologies, our fitting model is:

$$\mathrm{Im}\left[\frac{1}{\varepsilon(0,\omega)}\right] = \sum F(\omega) A_i \frac{\gamma_i \omega}{(\omega^2 - \omega_{p,i}^2)^2 + \gamma_i^2 \omega^2}$$

For outer-shell electrons, $F(\omega)$ represents a smooth exponential switching function:

$$F(\omega) = 1 + e^{-\Delta_i(\omega - \omega_{th,i})}$$

where Δ_i and $\omega_{th,i}$ are additional fitting parameters. For inner shells (K and L shells) with sharp edges in the optical ELF, $F(\omega)$ is a simple step function $\Theta(\omega - \omega_{th,i})$. For plasmons and conduction band electrons, $F(\omega)$ can be set to 1.

Fig. 2 [Figure 2: see original paper] compares the fitted ELF (solid lines) with experimental ELF (circles), showing contributions from each electronic shell.

The experimental optical ELF, covering electron energies from 0.005 eV to 1 MeV, was derived from databases of Palik, Windt, and EPDL97, with high-energy optical ELF calculated using photoionization cross sections:

$$\mathrm{Im}\left[\frac{1}{\varepsilon(0,\omega)}\right] = \frac{n_m c\sigma_{phot}}{2\pi e^2}$$

where n_m is atomic density, c is speed of light, and σ_{phot} is photoionization cross section.

The fitting results were validated using two sum rules (f-sum and ps-sum) and the mean ionization potential. A partial f-sum rule for fitted oscillators distinguished contributions to electronic shells. We used 28 oscillators to describe the optical ELF, achieving good agreement with experimental data as shown in Fig. 2.

During fitting, the plasmon peak was set at 25.42 eV, near the 24.8 eV value in Egerton's book. The f-sum rule verification yielded $Z_{eff} = 78.05$ (ideal: 79.0), while the ps-sum rule gave 1.0908 (ideal: 1.0). The mean ionization potential from the fitted ELF was 736.45 eV. These values agree well with experimental ELF, with only small deviations in high-energy regions (L and K shells), likely due to Drude function limitations. Better experimental ELF data would improve fitting accuracy. Partial f-sum rule results are also shown in Fig. 2, enabling calculation of inelastic mean free paths (IMFPs) for different shells.

IMFP calculation requires extrapolating momentum loss q from the optical limit to $q > 0$. For the extended Drude model, extrapolation used dispersion relations:

$$\mathrm{Im}\left[\frac{1}{\varepsilon_D(q,\omega)}\right] = \sum A_i \frac{\gamma_i(q)\omega}{(\omega^2 - \omega_{p,i}^2(q))^2 + \gamma_i^2(q)\omega^2}$$

Here, $\omega_{p,i}(q)$ describes plasmon dispersion and $\gamma_i(q)$ is the q-dependent damping constant representing broadening effects. While γ_i is typically constant, alternative dispersion relations include: (1) $\omega_{p,i}(q) = \omega_{p,i} + \gamma_i$; (2) $\omega_{p,i}(q) = \sqrt{\omega_{p,i}^2 + \alpha q^2}$; or (3) $\omega_{p,i}(q) = \sqrt{\omega_{p,i}^2 + \beta q^2}$ and $\gamma_i(q) = \sqrt{\gamma_i^2 + \delta q^2}$. The third method, presented by Ritchie et al. and proven more comprehensive, was chosen for conduction band and outer shells, while the first method was used for inner shells. This constitutes our first inelastic model, labeled "Ritchie."

For the Mermin model, extrapolation uses the Mermin dielectric function:

$$\varepsilon_M(q,\omega) = 1 + \frac{(\varepsilon_L(q,\omega+i\gamma)-1)(\varepsilon_L(q,0)-1)}{\varepsilon_L(q,\omega+i\gamma)-\varepsilon_L(q,0)}$$

where ε_L is the Lindhard dielectric function and $\varepsilon_L(q,0)$ is its static limit. This second inelastic model is labeled "Mermin."

A significant advantage of both models is that fitted oscillators can approximate contributions to specific electronic shells or plasmons. Combined with shell-divided ELF, this enables calculation of IMFPs for different electronic shells.

The general IMFP calculation including relativistic high-energy corrections is:

$$\lambda_{inel}^{-1}(E) = \int d\omega \int_{q_-}^{q_+} f_{ex}(q,E)F(\omega)\mathrm{Im}\left[\frac{1}{\varepsilon(q,\omega)}\right]\frac{2\pi e^2}{\omega}dq$$

where E is incident electron kinetic energy, c is speed of light, W_+ is maximum energy loss, W_- is minimum energy loss, and q_+ and q_- are maximum and minimum momentum transfers. The momentum transfer limits are:

$$q_\pm = \sqrt{E(2+E/c^2)} \pm \sqrt{(E-\omega)(2+(E-\omega)/c^2)}$$

The Ochkur exchange correction is $f_{ex}(q,E) = 1 - q^2/(2E)$. For collective excitations, $f_{ex} = 1$. As noted, $F(\omega)$ is either an exponential switching function or simple step function.

