

Uniform Factor Modeling with the Relativistic Stopping Power of (IV) Silicon-Carbide (Si-C) Targeted Semiconductor Material against the Sourced Energetic Radiation.

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Abstract: Ion irradiation is used to analyze and modify the structure of condensed matter. It can for instance be used to form and shape nanocrystals in solids as the understanding of the fundamental processes that take place in material under ion irradiation is important for all these applications of ion beams, and great interest from a basic science point of view. The mechanisms involved during ion irradiation-induced displacement of atoms in uniform bulk solids are fairly well understood and described in the literature, but many unresolved questions remain regarding the structural modification caused by electronic interactions, and the radiation response of materials with phase boundaries. Especially ion irradiation of nanomaterials is a topic that is under active research. The short-lived collision cascades caused by energetic ions in solids cannot be studied in experiments and are therefore often modeled in computer simulations. Such simulations can give a host of valuable information about processes that occur in nature. It is necessary to validate simulation results by either some other computational method or ideally by experiments. In this article, molecular dynamics simulations were conducted through an online based simulation at maximum and minimum energy levels of 10 and 90 MeV in studying the nature of nuclear-stopping potentials of silicon-carbide semiconductor materials with a uniform factor theory. Logarithmic models were eventually deduced both from the silicon-carbide [$y = 0.3110 \ln(x) + 2.1812$ ($R^2 = 0.9845$)] and empty material systems [$y = 0.4098 \ln(x) + 1.9024$ ($R^2 = 0.9998$)]. Meanwhile, the integration of computer simulations and experimental observations are actively required to explain the complex processes during ion irradiation.

Keywords: Nuclear stopping power, relativistic, silicon-carbide, semiconductor and logarithm models.

1.0 INTRODUCTION

Part of the effective experimental techniques for testing the structure of matter has been charged particle beams. In the famous Geiger-Marsden experiment, it was early experiments on charged alpha particles occurring on thin gold foils that helped to develop the Rutherford planetary atom model in 1911, with Niels Bohr modification in 1913[1]. Years after these developments, a research team with the CERN project engaged colliding beams of particles to investigate the nature of the universe and the processes in explaining the structure of the atom [1]. Ion beam technology has progressed immensely in the hundred years that have passed since the Geiger-Marsden experiment and has performed an important role in the evolution of the modern computer via silicon doping for integrated circuits. Although Bohr may be renowned for establishing the atomic model on quantum physics and developing the concept of how charged particles are associated with the matter or the stopping theory as regarded in contemporary times [2]. Moreover, since then, the models illustrating ion energy loss have been modified by Bethe, Fermi, Lindhard, and several others. In the analysis of solid-ion relationships, theoretical models, such as binary collision approximation and

molecular dynamics simulations, the models have proven to be incredibly valuable. For the regulated use of the beams of ions in technological processes, knowledge of the processes that occur when ions interact with the matter has been crucial. The most significant industrial process involving ion beams is probably silicon ion implantation doping in the manufacture of the small integrated circuits that make up modern computers [1]. Although other doping approaches have been used as the dominant approach in today's semiconductor industry is ion beams [1]. In the microchip, the fundamental operating mode is the same as in the 1970s approach. However, there are experimental attempts to replace traditional microchips with optical functionality alternatives. A proposed material for such optoelectronic circuits is semiconductor silica nanocrystals formed by ion implantation and annealing [3]. In modern technology ranging from nuclear fission/fusion reactors to semiconductor devices for space flights, to cancer therapy focused on ion beam radiation [4]. Understanding the stopping mechanism of highly energetic ions in condensed matter structures has significant implications. In a substance in the stopping step, the dynamic strength of irradiating energetic ions is dissipated, a fundamental process in which

stored energy becomes available through different mechanisms to cause structural transitions. Functionally, according to the nature of excitation emitted, the stopping phase is classified into two as low ion velocities where the main impact is the Nuclear stopping, which contributes mainly to excitation of the lattice and displacement of the nuclei and the related electronic excitations at high rates in Kev, thus the phrase 'electronic stopping'. In general, the mean rate of energy transmission from the ion to the target material is determined in terms of the unit distance of motion of the projectile ion, and this is considered stopping power [5]. In condensed matter, the stopping ability of a radiating species is characterized by the kinetic energy potential (E) against the unit length.

