COMSOL Conference 2024 Florence

Monte-Carlo Model for Radiation **Transport in Solid X-Ray Targets**



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Austria

INTRODUCTION

CENUMERICS

- engineering consultancy founded in 2005
- in Innsbruck, Austria
- mathematical modeling and numerical simulation
 - multiphysics modeling
 - component and process simulation
 - application and software development
 - COMSOL Application Builder
 - COMSOL Physics Builder
 - C/C++, Java





INTRODUCTION



PLANSEE

- founded in 1921 for production of molybdenum (Mo) and tungsten (W) wires
- 1,000 MEUR turnover; 3,500+ employees worldwide (2023/24)
- world market leader in powder-metallurgical (P/M) production of refractory metals



used in wide range of high-tech applications and industries



- unique combination of material properties
 - high melting point
 - excellent high temperature strength



X-RAYS

High-energy electromagnetic radiation

- discovered 1895 by CONRAD RÖNTGEN
- energy range above UV light
- good penetration of solid matter ($\rho \approx 0$)
- widely used in medical diagnostics and material testing

Production using high-vacuum X-ray tubes

- electrons e⁻ thermionically emitted from cathode (C)
- accelerated to anode (A), voltage 10¹...10² kV, formation of e-beam
- impact on target or focal track (T)
- cascade of atomic interactions within target material
- emission of X-ray photons γ as:
 - (1) bremsstrahlung \rightarrow continuous spectrum
 - (2) characteristic X-rays \rightarrow discrete spectrum
- escaping by tube window (W) \rightarrow utilizable radiation



Ref: wikipedia:User:ChumpusRex, X ray tube in housing, Accessed: 2024-08-28



X-RAYS

Low efficiency, high heat dissipation

- only 0.1...1% as photon emission
- significant thermo-mechanical loads

Concepts for increased power

- active cooling of stationary anodes
- rotating anodes
- rotating envelope anode
- line-focus-principle (target inclination, stretched beam)

Motivation for study

- numerical model for radiation transport in X-ray target
- gain insight into performance of target, emitted spectrum, heat dissipation, influence of main design parameters





Ref (top, bottom): PLANSEE

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Modeling of radiation transport

- transport of high-energy electrons and photons (particles) through matter (medium)
- interaction with atoms and molecules
- energy transfer and secondary particle emission (cascade, particle shower)
- energy deposition within medium

Monte Carlo method

- particle-based approach
- history of particles discretized as random sequence of
 - (1) free "flights" (sampled from mean free path length)

(2) subsequent particle-interactions (sampled from relative interaction probability)

- change of flight direction and energy
- possible emission of secondary particles

tracked until energy absorption



$$\xi(E) = -\lambda_{\mathsf{T}} \log \xi, \qquad \xi \in [0, 1]$$

 $\mathbf{x}_{n+1} = \mathbf{x}_n + s \mathbf{t}_n;$ $\mathbf{t}_n = \mathbf{T}(\theta, \varphi) \mathbf{t}_{n-1};$ $\theta = f(E, \ldots), \quad \varphi = 2\pi\xi$

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INTERACTION MODEL

Relevant atomic interactions

electrons



Ref: reproduced from [Poludniowski et al., 2022]



target

IMPLEMENTATION

Monte Carlo model implementation

- using COMSOL Multiphysics 6.1
 - no ready-made interface for coupled electron-photon transport
 - COMSOL "Particle Tracing Module" allowing custom implementation
- main features:
 - particle types:
 - electrons
 - photons
 - excited target atoms (energy transfer to medium)
 - particle state variables:
 - particle energy E (Note: "massless" formulation)
 - quantities for sampling and statistics
 - interaction model:
 - using Velocity Reinitialization and Secondary Emission features
 - interaction data (cross sections etc.) for Mo, W, Re from EPICS-database (IAEA)
 - random sampling methods [Salvat, 2019] implemented in extensive function library (native/external C++)
 - domain accumulators: energy deposition (absorbed dose)
 - boundary accumulators: fluence and energy fluence

