

Geant4 simulations of surface contaminations and roughness and their influence on low energy background spectra

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Christoph Grüner

- on behalf of the
CRESST collaboration



COMENIUS
UNIVERSITY
BRATISLAVA

EBERHARD KARLS
UNIVERSITÄT
TÜBINGEN



The CRESST experiment

CRESST is a direct detection dark matter experiment, probing the parameter space for low mass ($\lesssim 1 \text{ GeV}/c^2$) WIMPs [1].

Placed at LNGS (Italy),
~1400 meter below the Gran
Sasso mountains.

Two channel approach:

- Phonons with cryogenic crystals ($\sim 15 \text{ mK}$)
- Scintillation light with a light detector

Various detector modules
with different crystal
materials are used [2–4].
Here focused on CaWO_4 .

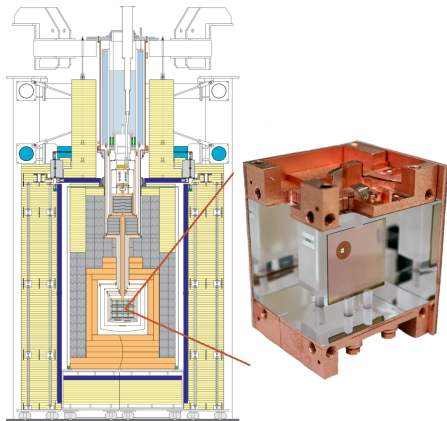
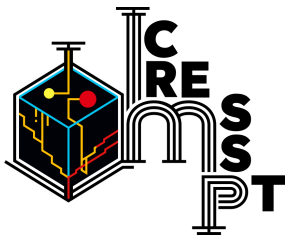


Figure 1: Sketch of experimental setup and photo of a detector module.

For more information see previous talk by Samir Banik, Thursday 15:20

Measured EM-background is investigated with simulations.

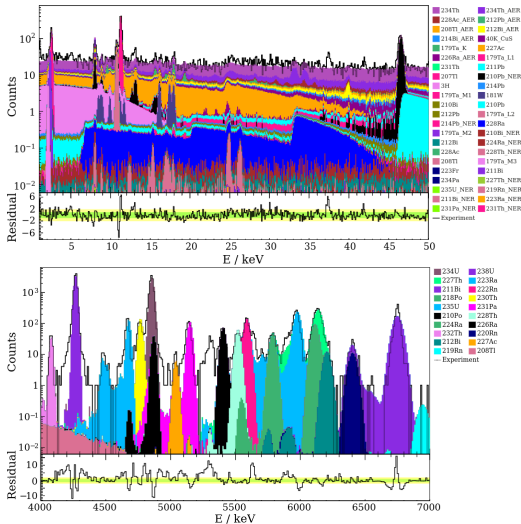
ImpCRESST is a Geant4/Root based simulation tool, developed for rare-event experiments and used by CRESST [5].



With **CrestDS** the detector resolution (time-, energie resolution) is applied to the data.

With a **Gaussian fit method** or a recently developed **Likelihood Normalization method** [6] the generated templates are fitted to the measured data.

Background spectrum



Total coverage of 99.6%, but some details are missing. (e.g.: there are gaps in the high energy range.)

This is a hint for:

- isotopes/contaminants are missing in the simulation
- effects are underestimated/not included

Figure 2: Simulated bulk contamination fitted to experimental data using a Likelihood fit method [6]. For fitting the program BLISS is used.

Background spectrum: Contamination

Surface could be contaminated with ^{210}Pb , because of ^{222}Rn .

^{210}Pb decays to ^{206}Pb .

^{210}Po is a bottleneck:

- Half-life 138 days
- α -decay
- Q-value 5.408MeV

Surface ^{210}Po is measured by CRESST [7].