$$S = -\frac{dE}{dx} \tag{1}$$

With the recognition that there is a force component to the stopping power, hence the stopping force that consists of two components: the nuclear stopping power (Sn), which entails the loss of energy due to collisions with the target nuclei, and the (Se) electronic stopping power, which results from the excitation of the target electrons. The electronic component becomes the vastly dominant contribution as soon as the kinetic force with the impinging ions is greater than a few tens of Kev/amu. The net stopping effects is given as the addition of the two forms of stopping:

$$S = S_n + S_e \tag{2}$$

The first reliable and acceptable theories to study the phenomena of stopping power were proposed by Bohr [7] and Bethe [8]. In reality, the earlier works were conducted by Thomson and Darwin [9] as they decided to solve numerous limitations and problems. In many applications, the work of both Bohr and Bethe is still being used, as only in the case of swift particles can a nice result be achieved compared to the experimental data. The electronic stopping theory of Bohr considers the energy transfer from a point charge projectile to classical electrons harmonically attached with a resonance angular frequency to the atoms of the target, say! The following formula of the electronic stopping power cross-section was obtained by Bohr within a classical perturbation process.

$$S(Z, v) = \frac{4\pi Z^2 e^4}{m_e v^2} L_{Bohr} \tag{3}$$

With the Bohr stopping number

$$L_{Bohr} = \sum_j f_j \ln \left(\frac{C m_e v^3}{Z e^2 \omega_j} \right), \tag{4}$$

As C=1:1229, fj values reflect the distinct relative contributions as J values that are subject to $\sum_j f_j = 1$. Bohr's theory is only applied for weak interactions as the classical perturbation principle was derived with the stopping model. Furthermore, to simplify the problem, Bohr considered two estimations as to the dipole interpretation and interaction of the particle with the electrons with treatment on the premise that the strength of the relationship of the Coulomb does not differ extensively with the electron's range of movement. Also, the momentum estimation in which the direction of the projectile does not change as the targeted radiations (electrons) remain static. The impact parameter between the direction of the particle and the target nucleus is limited to maximum and minimum values, bmax and bmin, in the Bohr method. Bethe [8] has derived an alternative stopping power formula. In terms of quantum mechanics, unlike Bohr, for the case of the high-velocity projectile, Bethe derived a stopping formula. It is possible to express the classical expression Bethe stopping formula for a free electron gas target as [10]

$$S(Z, v) = \left(\frac{Z e \omega_p}{v} \right)^2 \ln \frac{2 m_e M_p v^2}{(m_e + M_p) \omega_p \hbar} \tag{5}$$

Where v, Ze, and Mp represent the velocity, charge, and mass of the projectile. P refers to the classical frequency of plasma that is acquired with the relation

$$\omega_p = \sqrt{\frac{4\pi n e^2}{m_e}}$$

Where n is electron number density and I is the electron mass. Also, the stopping power in Eq 5 for heavy projectile Mp Me. decreases to:

$$S(Z, v) = \left(\frac{Z e \omega_p}{v} \right)^2 \ln \frac{2 m_e v^2}{\omega_p \hbar} \tag{6}$$

Two hypotheses have been used in this derivation: the Coulomb excitation and ionization of the target electrons resulted in the stopping. The stopping letter L Bethe reads, thus,

$$L_{Bethe} = \sum_j f_j \ln \left(\frac{2 m_e v^2}{\hbar \omega_j} \right), \tag{7}$$

About when $\sim J$ is the intensity equivalent to the jth electron excitation in the target atom and fj is a standardized power

of the oscillator. In theory, the electronic activation of j th is quite

difficult to calculate, rather we can compute the expected excitation energy. The average energy for excitation is characterized as

$$\ln I = \sum_j f_j \ln(\hbar\omega_j). \tag{8}$$

It can be approximated empirically using a widely used scaling relationship [10]:

$$I \approx Z_2 \times 10 \text{ eV} \tag{9}$$

The results with the electronic stopping effect of proton passing through Si target to judge the accuracy of using both Bohr and Bethe theories in the prediction.

