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METHODS OF MONTE CARLO ELECTRON TRANSPORT
IN PARTICLE-IN-CELL CODES

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An algorithm has been implemented in CCUBE and ISIS to treat electron transport in materials using a Monte Carlo method in addition to the electron dynamics determined by the self-consistent electromagnetic, relativistic, particle-in-cell simulation codes that have been used extensively to model generation of electron beams and intense microwave production. Incorporation of a Monte Carlo method to model the transport of electrons in materials (conductors and dielectrics) in a particle-in-cell code represents a giant step toward realistic simulation of the physics of charged-particle beams. The basic Monte Carlo method used in the implementation includes both scattering of electrons by background atoms and energy degradation. Two methods were used to model the elastic scatterings. One is the theory due to Goudsmit and Saunderson and the other is given by Moliere, Hanson, and Bethe. In applying the former method, small angle scatterings were represented by Gaussian distributions with appropriate widths for the individual electrons and large angle scatterings were treated by the screened Coulomb distribution. In using the latter method, all scatterings were treated as small angle events; and, therefore, only the Gaussian term of the distribution was included. For energy degradation, it is assumed that the electrons are subjected to a slowing down force throughout their transport and that the force acts in a direction opposite to the electron's momentum. The energy loss is computed by using Bethe's formula, which treats the energy loss of incoming electrons in matter due to excitation and ionization of bound electrons in the stopping substance. Tests of the codes yielded electron transmission probability and its energy range relation, which agreed very well with empirical results. Furthermore, our results showed that space-charge effects could significantly affect the physics of electron transport. Further inclusion of photonic transport can lead to a new generation of numerical simulation tools.

METHODS OF MONTE CARLO ELECTRON TRANSPORT IN PARTICLE-IN-CELL CODES

INTRODUCTION

Particle-in-cell simulation techniques and Monte Carlo transport methods are well established numerical tools in the study of the evolution of a system of charged particles. However, the emphases of the two type of numerical codes are very different. Particle-in-cell simulation codes which have been extensively applied in plasma physics deal with the phenomena of collisionless plasmas where the self-consistent electromagnetic fields are very crucial. On the other hand, Monte Carlo codes which are often used to determine the transport characteristics of charged particles by modeling the scattering processes in various materials but neglecting the self-consistent fields. Consequently, these two types of codes are only applicable in different regimes where certain physical processes can be ignored. However, there are numerous physical phenomena which require the physics of atomic scatterings and self-consistent electromagnetic fields. The propagation of intense charged particle beams and the generation of microwaves by relativistic electron beams are just two examples from the current research topics of charged particle beam physics.

PARTICLE-IN-CELL SIMULATION

In a particle-in-cell simulation, a system of charged particles such as a plasma, is modeled by a large number of computational particles which move in a spatial grid according to the self-consistent electromagnetic forces and any applied external electromagnetic fields. The trajectories of the computational particles are calculated on a microscopic level by making use of Maxwell's equations subjected to appropriate boundary conditions and the Lorentz force equation in a self-consistent manner. The microscopic representation of the plasma can accurately (within the limit of numerical algorithm) yield the desired macroscopic quantities which characterize the space and time evolution of the system. Due to limitation of computer time and memory, the number of computational particles in a simulation plasma is far less than in a real plasma, and space and time are necessarily treated as discrete rather than continuous. The use of a finite time step and grid spacing puts an upper limit on the frequency and a lower limit on the wavelength that the particle simulation model can accurately describe. The maximum frequency is limited according to $\omega_{\max} \Delta t \leq 0.5$, whereas the shortest wavelength is on the order of several grid spacings. In addition, discretization of space and time can lead to problems of accuracy and stability of simulation codes, which must be carefully dealt with.

In recent years, the application of particle-in-cell codes to the physics of charged particle beam has been very widespread. PIC codes such as CCUBE¹ and ISIS² were developed for this purpose. In the generation and transport of high current charged particle beams, the dynamics is dominated by the self-consistent fields. However, in order to obtain an accurate description of the beam quality which is often important in the applications of charged particle beams, atomic scatterings suffered by the electrons as they go through the anode foil must be included in the simulation. Incorporation of a Monte Carlo method to model the transport of electrons in materials (conductors and insulators) in a particle-in-cell code represents an important step toward realistic simulation of the physics of charged particle beams.

THE MONTE CARLO METHOD IN PIC CODES

The basic Monte Carlo method used to treat electron transport includes scatterings and energy degradation by background atoms. Velocity scattering of ions is a negligible effect and, therefore, only energy degradation is included. A continuous slowing-down force is assumed to act in a direction opposite to the electron's momentum. Thus, the equation of motion is given by

$$\frac{d\vec{p}}{dt} = -e \left[\vec{E} + \frac{\vec{p} \times \vec{B}}{\gamma c} \right] - A(\gamma) \frac{\vec{p}}{p} \quad (1)$$

where $A(\gamma)$ depends on the energy of the electron and the atomic number of the material. The energy loss is computed by an approximation to Bethe's formula³ which treats the energy loss of incoming electrons in matter due to excitation and ionization of bound electrons in the stopping substance. The mean change of energy $d\epsilon$ per track length ds is

$$-\frac{1}{mc^2} \frac{d\epsilon}{ds} = 2\pi N Z r_o^2 \frac{\gamma^2}{p^2} \psi \quad (2)$$

Here N is the density of the matter of atomic number Z , $r_o = e^2/mc^2$ is the classical radius of the electron, and

$$\psi = \ln [(mc^2)^2 (\gamma-1) p^2 / 2I^2] - (2/\gamma - 1/\gamma^2) \ln 2 + 1/\gamma^2 + (1-1/\gamma)^2 / 8 \quad (3)$$

In Eq. (3), I is the mean excitation potential. For aluminum, $I = 150$ eV. One can simplify the calculation by approximating Eq.3 to be

$$\psi = 2 \ln (mc^2/I) + 3.42 \ln(p) - 1.71 \quad (4)$$

Substituting the value of I for aluminum, one has

$$\psi = 14.57 + 3.42 \ln(p) \quad (5)$$

This approximation is accurate to 1% for electron energies between 25 KeV and 5 MeV⁴.

