

Monte Carlo Modeling For Electron Microscopy And Microanalysis Oxford Series In Optical And Imaging Sciences

The implicit SNB (iSNB) non-local multigroup thermal electron conduction method of Schurtz et. al. [Phys. Plasmas 7, 4238 (2000)] and Cao et. al. [Phys. Plasmas 22, 082308 (2015)] is adapted into an electron thermal transport Monte Carlo (ETTMC) transport method to better model higher order angular and long mean free path non-local effects. The ETTMC model is used to simulate the electron thermal transport within inertial confinement fusion (ICF) type problems. The new model aims to improve upon the currently used iSNB, in particular by using finite particle ranges in comparison to the exponential solution of a diffusion method and by improved higher order angular modeling. The new method has been implemented in the 1D LILAC and 2D DRACO multiphysics production codes developed by the University of Rochester Laboratory for Laser Energetics. The ETTMC model is compared to iSNB for several direct drive ICF type simulations: Omega shot 60303 a shock timing experiment, Omega shot 59529 a shock

timing experiment, Omega shot 68951 a cryogenic target implosion and a NIF polar direct drive phase plate design. Overall, the ETTMC method performs at least as well as the iSNB method and predicts lower preheating ahead of the shock fronts. This research was supported by University of Rochester Laboratory for Laser Energetics, Sandia National Laboratories and the University of Wisconsin-Madison Foundation.

This work establishes a framework for Monte Carlo simulations of complex, modulated electron fields produced by Varian's TrueBeam medical linear accelerator for investigations into modulated electron radiation therapy (MERT) and combined modulated photon and electron radiation therapy (MPERT). Both MERT and MPERT have shown potential for reduced low dose to normal tissue without compromising target coverage in the external beam radiation therapy of some breast, chest wall, head and neck, and scalp cancers. This reduction in low dose could translate into the reduction of immediate radiation side effects as well as long term morbidities and incidence of secondary cancers. Monte Carlo dose calculations are widely accepted as the gold standard for complex radiation therapy dose modelling, and are used almost exclusively for modelling the complex electron fields involved in MERT and MPERT. The introduction of Varian's newest linear accelerator,

the TrueBeam, necessitated the development of new Monte Carlo models in order to further research into the potential role of MERT and MPERT in radiation therapy. This was complicated by the fact that the field independent internal schematics of TrueBeam were kept proprietary, unlike in previous generations of Varian accelerators. Two approaches are presented for performing Monte Carlo simulations of complex electron fields produced by TrueBeam. In the first approach, the dosimetric characteristics of electron fields produced by the TrueBeam were first compared with those produced by an older Varian accelerator, the Clinac 21EX. Differences in depth and profile characteristics of fields produced by the TrueBeam and those produced by the Clinac 21EX were found to be within 3%/3 mm. Given this information, complete accelerator models of the Clinac 21EX, based on its known internal geometry, were then successfully modified in order to simulate 12 and 20 MeV electron fields produced by the TrueBeam to within 2%/2 mm of measured depth and profile curves and to within 3.7% of measured relative output. While the 6 MeV TrueBeam model agreed with measured depth and profile data to within 3%/3 mm, the modified Clinac 21EX model was unable to reproduce trends in relative output as a function of fieldsize with acceptable accuracy. The second approach to modelling TrueBeam electron

fields used phase-space source files provided by Varian that were scored below the field-independent portions of the accelerator head geometry. These phase-spaces were first validated for use in MERT and MPERT applications, in which simulations using the phase-space source files were shown to model depth dose curves that agreed with measurement within 2%/2 mm and profile curves that agreed with measurement within 3%/3 mm. Simulated changes in output as a function of field size fell within 2.7%, for the most part. In order to inform the positioning of jaws in MLC-shaped electron field delivery, the change in output as a function of jaw position for fixed MLC-apertures was investigated using the phase-space source files. In order to achieve maximum output and minimize treatment time, a jaw setting between 5 and 10 cm beyond the MLC-field setting is recommended at 6 MeV, while 5 cm or closer is recommended for 12 and 20 MeV with the caveat that output is most sensitive to jaw position when the jaws are very close to the MLC-field periphery. Additionally, output was found to be highly sensitive to jaw model. A change in divergence of the jaw faces from a point on the source plane to a $3 \times 3 \text{ mm}^2$ square in the source plane changed the shape of the output curve dramatically. Finally, electron backscatter from the jaws into the monitor ionization chamber of the TrueBeam was measured

