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(Research Article)

Absorption, backscattering and transmission properties assessment of electrons and photons in BeO and NaCl materials by Monte Carlo method

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Abstract

The simulation by the Monte Carlo method has proved to be effective in highlighting the absorption properties, of backscattering and transmission when propagating 5 KeV electron beams through 150 µm thick of each of the BeO and NaCl materials. Despite the fact that a very small fraction of the primary electrons was transmitted in the materials, several microscopic phenomena occurred at the level of the electronic sub-layers. This is the characteristic line, fluorescence and bremsstrahlung. The energy of the incidence electrons was higher than that of the sub-shells of atoms in the materials studied. The sub-shells concerned were for oxygen: KL2, KL3, KM2, KM3, L3M1, L3M3, L2M1, L1M3, L1M2, chlorine: L1M2, sodium: KL2 and KL3. Due to their properties, the use of BeO and NaCl can improve performance in the manufacture of advanced technology devices such as synchrotron, clinical particle accelerator and X-ray tube.

Keywords: Absorption; Backscatter; Transmission; BeO; NaCl; Monte Carlo

1. Introduction

The phenomenon of braking radiation concerns particles carrying an electric charge whose speed is close to light. It occurs when this ultra-relativistic particle interacts with a strong electric or magnetic field. Radiation emitted when an energy-charged particle is incident on an atom or molecule and accelerated as a result of interaction with the Coulomb field [1]. It is important to understand the processes involved in brake radiation emissions for research in a wide variety of fields, including astronomy, medical physics and fusion reactor design. Although there have been many studies on the emission of Bremsstrahlung resulting from interactions of electrons with conductive targets, there have been far fewer experiments conducted to study the noise emitted by electrons interacting with isolating or molecular targets [1, 2, 3]. In a recent study, braking radiation was produced by bombarding beryllium oxide (BeO) and sodium chloride (NaCl) with an incident electron beam of 5KeV energy [1]. Indeed, BeO is a white crystalline oxide. It is an electrical insulator with thermal conductivity [**Error! Bookmark not defined.**]. BeO is one of the most widely used nanomaterials in a wide range of applications, including nuclear as a neutron moderator and reflector. It is also used as a structural ceramic for electronic lamps and gas lasers. As for NaCl, also known as salt, it is an essential compound used by our body known as crystalline metals. NaCl is used in medicine to treat a body's loss of water, depletion and diluted other drugs perfusion. It also allows to absorb and transport nutrients, maintain blood pressure, maintain the proper balance of fluids, transmit nervous signals to contract and relax muscles [1]. Various simulation software, including GEANT 4, MCNPX and PyPENELOPE, have been designed to simulate the interactions between particles and materials.

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Most of these simulation programs rely on several scattering theories for electron transport to reduce the computation time [1, 2]. PENELOPE means penetration and energy loss of positrons and electrons in matter. It uses the Monte Carlo method for simulating many devices such as dosimeters and material structures. It will therefore be a tool of choice for simulating the interaction between electron beams and BeO and NaCl materials in order to evaluate absorption, transmission and diffusion properties. PENELOPE combines numerical and analytical cross sections (DCS) to describe the different mechanisms of interaction. These sections are the result of approximate physical models and therefore affected by systematic uncertainties. The interaction mechanisms considered in PENELOPE, and the corresponding DCS, are as follows: Elastic scattering of electrons and positrons where these cross sections have been calculated using the ELSEPA program,[3] inelastic collisions of electrons and positrons [3], ionization by impact of electrons [1], Brake radiation emission by electrons and positrons photons, incoherent scattering (Compton) of photons [6], photons photoelectric absorption [3], Production of electron-positron pairs [8]. Adamson et al. have conducted studies on the surface charge effects of BeO and NaCl. In our work, we will try to provide additional information on the properties of particle in order to explain the propagation of microscopic electrons.