Two methods were used to model the elastic scatterings between the electrons and the atoms. One is the theory due to Goudsmit and Saunderson and the other is given by Moliere, Hanson, and Bethe. In applying the former method, small angle scatterings were represented by Gaussian distributions with appropriate widths for the individual electrons and large angle scatterings were treated by the screened Coulomb distribution. In using the latter method, all scatterings were treated as small angle events; and, therefore, only the Gaussian term of the distribution was included. However, we found that the latter method provided satisfactory results in almost all the cases studied and we can readily vectorize the algorithm resulting in a significant increase in computational speed.

The scattering of an electron is carried out in a reference frame in which the z axis is colinear with the electron velocity. The scattering can then be specified by two angle variables, the polar angle θ and the azimuthal angle ϕ . The polar angle θ is determined by the scattering theory and the angle ϕ is chosen randomly with a uniform distribution between 0 and 2π . The velocity components of the electron in the lab frame are then obtained through the construction of a rotation matrix.

The calculations of scattering and energy degradation can be subcycled during every time step in the ISIS calculation. The number of Monte Carlo subcycles depends on the ratio of the range of the electron to the distance it is expected to travel during one time step. We have found that a few Monte Carlo subcycles per time step, in general, are sufficient to model the physical process accurately.

We have tested the Monte Carlo implementation by modeling the transport of monoenergetic electron beams in aluminum. The aluminum is treated as having infinite conductivity and, therefore, the electron beam is current and charge neutral. A monoenergetic beam was injected from the left boundary of a cylindrical block of aluminum with a radius of 11.43 cm. The electron beam had a radius of 1.0 cm. Figure 1 shows the electron transmission probability curves through aluminum as obtained from simulations with electron beams of various kinetic energies. From the transmission probability curves, one can obtain the extrapolated electron range by extending the linear portion of the curve to intercept the range axis. Figure 2 shows the extrapolated range of electrons impinging on aluminum as a function of the kinetic energy of the electron beam. The circles represent numerical results obtained from our calculations and the solid curve is the empirical relationship developed by Katz and Penfold⁵:

$$R_0(\text{cm}) = 0.1963E(\text{MeV}) - 0.0393, \quad (6)$$

where the kinetic energy of the electron, E , is greater than 0.6 MeV. It is evident that our numerical results agree well with the empirical curve.

Electron transmission through various materials have also been studied using ISIS and the results are compared with those obtained by CYLTRAN,⁶ a cylindrically symmetric two dimensional electron-photon transport code. The transmission probability curves of 2.0 MeV electrons through silver, aluminum, carbon, and beryllium are shown in Fig. 3. The comparison between the two codes shows a maximum deviation of less than 10% in light elements

and the agreement becomes very good in heavier elements. This is probably due to the fact that our algorithm only takes into account energy loss due to excitation and ionization. In any case, the overall agreement is quite good.

The space charge effect on the energy-range relation was investigated by simulations of electron beams of progressively higher density. Figure 4 shows the electron transmission probability curves of a 2.0 MeV electron beam impinging on a dielectric material with the same density and atomic number as aluminum. The current of the electron beams used in the five cases ranged from 1.0 ampere to 75,000 amperes. The space charge effect was shown to be significant at currents greater than 10 kA. The extrapolated range was shortened as the density of the electron beam increased. However, the curves for higher density beams had longer tails. This is due to the fact that the space charge effect diminished when the current was depleted below 10 kA. Further increase in the beam current results in virtual cathode formation which is a highly nonlinear phenomenon due to space charge effect. In a regime where space charge effect and Monte Carlo transport are equally important, the particle-in-cell Monte Carlo method is the only appropriate approach to the physical problems.

CONCLUSIONS

We have extended the application of Monte Carlo methods to include transport of charged particles in materials in addition to the dynamics determined by the self-consistent electromagnetic fields in particle-in-cell codes. This type of Monte Carlo-PIC codes would be extremely useful in the simulation of intense charged particle beams. Further inclusion of photon transport is being developed. In the treatment of photon transport, a thick target model⁷ can be used to calculate the bremsstrahlung cross section of electrons along their paths in a time step. Photons with the appropriate energy spectrum are created at the positions of the electrons. Subsequent Compton and photoelectric effects are included by considering the appropriate cross sections and, thereby, secondary electrons are appropriately created. Successful development of this can lead to a new generation of numerical codes.

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Figure 1. Transmission probability curves of monoenergetic electron beams in aluminum.

Figure 2. Range calculation for monoenergetic electrons with different initial energies in aluminum. The circles are the results obtained from the PIC simulations with the Monte Carlo model. The solid curve is the empirical curve given by Katz and Penfold.

Figure 3. Comparison of 2.0 MeV electron transmission probability in silver, aluminum, carbon, and beryllium between ISIS and CYLTRAN.

Figure 4. Transmission probability curves of 2.0 MeV electron beams in aluminum-like dielectric with increasing current (1.0 A, 10.0 kA, 50 kA, and 75 kA) show the range shortening due to space charge effects.