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Model Builder
A (B) Global Definitions
Pi Parameters Pi Consult assessmenters (defend)
Pi Material property parameters (pgr13)
P) Collision scaling parameters (par12)
Auxiliary parameters (grp23)
▲ for Functions
Common functions (grp24)
Random number generator functions (grp I) Rational interpolation (RITA) generic sampling functions (grp27)
Probability density functions (PDF) and sampling functions (grp15)
 Detector plane intersection point (grp2) Atomic electron and photon interaction data from FADI /FEDI /FPDI (grp22)
Atomic data from EADL (grp1)
Atomic photon interaction data from EPDL (grp2)
Atomic electron interaction cross sections from EEDL (grps) Analytic - Emission by collision type (by type) (an23)
Analytic - Fibonacci number (fib) (an24)
Q Analytic - Equal comparison with tolerance (equals) (an153) Analytic - Efficiency actimate (Koch and Motz 1959) Equ. (IV-16) (see also comments) (antion) (an154)
Pandyus - Entering estimate (exchange results (grp33)
Gaussian electron beam functions (grp32)
 B Geometry Parts Shared Properties
(a) Materials
" Method Calls Detrings Forme
Component 1 (comp1) (comp1)
Definitions
Materials
A 🔆 Charged Particle Tracing - D_Solid (cpt) (cpt)
Wall (default, unused) - Disappear (wall1)
Photon (γ) (pp2)
Excited Target Atom (A* / A+) (pp3)
Mandatory Auxiliary Dependent Variables (grps) 6 Auxiliary Dependent Variable 1 - Shower number (gux1)
Auxiliary Dependent Variable 2 - Energy (aux2)
Optional Auxiliary Dependent Variables (grp26) Optional Auxiliary Dependent Variables 2 _ Collision Count (grp21)
 Jai Auxiliary Dependent Variable 4 - Previous Collision Type (aux4)
Maximiary Dependent Variable 5 - Collision Count - Electrons, Elastic Scattering (aux5)
 Jes Auxiliary Dependent Variable 6 - Collision Count - Electrons, Inelastic Scattering (aux6) Auxiliary Dependent Variable 7 - Collision Count - Electrons, Bremsstrahlung Emission (aux7)
Auxiliary Dependent Variable 8 - Collision Count - Photons, Photo-Electric Absorption (aux8)
In Auxiliary Dependent Variable 9 - Collision Count - Photons, Coherent (Rayleigh) Scattering (aux9)
Release from Grid - Electron Pencil Beam (relg1)
Velocity Reinitialization - Energy and Particle Absorption in Solid Medium - D_Solid (vre7)
Accumulator - Energy Absorption - D_Solid (vacc1) Accumulator - Electron Absorption - D_Solid (vacc2)
 Accumulator - Photon Absorption - D_Solid (vacca)
Accumulator - Excited Target Atom Absorption - D_Solid (vacc4)
Equation View (Info) Electron Interactions (ara6)
Image: Provide the state of
$(2) \text{ Inelastic Scattering (e + A \rightarrow e + A^* / 2e + A^*) - D_Solid (we2)}$ $(3) \text{ Remestrablung Emission (e + A \rightarrow e + X^* + A) - D_Solid (we3)}$
(b) bit matching characterize (c) + + + + + + + + + + + + + + + + + + +
▷ = (4) Photo-Electric Absorption ($\gamma + A \rightarrow e + A$) - D_Solid (vre4)
b = (6) Incoherent (Rayleign) Scattering ($y + A \rightarrow y + A$) - D_Solid (<i>web</i>) b = (6) Incoherent (Compton) Scattering ($y + A \rightarrow y + e + A$) - D_Solid (<i>web</i>)
🖌 📟 Wall - B_SolidBoundary - All Particles Disappearing with Fluence and Energy Fluence Accumulators (wall3)
Accumulator - B_SolidBoundary - Electron Energy Fluence (bacc1)
 Accumulator - B_SolidBoundary - Electron Fluence (bacc3)
Accumulator - B_SolidBoundary - Photon Fluence (bacc4)
Equation view (unio) 4 Wall - B_Target - Particles Conditionally Freezing or Disappearing with Fluence and Energy Fluence Accumulators (wall4)
Accumulator - B_Target - Electron Energy Fluence (bacc1)
Accumulator - B_Target - Photon Energy Fluence (bacc2) Accumulator - B_Target - Photon Energy Fluence Caught by Detector (bacc3)
 Accumulator - B_Target - Electron Fluence (bacc4)
Accumulator - B_Target - Photon Fluence (bacc5)
Accumulator - B_larget - Photon Fluence Caught by Detector (bacc6) Reflected Incident Electron Clone - B Target (sem1)
Equation View (info)
Wall - B_Interface - Pass Through (wall5)
Global ODEs and DAEs (ge) (ge)
Global ODEs and DAEs 2 (ge2)
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 a countainy one - b_iniger - renet and Gaussian e-beam proton energy nuerce per incident electron (gopsi) (gopsi) a Domain DAE - D_Solid - Pencil and Gaussian e-beam dose per incident electron (dode) (dode)
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5 Study 1 - Small sample, all steps stored, all variables, all probes, in:

APPLICATION



Typical rotating X-ray anode with graphite body



Ref: PLANSEE



APPLICATION

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System



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October 22-24 COMSOL Conference 2024 Florence



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sample size: $N_{\rm e} = 3 \cdot 10^5$

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Results for GAUSSIAN electron beam

Absorbed dose per incident electron \bar{D}

Solid body

Focal spot section $\eta = 0$

transformation from electron pencil beam to arbitrary finite beam using convolution theorem (beam shape as kernel)

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SUMMARY AND OUTLOOK

Summary

- Implementation of Monte Carlo model in COMSOL Multiphysics
- radiation transport in solid X-ray targets
- focus on bremsstrahlung emission (continuous spectrum)
- state-of-the art sampling methods
- convolution of pencil electron beam results to arbitrary finite e-beam

Outlook

- model enhancement
 - performance improvements, increase sample size
 - radiative transitions and characteristic X-ray production
- model application
 - assessment of main parameters: tube voltage, target angle, thickness
 - better understanding of heat source distribution for use in nonlinear cyclic thermo-mechanical FEA

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Monte-Carlo Model for Radiation Transport in Solid X-Ray Targets

Dr. Christian Feist

...thanking you for your attention and looking forward to your questions