2. Material and Methods

2.1. Material

This work was done with a Monte Carlo simulation code using the PyPENELOPE software which is a version of PENELOPE executed by the Python program as it has been the case in several works[9, 10, 11]. PyPENELOPE was installed on the Windows operating system of the Dell Compute Machine branded Intel(R) Core (TM) i5-6300U processor CPU @ 2.40GHz , 8 GB RAM, 500 GB hard disk. PyPENELOPE is one of the best tools for evaluating particle transport in the material describing different types of interaction.

2.2. Methods

The BeO and NaCl materials studied by Adamson et al. have conducted studies on surface load effects that showed certain physical properties but without giving particle propagation characteristics related to absorption properties, of the back-scattering and transmission of electrons and photons in matter.

In this work, we simulated an incident beam of primary electrons and sent it perpendicularly on the surface of BeO and NaCl materials under optimal conditions to study the propagation effects. Our beam source was at the initial coordinate position (0; 0; 0) under a polar angle range of zero to 180. The duration of a simulation was about 500 seconds, the number of electrons corresponded to 155400 for BeO and 118900 for NaCl. The beam diameter was set at 10 µm. Multi-layer geometry was used with a thickness of 150 µm for both materials. BeO has a density of 0.178 g/cm^3, purity 99.95% and NaCl of 0.432 g/cm^3, purity 99.9%. The version 0.2.10 of PyPENELOPE was used for simulations. All simulations were performed using a beam energy of 5.0 keV. The PyPENELOPE interface allows users to enter the chemical formula for a given target and weight fractions are automatically calculated.

For all simulations performed, the default settings were used. Parameters C1 and C2, which control the simulation of elastic scattering for electrons and positrons respectively, have both been set to 0.2. The values for the WCC and WCR parameters, which are the cut-off energy losses for inelastic collisions and the Bremsstrahlung emission, respectively, were set at 50 eV. Similarly, the values of electron and photon absorption energies (EABS1 and EABS2, respectively) were set at 50 eV. The default interaction forks were also used for all simulations.

3. Results and discussion

3.1. Particle propagation Statistics and probability

Statistical data from the simulation of the impact of electrons with an energy of 5KeV on BeO and NaCl materials are presented in the tables below.

Table 1 Fraction absorbed, backscattered and transmitted of primary and secondary irradiations simulated through the BeO material

	Primary electron		Secondary electron		Secondary Photon	
BeO	**Fraction**	**Uncertainty**	**Fraction**	**Uncertainty**	**Fraction**	**Uncertainty**
Absorption	0,9191	0,002076	19,03	0,03496	0,001069	$3,924\times10^{-05}$
Backscatter	0,08908	0,002744	0,008141	$6,685\times10^{-4}$	0,0005586	$3,213\times10^{-05}$
Transmission	$1,024\times10^{-08}$	$2,303\times10^{-09}$	$1,024\times10^{-08}$	$2,303\times10^{-09}$	$6,252\times10^{-06}$	$5,464\times10^{-08}$

Table 2 Fraction absorbed, backscattered and transmitted of primary and secondary irradiation simulated through the NaCl material

	Primary electron		Secondary electron		Secondary Photon	
NaCl	**Fraction**	**Uncertainty**	**Fraction**	**Uncertainty**	**Fraction**	**Uncertainty**
Absorption	0,8126	0,003395	17,71	0,05374	0,001727	$6,283\times10^{-10}$
Backscatter	0,2038	0,004452	0,01639	$1,056\times10^{-3}$	$5,516\times10^{-4}$	$3,875\times10^{-5}$
Transmission	$7,125\times10^{-10}$	$9,559\times10^{-10}$	$7,125\times10^{-10}$	$9,559\times10^{-10}$	$6,874\times10^{-7}$	$1,327\times10^{-6}$

3.2. Energy distribution

3.2.1. Backscattered Particles

The probability density of the backscattered particles as a function of energy is shown in the figure 1.

