

TITLE OF THE PROJECT

GECO - GEANT4 CRYSTAL OBJECTS

NAME OF THE PRINCIPAL INVESTIGATOR

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Geant4 + Crystal Objects = the exploration of novel physical effects.

e.g., enhancement of the production yield of radioisotope in crystals against amorphous.

ABSTRACT

A fundamental aspect of a successful physics experiment is the availability of a reliable and precise simulation code. In particular, Geant4 has seen a large expansion of its user community in recent years. Currently, the toolkit does not allow the simulation of particles interacting with other than amorphous states of matter. The development of the Geant4 extension for the handling of crystal structures would allow the simulation of the mutual influence of various physics fields, and the exploration of novel applied physical effects. As an elective outcome of the project, the enhanced Monte Carlo code will permit the combination of solid-state and nuclear effects for the study of nuclear interaction rate in crystals. Indeed, an enhancement of the yield for the production of radioisotope in crystalline targets against amorphous material has been predicted. The aim of this project is to develop a general framework for the management of solid-state structures in the Geant4 kernel and to validate it against experimental data.

1. SCIENTIFIC BACKGROUND

Physics experiments usually take advantage of the most recent technologies and materials for the design and construction of their experiments. Because semiconductor companies invested many resources in R&D in order to produce high quality crystalline materials for information technology, samples of such materials can be easily bought on the market. The widespread use of semiconductors and all the possible dresses they can wear in an experimental apparatus have brought physicists to adopt such materials for a wide range of applications, spanning from detection to manipulation of charged and neutral beams.

1.1 APPLICATIONS

1.1.1 NUCLEAR INTERACTION RATE MODIFICATION

Radioisotopes are adopted in nuclear medicine to provide diagnostic information about the functioning of humans or information on how to treat them. The expensive cost of the prime materials for the production via cyclotron obliges the search for new solutions to enhance the production rate with minor upgrades of the current instrumentations. Oriented ordered structure can modify particle trajectories inside a medium leading to a sensible variation of the interaction rate with atomic nuclei. Under particular orientation of the crystal with respect to the incident beam, the probability of inelastic interaction with nuclei can be enhanced up to two times with respect to the standard rate. An elective application of such phenomenon is the possibility to enhance the production yield of radioisotopes by properly aligning the crystalline target with the impinging beam, e.g., a tens of MeV proton beam which impinges on a crystalline Ni⁶⁴ target aligned under anti-channeling condition¹.

1.1.2 SEMICONDUCTOR DETECTOR

The trackers adopted in astrophysics and high-energy physics are usually made of semiconductor materials. Ionizing radiation crossing material generates electron-hole pairs, which drift under the effect of the existing electric field, generating a charge signal proportional to the energy of the particle. Semiconductor detectors are currently adopted in a wide area of physics applications from track reconstruction in high-energy accelerators (ATLAS², CMS³) and in detection of astrophysics radiation from the Universe (AMS⁴, PAMELA⁵, FERMI-LAT⁶) to X-ray detection for medical imaging and diagnostics (SYRMEP⁷) or in semiconductor-based nuclear particle counters, such as HPGe detectors used for gamma-spectrometry.

1.1.3 DARK MATTER DETECTION WITH CRYSTALS

Thallium-doped sodium iodide scintillating crystals were used in dark matter experiments with low background at the Gran Sasso Laboratory of INFN by the DAMA/LIBRA experiment⁸, which pointed out that trajectories of recoiling nuclei may be modified by the presence of the crystalline structures⁹. High-purity germanium detectors are adopted by the CDMS experiment¹⁰ experiment for the same purposes at the SNOLAB cave and the COGENT experiment¹¹ at Soudan Underground Laboratory. Dark matter particles may scatter on target nuclei in the lattice, which vibrates and induces the creation of phonons, collected at the surface by deposited superconducting thin films. Recoiling nuclei may produce electron-hole pairs also recorded by the CDMS detector.

1.1.4 CHANNELING EFFECT AND BEAM OPTICS

Crystalline targets are currently adopted as beam optics for high-energy accelerators. Bent crystals were proved to work as beam manipulator for positive (INFN-H8RD22¹²) and negative

(INFN-ICE-RAD¹³) particles, and as the leading actors of an innovative collimation scheme for the SPS synchrotron with the UA9 experiment, which demonstrates the possibility of reaching a 20 times reduction of the beam losses for protons¹⁴ and 7 times for Pb ions¹⁵. Such results pushed forward the installation of two bent silicon strips into the LHC for beam collimation with the LUA9 experiment¹⁶.