and simulated to enable accurate absolute dose calculations. Two approaches were presented for measuring backscatter into the monitor ionization chamber without specialized electronics by turning off the dose and pulse forming network servos. Next, a technique was applied for simulating backscatter factors for the TrueBeam phase-space source models without the exact specifications of the monitor ionization chamber. By using measured backscatter factors, the forward dose component in a virtual chamber was determined and then used to calculate backscatter factors for arbitrary fields to within 0.21%. Backscatter from the jaws was found to contribute up to 2.6% of the overall monitor chamber signal. The measurement techniques employed were not sensitive enough to quantify backscatter from the MLC, however, Monte Carlo simulations predicted this contribution to be 0.3%, at most, verifying that this component can be neglected.

Monte-Carlo Simulation of Electron Transport in III-V semiconductor Heterostructures

The Macro Response Monte Carlo Method for Electron Transport

Monte Carlo Simulation of Electron-induced Air Fluorescence Utilizing Mobile Agents

A model and computer code for the Monte Carlo simulation of relativistic electron and positron penetration through matter

*Measurement and Monte Carlo Simulation of
Electron Fields for Modulated Electron Radiation
Therapy*

A 3D model of a low voltage electron beam has been constructed using the ITS/ACCEPT Monte Carlo code in order to validate the code for this application and improve upon 1D slab geometry simulations. A line source description update to the code allows complete simulation of a low voltage electron beam with any filament length. Faithful reproduction of the geometric elements involved, especially the window support structure, can account for 90--95% of the dose received by routine dosimetry. With a 3D model, dose distributions in non-web articles can be determined and the effects of equipment modifications can be anticipated in advance.

For ten days at the end of September, 1987, a group of about 75 scientists from 21 different countries gathered in a restored monastery on a 750 meter high piece of rock jutting out of the Mediterranean Sea to discuss the simulation of the transport of electrons and photons using Monte Carlo techniques. When we first had the idea for this meeting, Ralph Nelson, who had organized a previous course at the "Ettore Majorana" Centre for Scientific Culture, suggested that Erice would be the ideal place for such a meeting. Nahum, Nelson and Rogers became Co-Directors of the Course, with the help of Alessandro Rindi, the Director of the School of Radiation Damage and Protection, and Professor Antonino Zichichi, Director of the "Ettore Majorana" Centre. The course was an

outstanding success, both scientifically and socially, and those at the meeting will carry the marks of having attended, both intellectually and on a personal level where many friendships were made. The scientific content of the course was at a very high caliber, both because of the hard work done by all the lecturers in preparing their lectures (e. g. , complete copies of each lecture were available at the beginning of the course) and because of the high quality of the "students", many of whom were accomplished experts in the field. The outstanding facilities of the Centre contributed greatly to the success. This volume contains the formal record of the course lectures.

Experimental Validation and Evaluation of Uncertainty in the Monte Carlo Modeling of Electron Irradiation of Complex Objects

PENELOPE, an Algorithm and Computer Code for Monte Carlo Simulation of Electron-photon Showers

Full Band and Beyond

Monte Carlo Modeling of Non-local Electron Conduction in High Energy Density Plasmas

Monte Carlo Simulation of the Electron-solid Interaction with Emphasis on Scanning Electron Microscopy

We present an ensemble Monte Carlo simulation of electron transport in bulk ZnS at high electric fields. Scattering mechanisms associated with polar optical phonons, acoustic phonons (through deformation potential coupling), intervalley scattering, and impurities (neutral and ionized) are included in a nonparabolic multi-valley model. The

simulated results show that energetic electrons are available for impact excitation at fields exceeding 1 MV/cm, and that transient effects are negligible in explaining measured efficiencies in ACTFEL devices ... ACTFEL, Electroluminescence, Monte Carlo, High-Field Transport, ZnS.