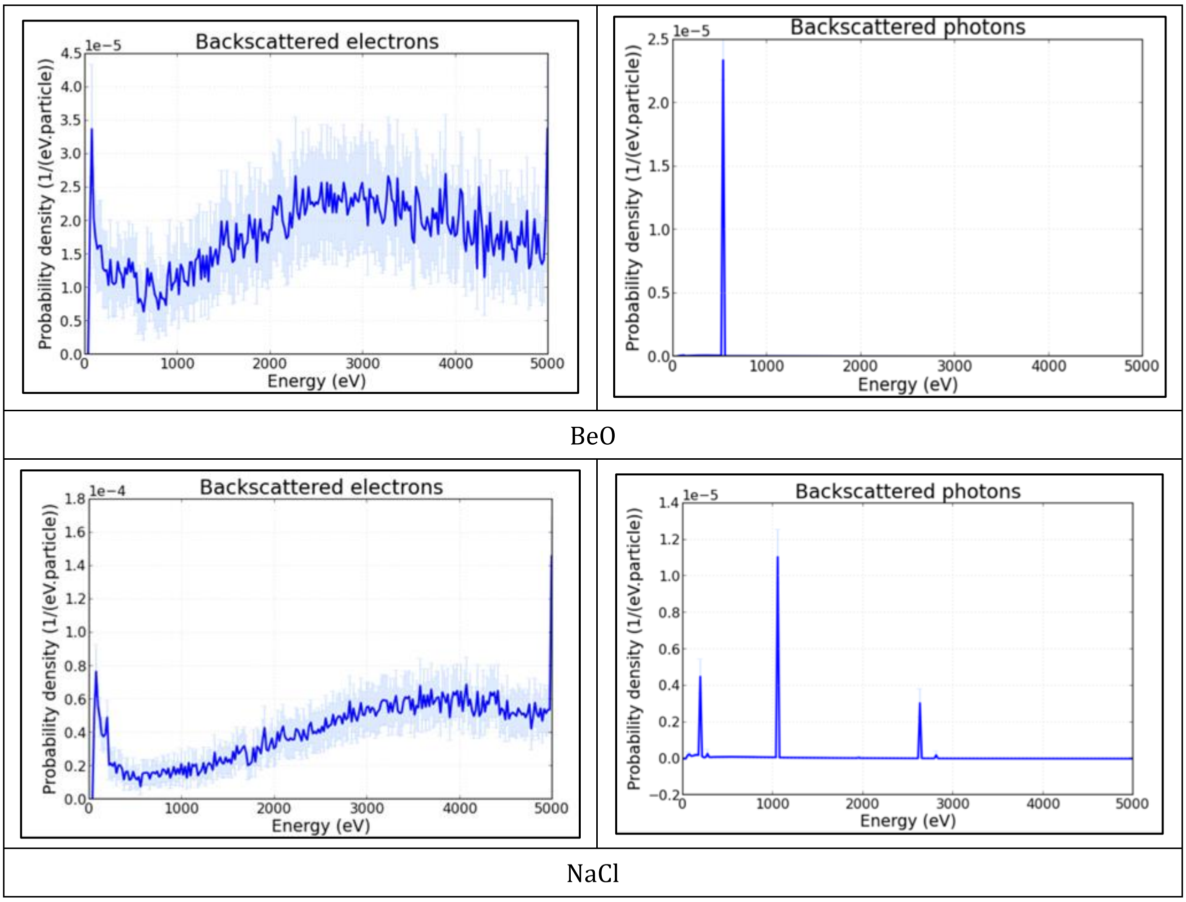


Figure 1 Probability density of backscattered particles as a function of energy

3.2.2. Transmitted Particles

The probability density of particles transmitted as a function of energy is shown in the following figure 2.