1.1.5 X-RAY DIFFRACTION FOR ASTROPHYSICS AND MEDICINE PURPOSES

Crystals also allow the manipulation of high-energy photon trajectories through diffraction under Bragg and Laue configurations. X- and gamma rays interacting with crystals can be reflected through diffraction. Such interactions can be exploited to focus photons for astrophysics and medical purposes. As an example, the LOGOS experiment¹⁷ tries to improve the achievable sensitivity of X-ray space lenses through the study of a diffracting component made of bent crystals. A Laue lens can also be used to concentrate hard X-rays for therapy purposes. For instance, high-energy radiation used in radiation therapy to kill cancer cells by damaging their DNA can be focused with a Laue lens, minimizing side effects.

1.2 THE AIM OF THE PROJECT

A fundamental aspect of the design of experimental apparatus and the interpretation of physics results for a successful physics experiment is the availability of a reliable and precise simulation code. Nowadays Monte Carlo simulations of the interaction of particles with matter are usually done with download-able toolkits such as Geant4^{18,19,20} and Fluka^{21,22}. Such Monte Carlo codes are continuously expanded and improved thanks to the collaborative effort of scientists from around the world.

Geant4 is a general-purpose object-oriented toolkit, which was initially developed for high-energy physics. The first application in a full experiment was the simulation of the detector response for the BaBar experiment at SLAC²³. Geant4 has seen a large expansion of its user community in recent years. Nowadays, applications simulated by Geant4 range from particle transportation in the LHC detectors²⁴ to calculations of dose distribution curves for a typical proton therapy beam line²⁵, and from radiation analysis for space instruments²⁶ to early biological damage induced by ionizing radiation at the DNA scale²⁷.

The signal response of a silicon detector, the diffraction from different planes, the manipulation of charged particles by channeling or the enhancement in the production of radiation experimentally observed are not available in the standard Geant4 package. Indeed, although Geant4 deals with the interaction of particles with matter, the toolkit does not allow the simulation of particles interacting with other than amorphous states of matter.

The possibility to have a software infrastructure inside the Geant4 kernel capable of managing crystal structures would allow the development of specific physics models for the description of such effects in the toolkit and their usage together with already existing physics processes, as the hadronic, electromagnetic and optical physics processes, for example.

The aim of this project is to develop and integrate the framework for the management of solid-state structures in Geant4, in order to allow the toolkit to simulate physics processes connected to solid-state physics, to prove this capability by inserting the channeling effect into the available Geant4 processes, and to validate the code against experimental data for an elective application, i.e., the enhancement of radioisotope production yield in crystalline targets against amorphous.

2. STATE OF THE ART

The Geant4 toolkit provides a diverse, wide-ranging, yet cohesive set of software components, which can be employed from simple one-off studies of basic phenomena and geometries to full-scale detector simulations for experiments at the Large Hadron Collider and other facilities.

All aspects of the simulation process have been included in the definition and implementation of the software components: the geometry of the system, the materials involved, the fundamental particles of interest, the generation of primary particles of events, the tracking of particles through materials and external electromagnetic fields, the physics processes governing particle interactions, the response of sensitive detector components, the generation of event data, the storage of events and tracks, the visualization of the detector and particle trajectories, and the capture for subsequent analysis of simulation data at different levels of detail and refinement.

The materials are made of a single element or a mixture of elements; elements are made of a single isotope or a mixture of isotopes. Because the physical properties of materials can be described in a generic way by quantities which can be either given directly, like density, or derived from the element composition, only concrete classes are necessary in this category. The materials category also implements facilities to describe surface properties for the tracking of optical photons.

Currently, the Geant4 kernel does not handle crystalline structures.

The state of matter description of the materials is limited to a set of three values, i.e., solid, liquid or gas, which define the limits for the density of the kind of state.