Monte Carlo method is an invaluable tool in the field of radiation protection, used to calculate shielding effectiveness, as well as dose for medical applications. With few exceptions, most of the objects currently simulated have been homogeneous materials that vary in density by a factor of 3 or less. In the irradiation of very heterogeneous objects, particularly layered or leafy food items, one will encounter air pockets within the bundle as a matter of course. These pockets will cause variations in density of up to three orders of magnitude. Air pockets in a tissue equivalent phantom were found to produce "hot spots" in the dose distribution and introduced significant deviations between the calculated and measured distribution of dose to the phantom. To date, very little published work had been done in the area of Monte-Carlo simulation of objects of such disparate densities. Before Monte Carlo methods can be used successfully in this regime, further code development and experimental validation will be necessary, of which this work is just a beginning. Phantoms were made of corrugated low-Z material similar in electron density to plant based material. These phantoms incorporated air gaps of comparable size to those found in the leafy objects of interest. Dimensions were chosen to bracket electron ranges in the material of the objects modeled. Monte Carlo analysis will provide a reasonable qualitative picture of the dose distribution, but

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such a picture is not yet sufficiently accurate in a quantitative sense. Air gaps within the plant material produced large discrepancies between calculation and measurement. Smaller air gaps were observed to produce greater discrepancy between calculation and measurement.

Response Matrix Monte Carlo Based on a General Geometric Local Calculation for Electron Transport

Raytracing Monte Carlo Method for Calculating Secondary Electron Emission and Sputtering Effects on Micro-Architected Structures

Monte Carlo Modeling for Electron Microscopy and Microanalysis

THE RESPONSE HISTORY MONTE CARLO METHOD FOR ELECTRON TRANSPORT (MONTE CARLO METHOD).

Penelope

A Response Matrix Monte Carlo (RMMC) method has been developed for solving electron transport problems.

This method was born of the need to have a reliable, computationally efficient transport method for low energy electrons (below a few hundred keV) in all materials.

Today, condensed history methods are used which reduce the computation time by modeling the combined effect of many collisions but fail at low energy because of the assumptions required to characterize the electron scattering.

Analog Monte Carlo simulations are prohibitively expensive since electrons undergo coulombic scattering with little state change after a collision. The RMMC method attempts to combine the accuracy of an analog Monte Carlo simulation with the speed of the condensed history methods. The combined effect of many

collisions is modeled, like condensed history, except it is precalculated via an analog Monte Carlo simulation. This avoids the scattering kernel assumptions associated with condensed history methods. Results show good agreement between the RMMC method and analog Monte Carlo. 11 refs., 7 figs., 1 tabs.

This book describes for the first time how Monte Carlo modeling methods can be applied to electron microscopy and microanalysis. Computer programs for two basic types of Monte Carlo simulation are developed from physical models of the electron scattering process--a single scattering program capable of high accuracy but requiring long computation times, and a plural scattering program which is less accurate but much more rapid. Optimized for use on personal computers, the programs provide a real time graphical display of the interaction. The programs are then used as the starting point for the development of programs aimed at studying particular effects in the electron microscope, including backscattering, secondary electron production, EBIC and cathodo-luminescence imaging, and X-ray microanalysis. The computer code is given in a fully annotated format so that it may be readily modified for specific problems. Throughout, the author includes numerous examples of how such applications can be used. Students and professionals using electron microscopes will want to read this important addition to the literature.