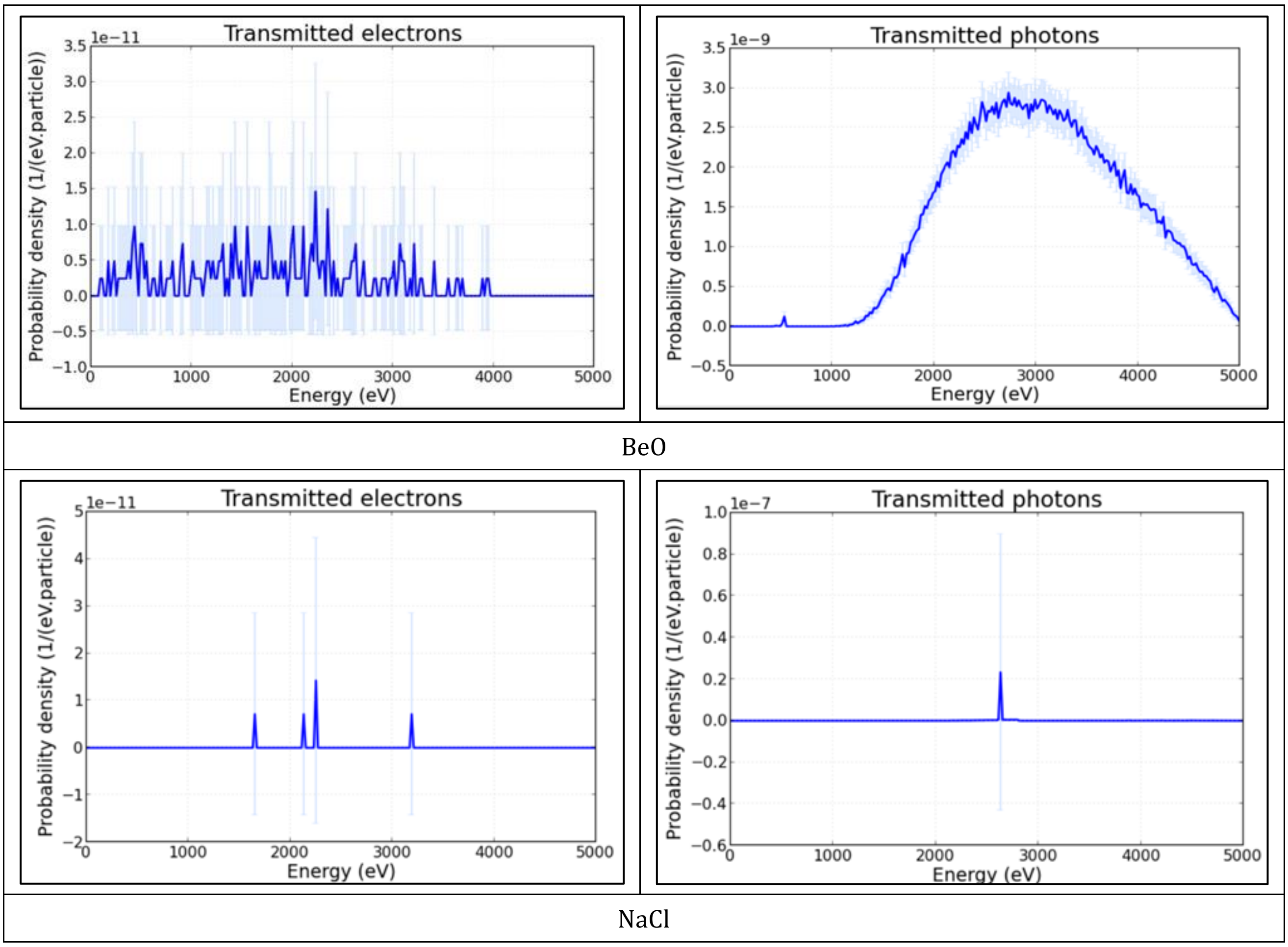
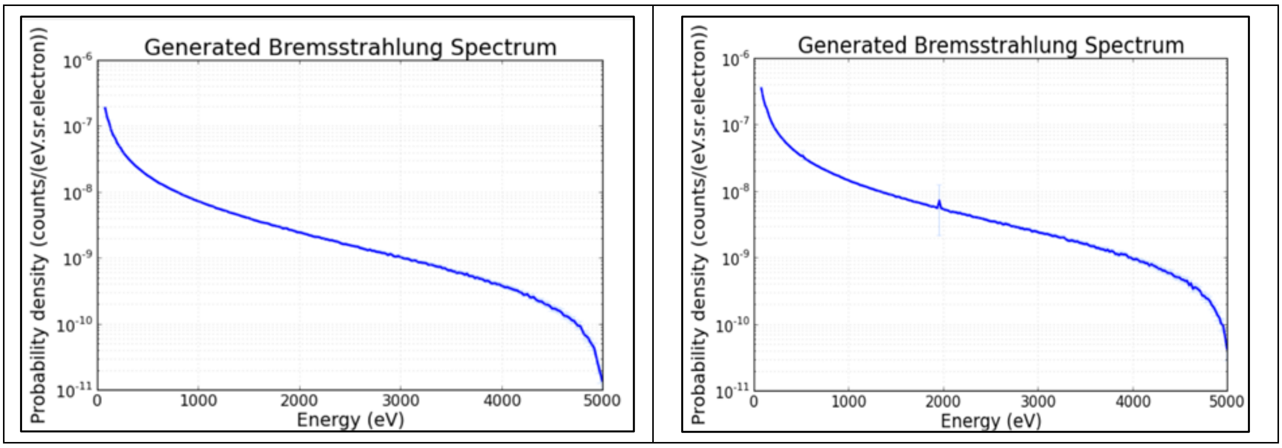