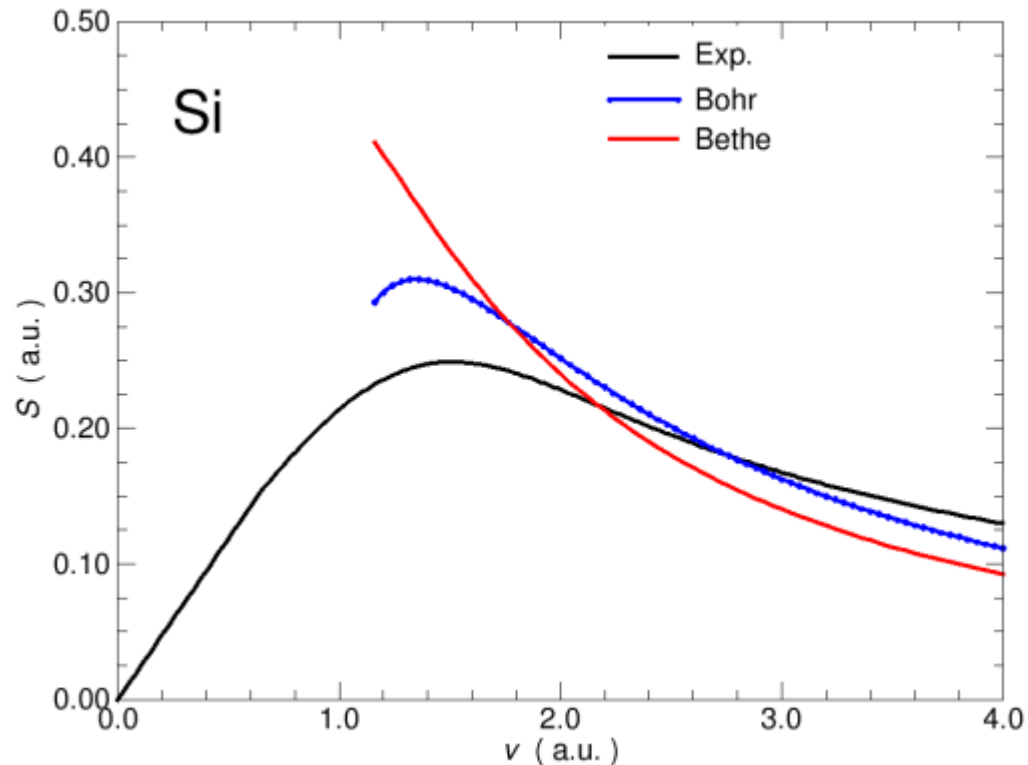


Figure 1. The projectile velocity was determined using both Bohr's formula (blue line) and Bethe's formula, electronic stopping power as a guide, an experiment from the PSTAR database[11] (black line).

Through sintering processes, silicon carbide materials can be bonded into durable ceramics products with typical applications in car brakes, clutches, and bulletproof vest with ceramic plates. Around 1907, electronic SiC uses with the light-emitting diodes and sensors in early devices were first displayed. SiC is often used in electronic semiconductor materials running at high voltages and temperatures [6]. The primary objective in modeling the electronic stopping potential is to simulate the stopping of any projectile against any stopping target medium. By applications, stopping power data is only required as input data for subsequent estimations [7]. Therefore, an empirical system, that provides desired stopping data, as the most direct method is adopted. The objective of this research is to mathematically model a theory of how material irradiation Carborundum is a

composite of semiconductors with silicon and carbide (SiC). It exists as the extremely scarce mineral moissanite in nature. Injury is affected by nuclear and electronic shielding of ions. Molecular dynamics simulations of ion irradiation in silicon carbide semiconductor.

2.0 METHODOLOGY

The SR-NIEL web base simulator was adopted in studying the Screened Relativistic of non-dissociated energy demands of electrons, protons ions, and neutrons passing through an absorber silicon carbide semiconductor (1 :1), based on the screened relativistic treatment for (elastic) Coulomb interactions on nuclei from low up to ultra-relativistic energies (10 to 100 MeV) under uniform form factor condition.

3.0 RESULTS AND DISCUSSION

Table 1. The simulated Silicon-carbide and non-semiconductor energy /nuclear stopping power profile

Energy (MeV)	Nuclear Stopping Power with SiC (MeVcm ² /g) X 10 ⁻⁴	Nuclear Stopping Power without SiC (MeVcm ² /g) X 10 ⁻⁴
10	2.85	2.85
15	3.01	3.01
20	3.11	3.13
25	3.20	3.22
30	3.26	3.30
35	3.31	3.36
40	3.36	3.41
45	3.39	3.46
50	3.42	3.51
55	3.45	3.54
60	3.47	3.58
65	3.48	3.61
70	3.50	3.64
75	3.51	3.67
80	3.52	3.70
85	3.53	3.73
90	3.54	3.75