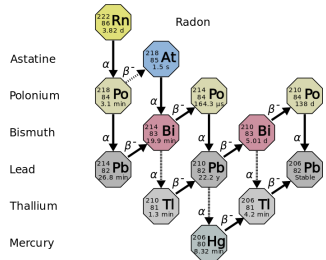
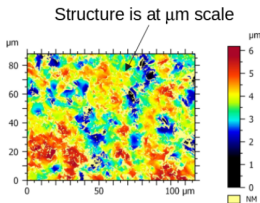


Figure 3: $^{222}\text{Rn} \rightarrow ^{206}\text{Pb}$ decay chain

Background spectrum: Surface roughness

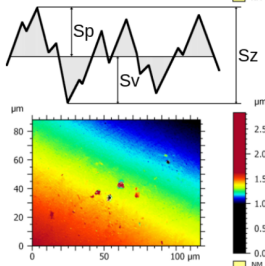
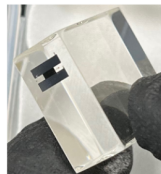
Diffused (TUM 84)



Parameter	Value [μm]
Sp	2.43
Sv	3.75
Sz	6.18



Polished (TUM 73)



Parameter	Value [μm]
Sp	1.52
Sv	1.31
Sz	2.83

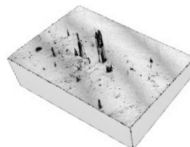


Figure 4: Surface profile of a diffused and polished crystal, grown at TUM [2]. Surfaces were examined by V. Mokina, using a LEICA DCM8 microscope.

Surface Roughness Module

Development of a **new Module** for Geant4 to simulate surface roughness and its contamination.

Module contains two main parts:

Surface Generator

Builds a patch of rough surface based on spikes.

Particle Generator

Samples vertices from the surface which are uniformly distributed to place nuclei.

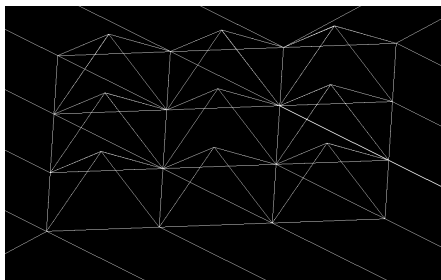


Figure 5: Patch of 3x3 spikes

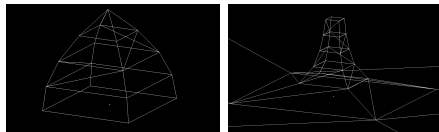


Figure 6: Other spike forms

Rough surface is represented by a G4Multiunion which contains spikes.

Up to 1000x1000 spikes possible.

Spikes can have different form and height.

Can calculate surface parameters to compare the generated surface to a real surface.

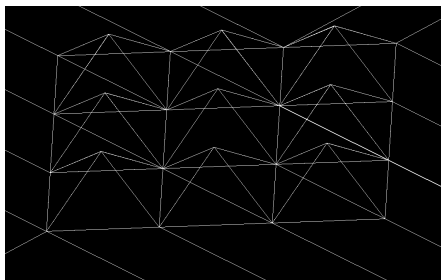


Figure 5: Patch of 3x3 spikes

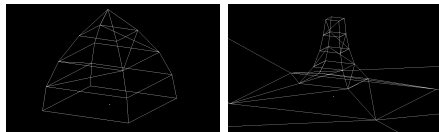


Figure 6: Other spike forms

Problem: G4Multiunion.Voxelize()

Voxelization is an optimisation routine to reduce the runtime with the tradeoff of an increased memory usage.

If spikes have different heights, the memory usage increases by $O((n_x \cdot n_y)^2)$. At 100x100 spikes, the memory consumption is in the range of GB.

Solution: Change the number of allowed Voxels

Change the class G4Voxelizer and implement a limit to the number of generated voxels in a certain direction.

Only one Layer of voxels in direction of spike height. Only a small change in runtime.

The **Particle Generator** places nuclei uniformly distributed on the generated rough surface.

Main part is the **Facetstore**, a singleton class which stores the rough surface as G4TriangularFacets.

The store is filled by the Surface Generator.

Downside: Currently a uniform placement of nuclei below the surface is not possible (but under development)

Used Physics

A slightly modified version of the physics list **G4EmStandard-Physics_Option4** was used for the following simulations. For Generic Ions the class **G4ScreenedNuclearRecoil** is implemented. It handles screened Coulomb collisions between nuclei.

```
} else if (particleName == "GenericIon") {  
    G4double energyLimit = 1 * MeV;  
  
    G4hMultipleScattering *NRmSc = new G4hMultipleScattering();  
    G4UrbanMscModel *model = new G4UrbanMscModel();  
    model->SetActivationLowEnergyLimit(energyLimit);  
    NRmSc->SetEmModel(model, 1);  
    ph->RegisterProcess(NRmSc, particle);  
  
    G4ionIonisation *ionIoni = new G4ionIonisation();  
    ionIoni->SetEmModel(new G4IonParametrisedLossModel());  
    ionIoni->SetStepFunction(0.1, 1 * um);  
    ph->RegisterProcess(ionIoni, particle);  
  
    G4ScreenedNuclearRecoil *nucrec =  
        new G4ScreenedNuclearRecoil("ScreenedElastic", "zbl");  
    nucrec->SetMaxEnergyForScattering(energyLimit);  
    ph->RegisterProcess(nucrec, particle);  
}
```

Figure 7: Changes of physics list for Generic Ions.