Figure 2 Probability density of particles transmitted as a function of energy

3.3. Spectrum of the photon Bremsstrahlung

During the incidence of primary electrons on BeO and NaCl, the electronic relocation on the layers of materials is illustrated by the presence of various phenomena such as the Bremsstrahlung photon spectrum, the characteristics and fluorescence of the sub-electronic transition layers. The figure 9 below shows the variation in particle probability density as a function of energy.



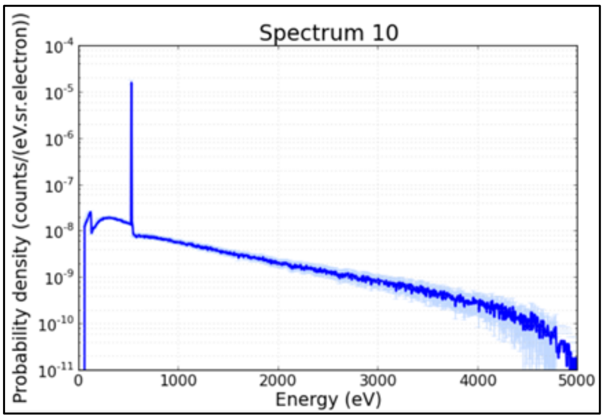
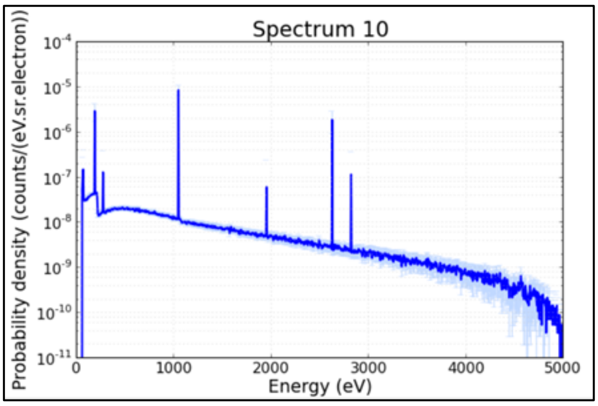
	
BeO	NaCl

Figure 3 Brake radiation photon spectrum, characteristic and fluorescence of the electron transition sublayers

4. Discussion

According to Tables 1 and 2, For the incidence of primary electrons, the fractions of particles transmitted are very small because more than 91.91% and 81.26% were absorbed by BeO and NaCl respectively. The backscattered fractions are 8.9% and 20.38% for BeO and NaCl respectively. Their collusion with the material will produce many interactions between electrical charges due to the exchange of photons.