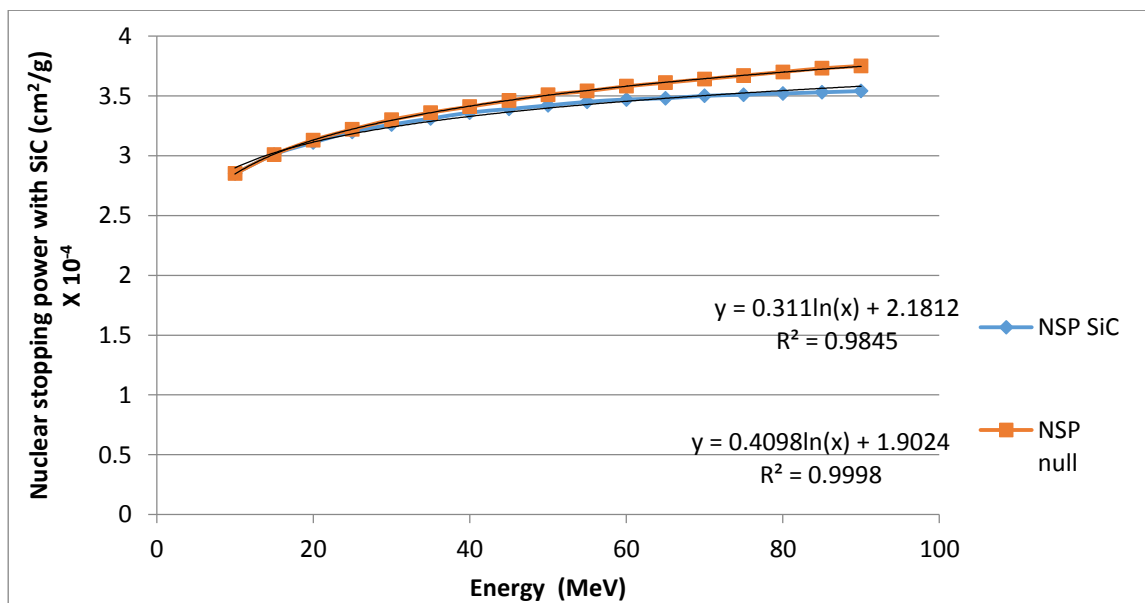


Figure 1. Logarithmic models with silicon-carbide semiconductor composite and without

The computed inputs and the outputs data concerning the energy and the stopping power of the silicon-carbide semiconductor material and without were depicted in table 1. Two distinct logarithmic models under uniform factor condition with the Si-C [NSP = 0.311 In (Energy) + 2.1812 at R2 of 0.9845] and without [NSP= 0.4098 In (Energy) + 1.9024 at R2 of 0.9998]. These outcomes justify the theoretical background of high-velocity sources of nuclear radiation (ions, protons, α particles, and electrons) discharge against an absorber and that higher velocity is necessary for the stopping effects just like in Figure 2.1 that shows that both the Bohr formula and Bethe formula are valid only for large velocity.

4.0 CONCLUSIONS

Two models that calculate the electronic stopping power of silicon carbide (SiC) and without SiC for protons and α -particles, under uniform dynamics simulations have been generated. The equations actively can be explored in determining the stopping power at any level or rate of energy generated by any classical radiation against the absorber under study. Despite this significant headway with the accurate estimation of the electronic stopping power of silicon carbide, associated physical quantities like temperature, density with other factor models could be explored further investigation into the accuracy of the stopping potentials of SiC and other semiconductor composites.

5.0 REFERENCES

1. Marie Backman (2012). Effects of nuclear and electronic stopping power on ion irradiation of silicon-based compounds. Helda.helsinki.fi. https://helda.helsinki.fi/bitstream/handle/10138/37606/backman_dissertation.pdf;sequence=1
2. Physics and physicists (2007). <https://physicsandphysicists.blogspot.com/2007/07/>
3. Mary Coan (2007). Silicon Quantum Dots Grown by Ion Implantation and Annealing. http://www2.ece.rochester.edu/courses/ECE580/docs/quantumdots_Coan.pdf
4. Dillon C. Yost and Yosuke Kanai (2018). Electronic stopping for protons and α -particles from first principles electron dynamics: The case of silicon carbide. <http://export.arxiv.org/pdf/1805.00557>
5. Michael F. L'Annunziata (2007). Stopping power. Stopping Power - An Overview <https://www.sciencedirect.com/topics/earth-and-planetary-sciences/stopping-power>
6. G. S. Was (2007). Fundamentals of Radiation Materials Science. Springer-Verlag, Berlin, Heidelberg.
7. N. Bohr. On the theory of the decrease of velocity of moving electrified particles on passing through matter. *Phil. Mag.*, 23(2):10–31, 1912.
8. H. Bethe. Zur theorie des durchgangs schneller korpuskularstrahlen durch materie. *Ann. Phys., Lpz.* 397:325–400, 1930.
9. C. G. Darwin. A theory of the absorption and scattering of the α rays. *Phil. Mag.*, 13:901–20, 1912.
10. J. Ortner and I. M. Tkachenko (2001). Stopping power of strongly coupled electronic plasmas: Sum rules and asymptotic forms. *Phys. Rev. E*, 63:026403.
11. M.J. Berger et al (2005): Computer programs for calculating stopping-power and range tables for electrons, protons, and helium ions (version 1.2.3).
12. En.wikipedia.org. (2020). Silicon Carbide. https://en.wikipedia.org/wiki/Silicon_carbide
13. James Ziegler et al (2010). The Stopping and Range of Ions in Mater. *Nuclear Instruments and Methods in Physics Research Section B Beam Interactions with Materials and Atoms* 268(11-12):1818-1823 10.1016/j.nimb.2010.02.091