A singleton for the managing of crystalline structure was first introduced with version Geant4.9.6²⁸ in an example code for the description of phonon propagation in a germanium crystal²⁹. The description of the crystal was limited to the managing of a pre-computed map of group velocities and the phonons were treated as particles. Recently, a new model suitable for Geant4 implementation was developed by the applicant³⁰ to simulate orientational effects of charged particles interacting with bent crystals under planar channeling and volume reflection. The capability to manage the potential calculated under the continuum approximation by Lindhard³¹ was added to the class for the description of the lattice. With the Geant4 10.00 version the code for channeling and volume reflection has been added in the “examples” category³².

4. DESCRIPTION OF THE PROPOSED RESEARCH ACTIVITY

The units involved in the project are three, the INFN section of Ferrara (FE), the INFN Laboratori Nazionali del Sud (LNS) and the INFN Laboratori Nazionali di Legnaro (LNL). The total amount of manpower required cover two years. The activities are summarized in Table [3]

TABLE 3: SUMMARY OF THE ACTIVITIES DIVIDED BY TASK.

Activities		Tasks	
a	Geant4 crystalline structures development	1	Open-source codes for solid state physics survey
		2	Implementation strategy
		3	Coding and engineering
b	Orientational effect development	1	Channeling process porting
		2	Wrappers of Geant4 physics process development
		3	Geant4 physics list for orientational effect engineering
c	Package validation	1	Design of the experimental setup
		2	Set-up of the experiment
		3	Data-taking
		4	Data analysis and comparison with simulations

4.A) CRYSTALLINE STRUCTURES AND THE GEANT4 KERNEL

The modification of the Geant4 kernel for the management of the crystalline structures will deal with two stages, a review of the published open source codes for the handling of solid-state physics processes and characteristics and the development of the code in collaboration with those responsible for the maintenance of the Geant4 kernel, the Geant4 team at SLAC (**Z.T.2**).

The review on the published open source codes will lead to the definition of the fundamental parameters needed by code. The study of existing free software under GPL license will help to define and summarize the fundamental parameters for the description of a crystalline structure and the expected capabilities of a code dealing with their management (**task a.1**). As a fundamental constrain, the software has to exploit the possibility of using the available online database, such as the Crystallography Open Database³³, an open-access collection of crystal structures of organic, inorganic, metal-organic compounds and minerals with hundreds of thousands of entries.

The second part of the activity will lead to the development of the code for the management of crystal structures in Geant4. Such development has strict requirements other than the correctness of the crystallographic description of the. Indeed, thanks to the intrinsic modularity of the Geant4 toolkit, the development of an extension for the code will allow the efficient integration of solid state physics with the other components, such as a complete set of physics processes, description of complex geometries, visualization, analysis and persistency tools. Therefore, from a semantic and logical computational point of view, a new package for the Geant4 kernel has to be harmoniously integrated into the existing framework in order to be compatible with the remaining code. In addition, because of the open source nature of Geant4 and the ongoing research for a collective development by the international collaboration, the design and the syntax have to be readable by physicist and modifiable by other suppliers of the service. As a consequence, the second part will deal with two stages, the definition of the implementation strategy (**task a.2**) and the code writing and engineering (**task a.3**).

4.B) ORIENTATIONAL EFFECTS OF CHARGED PARTICLES

Oriental effects of high-energy particles are a particular branch of the interaction between radiation and periodic structures. The most known process is the channeling, i.e., the trapping of a charged particle into the potential well generated by the planes or axes of a crystalline material³⁴. In the last decade, after the discovery of the volume reflection effect³⁵ predicted long before³⁶, the fundamental and technological research on orientational interactions has been pushed forward.

In particular, the INFN has been one of the main characters since the beginning of the tale, thanks to the involvement in the UA9 experiment for the application of orientational processes for the collimation of the SPS and LHC at CERN, and the fatherhood of the Gruppo V COHERENT and ICE-RAD projects for the study of the physics pillars of the orientational effects and the technological upgrading of the sample design, fabrication and characterization. In particular, the interpretation of the experimental data has been worked out thanks to available Monte Carlo codes. As an example, the DYNECHARM++ code, developed by the applicant³⁷, was involved in the simulation of coherent effects into $\text{Si}_{1-x}\text{Ge}_x$ crystals³⁸ in the field of the COHERENT project, in the systematic study of channeling efficiency vs. crystal curvature in bent crystals for the ICE-RAD project³⁹ and in the interpretation of the mirroring effect in ultra-thin straight crystals for the UA9 project⁴⁰.