The physics list is not part of the developed surface roughness module!

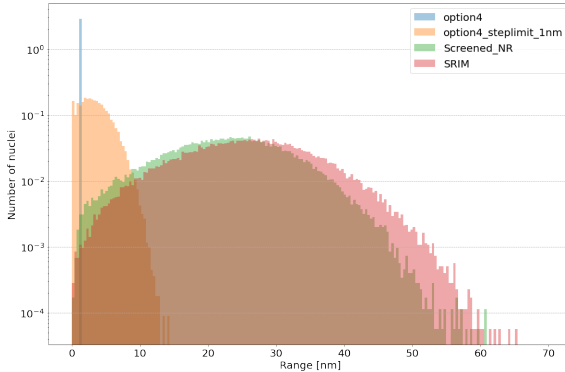


Figure 8: Penetration depth of ^{206}Pb nuclei with a kinetic energy of 103.08 keV inside a CaWO_4 -crystal. Two different physics for Generic Ions are used. Simulated data is compared with data generated with the SRIM simulation tool [8].

Simulation: ^{210}Po decay

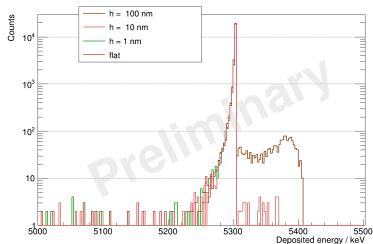
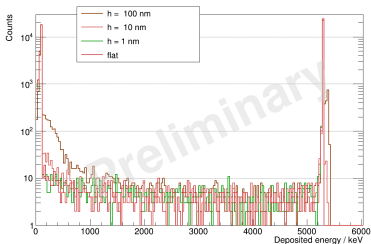


Figure 9: Sanity check of surface roughness implementation. The simulated energy deposition spectrum of a rough surface should approach the spectrum of a flat surface with decreasing spike height.

Simulation: ^{210}Po decay

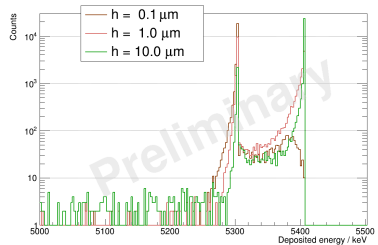
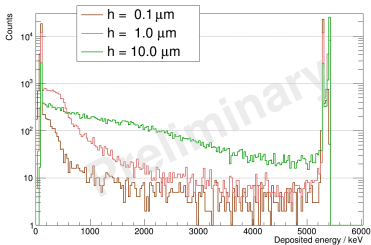
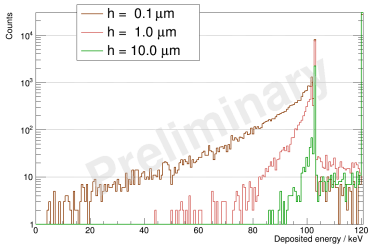
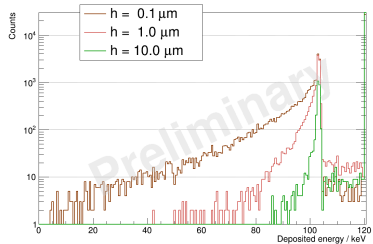


Figure 10: Energy deposition spectrum of ^{210}Po decay for different spike heights. A pyramid-like spike form is used.

Simulation: ^{210}Po decay



Raw energy deposition data



Detector resolution applied to data

Figure 11: Energy deposition spectrum of ^{210}Po decay for different spike heights. A pyramid-like spike form is used.