Regarding the secondary particles, only for the secondary electrons, a very large part is absorbed by both materials. 0.8% and 1.63% of secondary electrons are backscattered for BeO and NaCl respectively. Very small fractions of secondary photons are backscattered for both materials.

These fractions of the particles absorbed, backscattered and transmitted are due to an electron incidence of 5KeV on the materials. During the simulation, secondary particles were produced and interacted. The incidence energy of primary electrons was distributed at a microscopic level through the electron layers and sub-layers of the atoms that make up the materials chosen in our study. Figure 3 shows the probability density of secondary particles as a function of energy evolution in an interval of 0 to 5KeV. The same energy spectrum of the backscattered electrons was observed for both materials with a slightly low probability density for NaCl. For backscattered photons, a single peak was detected at 0.5KeV for BeO and three peaks were detected at 0.1KeV, 1KeV and 2.5KeV for NaCl. These peaks are justified by the energetic distribution of oxygen from BeO and KL2, KL3, KM2, KM3, L3M1, L3M3, L2M1, L1M3, L1M2 of chlorine and KL2 and KL3 of sodium from the NaCl material on the sub-shell KL2 and KL3.

The typical values of the bonding energy of the Be substrate K1s is 0.188KeV and those of Oxygen are 0.543 KeV and 0.04 KeV for the substrates K1s and L12s respectively [3]. Also, those of the sub-shell K1s, L_12s, $L_22p_{1/2}$, $L_32p_{3/2}$ give 1.070 KeV; 0.063 KeV; 0.0306 KeV; 0.0308 KeV and 2.822 KeV; 0.270 KeV; 0.202 KeV; 0.200 KeV for sodium and chlorine respectively [18**Error! Bookmark not defined.**]. The incidence of electrons with an energy of 5 KeV on BeO and NaCl materials is well above the typical values of electronic sub-shells. Therefore, it would justify the particle propagation properties in the materials studied. The analysis of shell and electron sub-shells has proved to be an effective means for the interpretation of microscopic interaction phenomena. A recent study on the MgO/TiO2 material from Allangba K.N.P.G et al. confirms this type of phenomenon at the level of the electronic sub-shells [4]. Indeed, these high-energy electrons must release energy to fill the lower energy gaps in the atom. These generated photons can be classified as radiation contamination for the material. Therefore, potential radiation contamination consists of generated X-rays, including the continuum (Bremsstrahlung), X-ray characteristics and fluorescence [5].

The particulate occupation of these shell and sub-shells of oxygen, chlorine and sodium are responsible for these phenomena. The electron exchanges an unobserved photon with the nucleus of the atom so it emits a photon that will be observed, the braking photon.

5. Conclusion

The Monte Carlo simulation method by PyPENELOPE software has proven to be a robust tool for particle propagation properties. The absorption, backscattering and transmission fractions to the propagation of materials, we were able to explain the displacement of primary and secondary particles on the electronic sub-shells of the atomic structures of beryllium, oxygen, sodium and chlorine according to their energy level. Under an incident energy of 5 KeV of primary electrons, despite a very low fraction of transmission of particles in BeO and NaCl materials, microscopic analysis showed by the density of probability as a function of energy, the presence of electron and secondary photon emission spectra. These secondary particles are responsible for several interactions that govern their propagation in the layers and sublayers of the constituent atoms of the material. This propagation causes phenomena such as characteristic underlayers, fluorescence and Bremsstrahlung. These interactions were produced on the sub-layers of oxygen, chlorine and sodium atoms. These properties can therefore improve the performance of other materials in the manufacture of advanced technology devices such as synchrotron, clinical particle accelerator and X-ray tube.

Compliance with ethical standards

Disclosure of conflict of interest

No conflict of interest to be disclosed.

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