The aim of first part of the activity is the integration of the DYNECHARM++ routine for orientational effects into Geant4 (**task 1**). From a physical point of view the routine has fewer restrictions than the channeling Geant4 model. However, it lacks in computational performance due to the heavier computation. A fundamental aspect to be inserted into the Geant4 kernel is the dynamic modification of the material density. Indeed, the material density experienced by the particle under coherent effects changes according to the particle trajectory. Thus, a wrapper class capable of managing the Geant4 processes and dynamically changing the density experienced by the particles will be developed (**task b.2**). The work will be done in close contact with the Geant4 team at IN2P3/LLR, responsible for the biasing code in the Geant4 collaboration (**Z.T.4**). Finally, a specific Geant4 physics list containing the channeling process will be developed (**task 3.c**).

4.C) RADIOISOTOPES PRODUCTION IN CRYSTALS

Oriented ordered structure can modify particle trajectories inside a medium leading to a sensible variation of the interaction rate with atomic nuclei. Under particular orientation of the target with respect to the incident beam (the anti-channeling condition⁴¹), the probability of inelastic interaction with nuclei can be enhanced up to two times with respect to the standard rate, leading to the increasing of the radioisotope production yield. The experimental observation of the phenomenon will pave the way to the exploitation of the process for the design of innovative crystalline targets, e.g., for the production of radioisotope for medicine. However, the fabrication of a crystalline target for such material will be expensive and require a long-time research.

In order to collect data on the phenomenon with no need of too expensive research of new targets, a well-known crystalline target together with an extensively adopted experimental setup with the need of minor improvements has to be used.

For the realization of the experiment a MeV-energy accelerator with a goniometer for the rotation of the crystalline target are needed. For the observation of the variation yield as a function of the crystal orientation, both the offline and online methods of the nuclear reaction

products can be exploited. The target has to be a common crystal with dislocation concentration less than 10^4 per cm^2 .

The best viable solution for the fulfillment of all the requirements is the realization of the experiment at the LNL. Indeed, the RBS-Channeling (Rutherford Backscattering-Channeling) line of the CN-LNL accelerator is equipped with a five rotational axes stage that allows orienting a crystal for the characterization via channeling effect. The line is suitable for the activation of a crystalline target and the measurement of the activity expect for minor upgrades. The LNL team is qualified for the obtaining of beam time, as proved by the HCCC and QDNS experiments at LNL of Prof. De Salvador. The design of the experimental setup (**task 3.a**) will be initiated during the first year (**Z.T.1**) and will be finalized (**task 3.b**) during the second year.

The measurement will be done with offline and online techniques. The online technique consists in the detection of the gamma prompt or the charged particles produced in a reaction. For such measurement, the experimental setup is ready except for an HPGe detector for the gamma prompt and a Si detector for the charged particles, which are available at LNL and have to be installed for the specific setup. The installation requires an update of the existing electronic chain (**Z.I.2**) and of the mechanical support (**Z.C.1**). The offline measurement requires the usage of a HPGe detector for the gamma of the decaying particle with an half-life of the order of hours. The setup external to the line for the measurement is available at LNL.

Because of the need for the usage of a crystalline target available on the market, the most promising solution are the elemental semiconductors, i.e., Silicon (Si), Germanium (Ge), and the compound semiconductors of the III-V group, i.e., arsenides (AlAs, GaAs, InAs), phosphides (AlP, GaP, InP), nitrides (AlN, GaN, InN). Such materials can be found as crystals as well as amorphous (sputtered targets) on the market and have to be bought (**Z.C.2** and **Z.C.3**).

Due to the large variety of isotopes in the crystals both the offline and online techniques will be analyzed. Indeed, due to the different thermal conductivity, electric conductivity, melting point and other physics characteristic important for irradiation, each isotope has to be studied under proper condition, even at low current (**task 3.c**). As an example, the natural Ge bombarded with deuteron⁴² can be used to produce ⁷¹As, which has a half-life 65.3 hours and a total cross section of ~ 10 mb, suitable for a offline measurement and the exploitation as a radionuclide for PET investigation.