Detailed Monte Carlo Simulation of Electron Elastic Scattering

Monte Carlo Simulation of Electron Trajectories in Thin Films

Monte Carlo Simulation of Electron Beam Scattering and Energy Loss in Thin Films on Thick Substrates

Monte Carlo simulation of neutral current radiative processes in deep inelastic electron-proton-scattering

Ensemble Monte Carlo simulation of electron transport in AlGaAs/GaAs heterostructures

Modeling ion beam induced secondary electron (iSE) production within matter for simulating ion beam induced images has been studied.

When the complex nature of ion beam interactions with matter is account for, a detailed quantitative model of the ion interactions with matter, Monte Carlo simulation will be the best choice to be able to compute and predict iSE yields faster and more accurately. In order to build Monte Carlo simulation software incorporated with a reliable database of stopping power tables, for wide variety of range of materials, there have been numerous attempts to experimentally measure ion stopping power tables and to tabulate the data. Experimental data for pure elements and compounds is almost totally absent and the ability of advanced software to calculate iSE production within matter for producing reliable predictions is limited. Despite the need having a complete set of experimental ion stopping power tables will not be easily obtained for at least several decades. This study explores the incorporation of a universal stopping power curve, calculated and published by the National Institute of Standards and

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Technology at Boulder, into a Monte Carlo simulation software that will be able to compute iSE yield for both pure elements and compounds. This new approach of modeling iSE generations for pure elements and compounds will contribute to quantify performance of the helium ion microscope and other ion microscopes.

"The scope of this thesis is the study of electron transportation and electron energy loss spectra using Monte Carlo and density functional theory calculations. In the first part, the electron transportations in the bulk materials and thin solid films were studied using Monte Carlo simulations based on the optical data model. The optical data model gives the benefit of the calculations of the backscattering and transmission coefficients from very low (about 100 eV) to high (about 500 keV) beam energies. The simulation results for backscattering and transmission coefficients are in good agreement with the available experimental data. Based on the Monte Carlo simulation results a new relation between backscattering and transmission coefficients of thin solid films was suggested enabling the estimation of one coefficient by having the other coefficient. A universal form for the signal-to-background ratio and the signal-to-noise ratio versus thickness divided by the inelastic mean free path was observed by Monte Carlo simulations in agreement with the available theoretical models. In addition, a

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simple equation was suggested for the estimation of the optimum thickness for the highest amount of signal-to-noise ratio. The equation implies that by having the value of one optimum thickness at a given beam energy the optimum thicknesses at other beam energies can be estimated. In the second part of the thesis, the fine structure of energy-loss near-edge structure (ELNES) obtained by the density functional theory calculations was introduced to the Monte Carlo simulations of the electron energy loss spectra. Density functional theory calculations successfully predicted the shape of energy-loss near-edge in comparison with the experimental measurements. Based on the suggested approach, the fine structure of an ionization edge can be introduced to the optical oscillator strength instead of the X-ray photoelectric data. X-ray photoelectric data does not contain the solid state effects and is appropriate for single atoms only. As a result of this approach, the total X-ray absorption coefficient can be calculated including the fine structure of inner-shell ionization edges. Using the Monte Carlo simulations with the new optical oscillator strength containing the fine structure of ionization edges, effect of different parameters of background removal for the ionization edges was studied. Monte Carlo simulations provided the optimum values for the optimization of the signal-to-background ratio calculations. In the third part of

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thesis, effect of temperature and pressure on the low-loss region of energy loss function were investigated. The energy loss function is in the direct relationship with the optical oscillator strength; hence it is important to study the parameters affecting the energy loss function. The density functional theory calculations were performed based on the change in the lattice parameter variation of solids with temperature and pressure. The results of density functional theory calculations are in the good agreement with the experimental temperature dependency of plasmon energy of aluminum. In addition, a new model for the temperature and pressure dependency of the plasmon energy of solids was suggested by combination of the free electron model and the pseudo-spinodal equation of state. The results of suggested model are in good agreement with the results of density function theory calculations. As well, the departure from the free electron behavior at high pressures was confirmed from the results of density functional theory calculations." --