Inelastic cross sections for each shell were calculated individually. For metals like Au, W_- equals zero. As proposed by Pablo et al., maximum energy loss W_+ depends on electronic shell: for plasmons and 5d electrons (collective excitations), $W_+ = E - E_F$; for outer- and inner-shell electrons, $W_+ = \min[E - E_F, (E + B_i)/2]$, where B_i is binding energy of the i-th shell. Binding energies were derived from the FFAST database. A classical Coulomb-field Born correction accounting for potential energy gained by incident electrons was added for outer- and inner-shell electrons by replacing kinetic energy E with $E' = E + 2B_i$ while keeping energy loss unchanged.

Fig. 3 [Figure 3: see original paper] compares calculated IMFP with experimental and theoretical data. Fig. 3a shows good agreement with experimental and previous theoretical results, with clear relativistic effects at high energies. Below 100 eV, the modified Ritchie model produces accurate IMFP similar to the Mermin model due to improved plasmon lifetime estimation by treating γ as a function of q. Fig. 3b compares inner-shell ionization cross sections with relativistic Gryzinski theory. The Ritchie model yields better inner-shell ionization data than the Mermin model, making it recommended for high-energy simulations. This is likely because plasmonic considerations in the Mermin model become invalid for inner shells, whereas simple q extrapolation in the Ritchie model remains applicable. Both models produce lower inner-shell cross sections than Gryzinski theory, possibly due to insufficient ELF accuracy for inner shells.

Following inelastic events, secondary electrons are normally generated with energy $E_S = W + E_F$ for Fermi electron excitation (conduction band and plasmon excitation) and $E_S = W - B_i$ for inner- and outer-shell ionization, where W is energy loss. We applied the improvement by Ding et al., which assumes the initial energy E' of the Fermi electron is proportional to the joint density of states (JDOS) of the free-electron gas: $P(E', W) \propto \sqrt{E'(E'+W)}$, where $E' < E_F$ and $E' + W > E_F$. Thus, the modified secondary electron energy is $E_S = W + E'$.

2.3 Surface Potential

For electron emission from metal surfaces, electrons must have kinetic energy exceeding both the Fermi level E_F and work function W_F (the potential barrier between metal surface and vacuum). Therefore, the simulation cut-off energy is set to $E_F + W_F$, and electrons below this limit are locally terminated, which also saves computational memory.

For surface escape, when an electron reaches the gold surface, its kinetic energy must satisfy:

$$E\cos^2\theta > U$$

where E is energy relative to the Fermi level, θ is the angle between electron trajectory and surface normal before emission, and $U = W_F$ is the potential barrier above the Fermi level. According to quantum theory, emission probability depends on the transmission coefficient T:

$$T = \frac{4\sqrt{1 - U/(E\cos^2\theta)}}{[1 + \sqrt{1 - U/(E\cos^2\theta)}]^2}$$

A random number R is generated and compared with T to determine emission: if $R < T$, emission occurs. Emitted electrons have kinetic energy $E - U$, while electrons entering the solid gain potential energy W_F above the Fermi level. In SEE simulations, the work function between gold surface and vacuum was set to 5.1 eV. For future development of water-gold interfaces, we will use the difference between work functions of the two materials and assume similar transmission coefficient calculations as for the surface-vacuum interface.

3 Results and Discussion

3.1.1 Secondary Electron Yield

To validate the code, we simulated SEE experiments and calculated the secondary electron yield (SEY) and backscattering coefficient (BSC) of gold. The simulation setup consisted of multiple groups of monoenergetic electron beams vertically bombarding an infinite gold plane, with emitted electron information collected at the surface. SEY is defined as the ratio of emitted secondary electrons (< 50 eV) to incident primary electrons, while BSC is the ratio of backscattered electrons (> 50 eV) to incident primary electrons. To obtain SEY and BSC, 1×10^6 particles were simulated, yielding an uncertainty of less than 1%. Fig. 4 [Figure 4: see original paper] presents calculated SEY and BSC compared with experimental data from Joy et al.

Experimental data were obtained using monoenergetic electron beams bombarding materials under vacuum conditions, similar to our simulation setup. Fig. 4a

shows that simulated SEY values agree well with experimental data, which is essential for calculating LEE emission from AuNPs. The Ritchie model produced larger SEY than the Mermin model, while BSC values were similar between models.

Fig. 4b demonstrates that without low-energy elastic scattering modifications, SEY values differ primarily below 1 keV. Calculations using only Mott cross sections overestimate SEY for primary electrons with energies < 400 eV compared to experimental values. The modified elastic cross sections significantly improve SEE description. The high SEY suggests that electrons emitted from ^{125}I can enhance LEE emission from gold nanoparticles.