The data collected during the experimental runs (**Z.T.3**) will be analyzed and compared to Geant4 simulations worked out with the developed new version of the code (**task 3.d**). The simulation will deal with the full reproduction of the experimental setup, with the online detectors and a “virtual” detector on the target. In such a way, the comparison between the experimental data and the simulation will furnish important information on the real isotope production rate in the crystalline target, thanks to the “virtual” detector.

5. MILESTONES AND TIMELINES

The milestones of the project will be four and are highlighted in Tab [1] as a black line.

Milestone	Date		Products
1	May 2016	1	survey on the available software for solid-state physics
2	December 2016	1 2	engineered code for crystal structure report of the design of the experimental setup
3	April 2017	1 2	code for the channeling effect report of the built experimental setup
3	December 2017	1 2	journal article on the validation of the code journal article on the experiment.

MILESTONE 1: MAY 2016

The FE unit will work on the survey of the available solid-state physics software (*task a.1*) and the beginning of the implementation strategy for the managing of the crystal structure into the Geant4 kernel together (*task a.2*) with the SLAC Geant4 team (see *Attachment A*). The products of the Milestone 1 will be the survey on the available software for solid-state physics.

MILESTONE 2: DECEMBER 2016

The FE and LNS units will initially define together with the SLAC Geant4 team to finalize the implementation strategy of the crystalline structures in the kernel (*task a.2*) and will be then involved in the writing of the Geant4 kernel code for the managing of crystalline structure (*task a.3*), by exploiting the survey worked out at Milestone 1. In the meanwhile, the LNL unit will work on the design of the experimental setup for the validation of the code (*task c.1*). The products of the Milestone 2 will be the engineered code for crystal structure in a private Geant4 release and the report of the design of the experimental setup.

MILESTONE 3: APRIL 2017

The FE unit will initially work to finalize the porting of the channeling model (*task b.1*). Then, they will work on a specific wrapping class for Geant4 processes (*task b.2*) in collaboration with the IN2P3 Geant4 team (see *Attachment B*) and on the development of the list of physics processes for Geant4 (*task b.3*). The FE and LNL units will finalize the mounting of the experiment setup (*task c.2*). The products of Milestone 3 will be the code for the channeling effect into the private Geant4 release and the report of the built experimental setup.

MILESTONE 4: DECEMBER 2017

During the last months, the FE and LNL units will collect the experimental data at the CN-LNL (*task c.3*). The data will then be processed analyzed by the FE unit. Finally, the Geant4-code will be validated against experimental data through the simulation of the experiment with the details of the experimental setup (*task c.4*). The products of the Milestone 4 will be a journal article on the validation of the code and a journal article on the experiment.

6. IMPACT

The main outcome of the project is the code for the managing of crystal structures for Geant4. The source code will be released on the Geant4 website. This result will involve a written survey of existing codes for solid state physics and of a journal article on the code itself. The code will be the cornerstone for the development of solid state physics processes in Geant4, e.g. the motion of electrons and holes in a semiconductor material or the diffraction of x-rays in crystalline structure. As reported in the introduction, the physics processes involved in solid-state physics may potentially touch the Monte Carlo simulation of many experiments.

The outcome of the second stage of the project is a general code for orientational effects in crystals validated against experimental data. The code may be used for the simulation of future INFN experiments involving orientational effects, such as for instance the LHC collimation (LUA9) and extraction (CRYSBEAM) via bent crystals and the study of orientational effects with GeV and sub-GeV electrons at SLAC and MAMI facilities (ICE-RAD).

Moreover, the observation of the enhancement of the yield for the production of radioisotope in crystalline targets against amorphous material may pave the way to the design of innovative crystalline target (see *Attachment C*). In fact, the production techniques of radioisotopes for medical purposes are a valuable and important field in nuclear medicine and, in particular, the expensive cost of the prime materials for the production via cyclotron obliges the search for new solutions to enhance the production rate with minor upgrades of the current instrumentations.

Once validated, the code could be exploited to simulate the impact of the usage of crystalline structure for various targets, i.e., the Ni^{64} . Therefore, the successful completion of the project may be the starting point for future projects involving the development of specific physics processes regarding solid-state physics, e.g., for Horizon 2020, the EU Framework Programme for Research and Innovation.

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