Monte-Carlo Simulation of High-Field Electron Transport in Alternating- Current Thin-Film Electroluminescent Devices

Monte Carlo and Density Functional Theory Simulation of Electron Energy Loss Spectra
Monte-Carlo Simulation in Electron Microscopy and Spectroscopy

The VCM++ Code System: Monte Carlo Simulation of Electron and Photon Transport for

Application in Radiation Treatment Planning
Monte Carlo Simulation of Electron Dynamics
in Quantum Cascade Lasers

X-ray microanalysis by analytical electron microscopy (AEM) has proven to be a powerful tool for characterizing the spatial distribution of solute elements in materials. True compositional variations over spatial scales smaller than the actual resolution for microanalysis can be determined if the measured composition profile is deconvoluted. Explicit deconvolutions of such data, via conventional techniques such as Fourier transforms, are not possible due to statistical noise in AEM microanalytical data. Hence, the method of choice is to accomplish the deconvolution via iterative convolutions. In this method, a function describing the assumed true composition profile, calculated by physically permissible thermodynamic and kinetic modeling, is convoluted with the x-ray generation function and the result compared to the measured composition profile. If the measured and calculated profiles agree within experimental error, it is assumed that the true compositional profile has been determined. If the measured and calculated composition profiles are in disagreement, the assumptions in the physical model are adjusted and the convolution process repeated. To employ this procedure it is

necessary to calculate the x-ray generation function explicitly. While a variety of procedures are available for calculating this function, the most accurate procedure is to use Monte Carlo modeling of electron scattering.

Monte Carlo simulation is now a well established method for studying semiconductor devices and is particularly well suited to highlighting physical mechanisms and exploring material properties.

Not surprisingly, the more completely the material properties are built into the simulation, up to and including the use of a full band structure, the more powerful is the method. Indeed, it is now becoming increasingly clear that phenomena such as reliability related hot-electron effects in MOSFETs cannot be understood satisfactorily without using full band Monte Carlo. The IBM simulator DAMOCLES, therefore, represents a landmark of great significance. DAMOCLES sums up the total of Monte Carlo device modeling experience of the past, and reaches with its capabilities and opportunities into the distant future. This book, therefore, begins with a description of the IBM simulator. The second chapter gives an advanced introduction to the physical basis for Monte Carlo simulations and an outlook on why complex effects such as collisional broadening and intracollisional field effects can be important

and how they can be included in the simulations. References to more basic intro the book. The third chapter ductory material can be found throughout describes a typical relationship of Monte Carlo simulations to experimental data and indicates a major difficulty, the vast number of deformation poten tials required to simulate transport throughout the entire Brillouin zone. The fourth chapter addresses possible further extensions of the Monte Carlo approach and subtleties of the electron-electron interaction. Complete Model Description of an Electron Beam Using ACCEPT Monte Carlo Simulation Code Monte Carlo Method for Simulation of Electron Transport in Semiconductors Device Modeling Based on Monte Carlo Simulation of Electron Transport in Group III-nitride Semiconductors Electron-Beam Interactions with Solids

particularly attractive for use on sub-MeV electrons, because analog Monte Carlo calculations are too time-consuming and condensed history calculations are inaccurate.

A Response Matrix Monte Carlo (RMMC) method has been developed for solving electron transport problems. This method was born of the need to have a reliable,

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computationally efficient transport method for low energy electrons (below a few hundred keV) in all materials. Today, condensed history methods are used which reduce the computation time by modeling the combined effect of many collisions but fail at low energy because of the assumptions required to characterize the electron scattering. Analog Monte Carlo simulations are prohibitively expensive since electrons undergo coulombic scattering with little state change after a collision. The RMMC method attempts to combine the accuracy of an analog Monte Carlo simulation with the speed of the condensed history methods. Like condensed history, the RMMC method uses probability distributions functions (PDFs) to describe the energy and direction of the electron after several collisions. However, unlike the condensed history method the PDFs are based on an analog Monte Carlo simulation over a small region. Condensed history theories require assumptions about the electron scattering to derive the PDFs for direction and energy. Thus the RMMC method samples from PDFs which more accurately represent the electron random walk. Results show good agreement between the RMMC method and analog Monte Carlo. 13 refs., 8 figs.