3.1.2 Secondary Electron Spectra

Secondary electron spectra are critical for analyzing LEEs emitted from AuNPs because DNA damage cross sections (for DSBs and SSBs) are highly energy-dependent. To obtain stable spectra, 1×10^7 electrons were simulated, with results shown in Fig. 5 [Figure 5: see original paper]. The spectra demonstrate that most emitted secondary electrons have energies below 30 eV, with a zero-loss elastic peak also observed.

The LEE peak occurs at 2.25–3.25 eV, similar to the 2.2 eV peak reported in ion-bombardment SEE experiments. This substantial LEE emission supports the feasibility of using sub-keV electrons combined with AuNPs as a high-flux LEE source.

3.2 Dosimetry Test

Dosimetry testing is critical for evaluating microdosimetric capabilities. The stopping power $S(E)$ for electrons of energy E can be calculated similarly to IMFP:

$$S(E) = \int \omega d\omega \int_{q_-}^{q_+} f_{ex}(q, E) F(\omega) \mathrm{Im}\left[\frac{1}{\varepsilon(q, \omega)}\right] \frac{2\pi e^2}{\omega} dq$$

Fig. 6 [Figure 6: see original paper] compares calculated stopping power with other theoretical calculations and experiments. Relativistic corrections are evident at high energies, showing good agreement with ESTAR and EEDL databases. With modifications, the Ritchie model produces accurate stopping power comparable to the Mermin model at low energies.

Energy deposition was tested using a semi-infinite gold model. Calculating energy deposition depth profiles provides information about energy distribution and uniformity in gold, verifying dosimetric correctness for future studies. Electron energy deposition as a function of depth in semi-infinite gold was calculated using both our developed code and Geant4 standard electromagnetic physics (option 4). Simulations were performed for 200 eV, 500 eV, 1 keV, 2 keV, and

10 keV electrons, with 5×10^6 electrons per test. Results are shown in Fig. 7 [Figure 7: see original paper].

Both inelastic models show similar trends. Fig. 7a demonstrates that our code's total energy deposition is approximately 89%–93% of Geant4's results, with the slight decrease due to greater secondary electron emission from the surface. Fig. 7b shows differences in energy deposition depth profiles. At low energies, our inelastic cross sections differ from the Livermore model (EEDL). Gibaru et al. suggested that Geant4 standard physics underestimates electron range, which is also observed in our comparisons. At high energies, depth profiles from both codes converge. Note that our detailed energy-straggling strategy is significantly slower than Geant4's multiple scattering approach.

A function for calculating energy deposition in 3D voxels was implemented for future microdosimetry studies. The method is demonstrated in Fig. 8 [Figure 8: see original paper], with voxel length set to 1 Å and maximum axis length of 1000 Å, using 1×10^7 electrons.

Fig. 8 shows the spatial distribution of energy deposition, demonstrating good symmetry that verifies particle transport in the Monte Carlo procedure. Energy deposition intensity in the X-Z plane is more comprehensive than depth profiles. At low energies, the X-Z plane projection forms an ellipse around the electron beam entry point, becoming more cylindrical at higher incident energies. The distribution demonstrates nanoscale precision, enabling visualization and analysis of electron energy deposition inside AuNPs under electron irradiation.

4 Conclusion

A Monte Carlo code was developed to simulate nanoscale electron transport in gold down to 0.5 eV above the Fermi level. Mott elastic scattering cross sections were calculated using ELSEPA. Electron-acoustic phonon cross sections were derived from fitted dispersion relations. Elastic cross sections were modified using a truncation method: Mott cross sections above 100 eV, electron-phonon cross sections at 0–50 eV, and interpolation between these regimes. Optical ELF data were fitted to 28 Drude oscillators categorized by electronic shell for cross section calculations using dielectric theory. Two inelastic models (Ritchie and Mermin) were employed. Exchange effects, Born corrections, and relativistic effects were carefully considered. The initial energy of Fermi electrons in conduction band excitations was refined from Fermi energy to values sampled from JDOS.

Simulated SEE results agree reasonably with experiments, with the quantum surface potential model playing an important role. Secondary electron spectra demonstrate high LEE yield from gold surfaces under keV electron irradiation, making this code significant for micro- and nanodosimetry studies. Inelastic stopping power and energy deposition depth profiles were validated. A 3D voxel function was implemented for future applications.

This code is planned for evaluating LEE emission in ^{125}I/AuNP systems and

shows significant potential for future microdosimetry studies. Planned improvements include considering small AuNP structures, implementing surface plasmon modes for specific AuNPs, adding more materials, and employing advanced geometry intersection algorithms.

Author Contributions

All authors contributed to study conception and design. Material preparation, data collection, and analysis were performed by Liheng Zhou, Shuiyan Cao, Tao Sun, Yunlong Wang, and Jun Ma. The first draft was written by Liheng Zhou, and all authors commented on previous versions. All authors read and approved the final manuscript.

Data Availability

The data supporting this study are openly available in Science Data Bank at https://www.doi.org/10.57760/sciencedb.j00186.00062 and http://resolve.pid21.cn/31253.11.sciencedb.j00186.

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