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



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## INTRODUCTION

#### **CENUMERICS**

- engineering consultancy founded in 2005
- **·** in Innsbruck, Austria
- mathematical modeling and numerical simulation
	- multiphysics modeling
	- component and process simulation
	- **EX application and software development** 
		- COMSOL Application Builder
		- **EXECOMSOL Physics Builder**
		- $\bullet$  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

- **In discovered 1895 by CONRAD RÖNTGEN**
- **Example 2** energy range above UV light
- good penetration of solid matter (*ρ* ≈ 0)
- widely used in medical diagnostics and material testing

## Production using high-vacuum X-ray tubes

- electrons e<sup>–</sup> thermionically emitted from cathode (C)
- $\blacksquare$  accelerated to anode (A), voltage  $10^1...10^2$  kV, formation of e-beam
- impact on target or focal track (T)
- cascade of atomic interactions within target material
- emission of X-ray photons y as:
	- (1) bremsstrahlung  $\rightarrow$  continuous spectrum
	- (2) characteristic X-rays  $\rightarrow$  discrete spectrum
- **E** escaping by tube window  $(W) \rightarrow$  utilizable radiation



Ref: [wikipedia:User:ChumpusRex, X ray tube in housing,](https://commons.wikimedia.org/wiki/File:Xraytubeinhousing_commons.png) Accessed: 2024-08-28



Mid-bin energy (keV)

## 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



#### Modeling of radiation transport

- transport of high-energy electrons and photons (particles) through matter (medium)
- **Example ration in the rations 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



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

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

## INTERACTION MODEL

#### Relevant atomic interactions

■ electrons



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

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## 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