Simulation: ^{210}Po decay

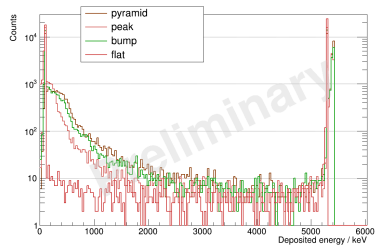
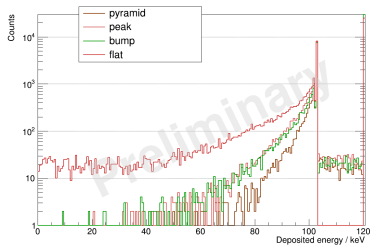


Figure 12: Energy deposition spectrum of ^{210}Po decay for different spike forms.

Fit of simulated templates

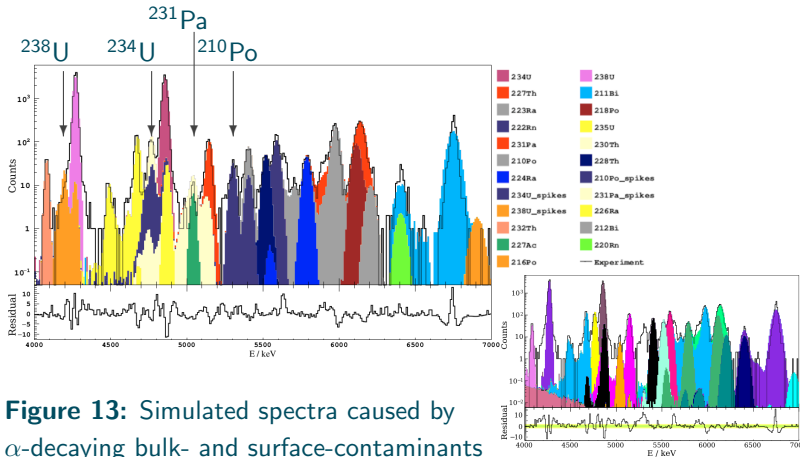


Figure 13: Simulated spectra caused by α -decaying bulk- and surface-contaminants (colored, filled histograms) fitted [5, 6] with BLISS to experimental data (black, open histogram) of CRESST's TUM40 detector [9]. The surface contaminants ^{210}Po , ^{231}Pa , ^{234}U and ^{238}U are placed on a rough surface [10].

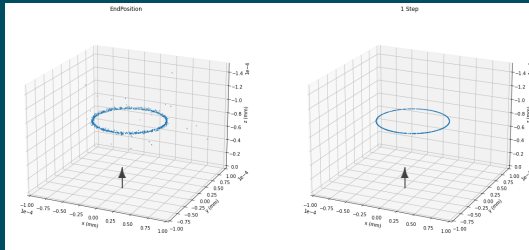
Summary and Outlook

- Geant4 based module for the simulation of surface roughness and surface contamination developed
- Capable of explaining some of the gaps between simulated and measured data (tails of alpha peaks, surface ^{210}Po)
- Module is still under development and will be improved further (nuclei placement below surface, more options to control surface)
- Prepare module for publication

Thank you!

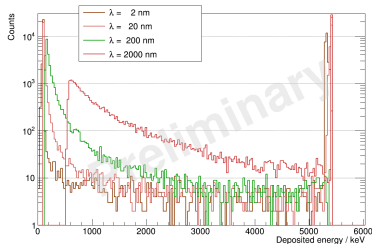
Questions?

Wanted! Have you seen this ring?

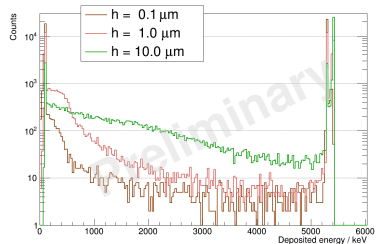


All nuclei enter the volume with the same kinetic energy at the position and the direction of the arrow.

Exponential depth distribution vs Surface roughness



Flat surface, exponential distribution



rough surface

Figure 14: Comparison of energy deposition spectrum of nuclei placed following a distribution $P(x; \lambda) \propto \exp(x/\lambda)$ normal to the surface (left) and a rough surface using a pyramid spike form (right).

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- [10] C. Grüner *et al.*, **“Geant4 simulations of the influence of contamination and roughness of the detector surface on background spectra in CRESST,”** *PoS*, vol. TAUP2023, p. 092, 2024. DOI: 10.22323/1.441.0092.