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Application of the Monte Carlo Method to Electron Scattering Problems

Monte Carlo Simulation of Radiative Processes in Electron-positron Scattering

Monte Carlo Device Simulation

A New Paradigm for Collaborative Scientific Simulation

A Rapid Method for Profile Deconvolution

The interaction of an electron beam with a solid target has been studied since the early part of the past century. Since 1960, the electron-solid interaction has become the subject of a number of investigators' work owing to its fundamental role in scanning electron microscopy, in electron-probe microanalysis, in Auger electron spectroscopy, in electron-beam lithography and in radiation damage. The interaction of an electron beam with a solid target has often been investigated theoretically by using the Monte Carlo method, a numerical procedure involving random numbers that is able to solve mathematical problems. This method is very useful for the study of electron penetration in matter. The probabilistic laws of the interaction of an individual electron with the atoms constituting the target are well known. Consequently, it is possible to compute the macroscopic characteristics of interaction processes by simulating a large number of real trajectories, and then averaging them. The aim of this book is to study the probabilistic laws of the interaction of individual electrons with atoms (elastic and inelastic cross-sections); to investigate selected aspects of electron interaction with matter (backscattering coefficients for bulk targets, absorption, backscattering and

transmission for both supported and unsupported thin films, implantation profiles, secondary electron emission, and so on); and to introduce the Monte Carlo method and its applications to compute the macroscopic characteristics of the interaction processes mentioned above. The book compares theory, computational simulations and experimental data in order to offer a more global vision.

Secondary electron emission (SEE) from inner linings of plasma chambers in electric thrusters for space propulsion can have a disruptive effect on device performance and efficiency. SEE is typically calculated using elastic and inelastic electron scattering theory by way of Monte Carlo simulations of independent electron trajectories. However, in practice the method can only be applied for ideally smooth surfaces and thin films, not representative of real material surfaces. Recently, micro-architected surfaces with micron-sized features have been proposed to mitigate SEE and ion-induced erosion in plasma-exposed thruster linings. In this thesis, an approach is made for calculating secondary electron yields from surfaces with arbitrarily-complex geometries using an extension of the raytracing Monte Carlo (RTMC) technique. Further, the model is extended to study the surface morphology evolution of micro-architected foam samples due to plasma exposure. Microfoam structures are studied with varying porosities as representative micro-architected surfaces and use RTMC to generate primary electron or particle trajectories and track secondary electrons or particles until their escape from the outer surface. Actual surfaces are represented as a discrete finite element meshes obtained from X-ray tomography

images of tungsten microfoams. At the local level, primary rays impinging into surface elements produce daughter rays of secondary electrons whose number, energies and angular characteristics are set by pre-calculated tables of SEE yields and energies from ideally flat surfaces. Depending on porosity and primary electron energy, the micro-architected geometries can reduce SEE by up to 50% with respect to flat surfaces.

A Code System for Monte Carlo Simulation of Electron and Photon Transport, Workshop Proceedings, Issy-les-Moulineaux, France 5-7 November 2001

Monte Carlo Simulation of Electron Swarms in Monte Carlo Simulation of KeV-electron Transport in Solid Media

Response Matrix Monte Carlo for Electron Transport Monte Carlo Simulation of Electron Transport in a Helium Gas

Monte Carlo Modeling for Electron Microscopy and Microanalysis Oxford University Press

Monte-Carlo Simulation in Electron Microscopy and Spectroscopy.

Application of Parallel Computing to the Monte Carlo Simulation of Electron Scattering in Solids

Proefschrift

Monte Carlo Transport of Electrons and Photons

Monte Carlo Modeling of Ion Beam Induced Secondary Electrons

Monte Carlo Simulation of Electron Transport Process in GaAs