Consultant Engineers for Numerical Simulatior Model Builder モーナル 天間・国・国・ XRayTarget\_3D\_cpt\_C61\_V8u.mph (root) 4 Global Definitions  $\blacktriangleleft$  P<sub>i</sub> Parameters Pi General parameters (default) Pi Material property parameters (par13)  $\triangleright$  Pi. Collision scaling parameters (pgr12  $\triangleright$   $\Box$  Auxiliary parameters (arp23) I \*\*\* Unused Parameters (par14) 4 roo Functions  $\triangleright \leftarrow$  Common functions (grp24)  $\triangleright$   $\leftarrow$  Random number generator functions (grp1) Rational interpolation (RITA) generic sampling functions (grp27)  $\triangleright$   $\uparrow$  Probability density functions (PDF) and sampling functions (arp15) Detector plane intersection point (arp2) 4 - Atomic electron and photon interaction data from EADL/EEDL/EPDL (grp22) Atomic data from EADL (grp1) Atomic photon interaction data from EPDL (grp2) Atomic electron interaction cross sections from EEDL (grp3) Analytic - Emission by collision type (by type) (an23) Analytic - Fibonacci number (fib) (an24)  $\frac{1}{2}$  Analytic - Equal comparison with tolerance (equals) (an153) Analytic - Efficiency estimate (Koch and Motz, 1959). Equ. (IV-16) (see also comments) (epsilon) (an154)  $\triangleright$   $\frac{1}{2}$  Pencil beam fluence and dose results (grp33)  $\triangleright$   $\pm$  Gaussian electron beam functions (am32) **D** Geometry Parts  $\triangleright$   $\equiv$  Shared Properties **E** Materials Method Calls **D** Settings Forms 4 Component 1 (comp1) (comp)  $\triangleright$   $\equiv$  Definitions  $\triangleright$   $\overline{A}$  Geometry 1 (geom 1) **中 Materials** Charged Particle Tracing - D\_Solid (cpt) (cpt) Mall (default, unused) - Disappear (wall1)  $\triangleright \ \leq \ \leq$  Electron (e) [pp I]  $\triangleright \ \blacksquare$  Photon (y) (pp2) Excited Target Atom (A\* / A+) (pp3) - La Mandatory Auxiliary Dependent Variables ... (am8) > fax Auxiliary Dependent Variable 1 - Shower number (aux1) > fax Auxiliary Dependent Variable 2 - Energy (aux2) 4 Optional Auxiliary Dependent Variables ... (grp26) > for Auxiliary Dependent Variable 3 - Collision Count (aux3) >  $\int_0^{\infty}$  Auxiliary Dependent Variable 4 - Previous Collision Type (aux4) > [a] Auxiliary Dependent Variable 5 - Collision Count - Electrons, Elastic Scattering (aux5) 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) Auxiliary Dependent Variable 9 - Collision Count - Photons, Coherent (Rayleigh) Scattering (aux9) Auxiliary Dependent Variable 10 - Collision Count - Photons, Incoherent (Compton) Scattering [aux10] > 333 Release from Grid - Electron Pencil Beam (rela1) A C Velocity Reinitialization - Energy and Particle Absorption in Solid Medium - D. Solid ... /we7 > Accumulator - Energy Absorption - D\_Solid (vacc1) Accumulator - Electron Absorption - D. Solid (vacc2) > Accumulator - Photon Absorption - D\_Solid (vacc3) Accumulator - Excited Target Atom Absorption - D\_Solid /vacc4 Eduation View (info)  $\triangleq$   $\Box$  Electron Interactions ... (arp6)  $\triangleright$  (1) Elastic Scattering (e + A - e + A) - D\_Solid (vre1)  $\triangleright$  (2) Inelastic Scattering (e + A - e + A\* / 2e + A+) - D\_Solid ... (vre2)  $\triangleright$  (3) Bremsstrahlung Emission (e + A - e + y + A) - D\_Solid \_ (vre3) Photon Interactions ... (grp7)  $\triangleright$  (4) Photo-Electric Absorption (y + A - e + A) - D Solid ... /vre4)  $\triangleright$  (5) Coherent (Ravleigh) Scattering (v + A - v + A) - D Solid (vre5)  $\triangleright$  (6) Incoherent (Compton) Scattering (y + A - y + e + A) - D\_Solid ... (vre6) 4 Wall - B\_SolidBoundary - All Particles Disappearing with Fluence and Energy Fluence Accumulators ... (wall3) > Cumulator - B\_SolidBoundary - Electron Energy Fluence [bacc] > Accumulator - B\_SolidBoundary - Photon Energy Fluence (bacc2) > Accumulator - B\_SolidBoundary - Electron Fluence (bacc3) > Accumulator - B\_SolidBoundary - Photon Fluence (bacc4, Equation View (info) 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) > E Accumulator - B\_Target - Photon Energy Fluence Caught by Detector (bacc3) > Accumulator - B\_Target - Electron Fluence (bacc4) > Accumulator - B\_Target - Photon Fluence (bacc5) > Accumulator - B\_Target - Photon Fluence Caught by Detector (bacc6) Reflected Incident Electron Clone - B Target (sem 1) Equation View (info) > Wall - B Interface - Pass Through (wall <sup>Buf</sup> Fouation View (info) Global ODEs and DAEs (ge) (ge) Global ODEs and DAEs 2 (ge2) (ge2) Boundary DAE - B\_Target - Pencil and Gaussian e-beam photon fluence per incident electron (gbphi) (gbphi) Boundary DAE - B\_Target - Pencil and Gaussian e-beam photon energy fluence per incident electron (gbpsi) (gbpsi) Bomain DAE - D\_Solid - Pencil and Gaussian e-beam dose per incident electron (dode) (dode) A Mesh 1 (mesh1) > nob Study 1 - Small sample, all steps stored, all variables, all probes, instantaneous electron release (std

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## APPLICATION

#### Typical rotating X-ray anode with graphite body



Ref: PLANSEE



## APPLICATION

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#### System



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sample size:  $N_e = 3.10^5$ 

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#### Results for GAUSSIAN electron beam

Absorbed dose per incident electron  $\bar{D}$ 

Solid body Focal spot section *η* = 0 Focal spot section *ξ* = 0





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

## 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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Dr. Christian Feist

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

![](_page_14_Picture_5.jpeg)