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EFFECTIVENESS OF GEANT4 IN MONTE CARLO SIMULATION STUDYOFPHONON CONDUCTION IN Sn HOST WITH SI NANOWIRE INTERFACE

C. Iheduru[1,3,*], M. A. Eleruja[1], B. Olofinjana[1], O. E. Awe[1,2], A.D.A Buba[3]

[1]*Department of Physics and Engineering Physics, Obafemi Awolowo University, Ile – Ife. Nigeria*

[2] *Department of Physics, University of Ibadan, Ibadan, Nigeria*

[3] *Department of Physics, University of Abuja, Abuja, Nigeria*

** iheduruc@gmail.com*

Article Info	Abstract
Received: 06.02.2019 *Accepted: 27.06.2019* **Keywords:** Ballistic conduction, heat flow, MC simulation, Silicon – Tin, Geant4.	We have explored the effectiveness of Geant4 by using it to simulate phonon conduction in Sn Host with Si Nanowire Interface. Our Monte Carlo Simulation shows that the effectiveness of the phonon conduction Geant4 simulation increases when the system attained a steady state of 100 time steps. We have simulated phonon conduction in Sn host with Si nanowire interface using a Geant4Condensed Matter Physics Monte Carlo simulation toolkit in a low cost and less powerful processing computer machine. In the simulation, phonons were displaced inside a computation domain from their initial positions with the velocities and direction vectors assigned to them. A time step was selected so that a phonon can move at most the length of one sub-cell in one time step. Our phonon conduction analysis of SiSn based alloy using Geant4 showed performance enhancement and reasonable predicted thermal values. Numerical predictions of the thermal profile simulations of the values of the temperature in each cell were all within ten percent of the average temperature of Silicon – Tin.

1. Introduction

Simulation study of phonon conduction in Silicon – Tin (SiSn) in High Energy Physics (HEP) and solid state physics using Monte Carlo technique often requires a package that can determine an experimental setup in real time, optimize the transport and shielding locations to obtain decent result in experiment, compare results simulated with experiment to ascertain avoidance of error in analysis or simulation code and correct the experimental results by comparing them with simulated results with inputs from theory [8]. When comparing with other methods such as Molecular dynamics, Fourier functions and their likes,

the Monte Carlo method using GEANT4 is among a few methods that can reduce time cost to compute large-scale data in less than an hour [6]. There have been various coded packages invented to achieve these goals. Some of these codes include Qwalk, Scienomics Chameleon and Zori. However, high computation cost, not beingfreely available under an open source license and delay in debugging these cod packages on time by developers are major drawbacks which hinders their effectiveness for simulation study of phonon conduction in Sn Host with Si Nanowire Interface [6].

The acronym 'Geant' was invented in the 1970's to name a code that simulated 'Ge'ometry 'an'd 't'racking for particle physics experiments. At a point it was also decided that the program would be given the form of a toolkit allowing the user to easily extend the components of all domains. This new phase of development led, in 1998, to the first production release of Geant4 [4], [2], a sophisticated C++ based Monte Carlo simulation toolkit maintained by an international collaboration and freely available under an open source license [8], [3] that has now been adopted by fields other than particle Physics, such as space science, material science, solid state physics and medical physics and nuclear science [6].
We then investigate in this work, the effectiveness of Geant4 for simulating phonon conduction in Sn host with Si nanowire interface. This is with a view to finding areas for improvement.

2. Computation methods and samples

The simulations are performed in computational platforms consisting of Intel Core i7 processors running at 2.13 GHz, with 8 Gb of random access memory RAM. The simulations are done for two models; gray model and non – gray model phonon conduction in bulk Sn, and phonon conduction in Si nanowires fixed in Sn host respectively. A simulation model with a sub-cell in Y and Z direction and analogously longer X dimension is first observed to substantiate the computation model and application. A Geant4 simulation run usually follows the following sequence; particles to be transported are specified, updating the Particle Time, determining the Interaction Length or Mean Free Path and transportation domain.

2.1 Particle Transport

The combined steps of the Geant4 kernel's stepping manager class produce particle transport in Geant4 [2]. (D. Brandt, 2011) suggests that Geant4 kernel's stepping manager class enables a sped up development schedule resulting in a fast, dependable and

authenticated simulations. The ensuing developed application is a very precise customised simulation which, at the top level, works in the same manner to other general purpose conduction codes. GEANT4 is mainly used for simulating the transport of particles through matter, with special application areas including high-energy, nuclear and accelerator physics [6]. (S.D. Monk et al., 2107) in his work suggest that the simulation kit basically comprises of a kernel which utilises the transportation functions, and a front end guided user interface (GUI) that is utilised to call the GEANT4 kernel as well as tailor the proposed model within developer-defined limits [3]. GEANT4 differs from other simulation packages in its capability to rewrite and modify selected parts of the computation. This is specifically important when building the needed computational physics engine that can be customised to suit a given assignment [6]. This permits developers to design tailored physics models which models the root physical processes to a stepped up level when contrasted to models used in other, more non-specific computational packages [1],[5],[7]. An unknown sample *x* is used to show combination and rejection method. The anticipated length at which interactivity was presumed to occur was found by polling all processes applicable at each step. Then it was found whether the particle will stay within the current volume long enough - otherwise it will cross into a different volume before this potential interactivity occurs. The most specific steps for finding the trajectory of a charged particle, including boundary crossing and the effects of external fields are the multiple scattering processes and the transportation process. Suppose the sample *x* is to be sampled in the interlude $[x_1,x_2]$ from the scattering f (x), the normalised probability density function can thus be written as [8]:

$$f(x) = \sum_{i=1}^{n} N_i f_i(x) g_i(x) \quad (1)$$

where $N_i > 0$, $f_i(x)$are normalised density functions on $[x_1, x_2]$,$g_i(x)$ are normalized probability functions and $0 \leq g_i(x) \leq 1$

It can be shown that the average trials to accept a value are$\sum_i N_i$ [1].

Practically, a method of sampling from the scattering $f(x)$ has the ensuing properties [7]:

a. every single sub scattering$f_i(x)$ can be analyzed easily;
b. the rejection functions $g_i(x)$ can be sampled quickly
c. the average number of tries is moderate. [7]

Therefore, the various likely decompositions of the scattering$f(x)$ are not the same in

practice (as they can be very divergent in speed of simulation) and it can be important to utilize the decomposition [8]. If our distribution is not normalized

$$\int_{x_1}^{x_2} f(x)d(x) = \boldsymbol{C} > 0 \tag{2}$$

the method can be used in the same manner; the mean number of trials in this case is thus $\sum_i N_i/C$, where C is the computation speed [5].

2.2 The Interaction Length or Mean Free Path

Simulation of average free path of a particle in a model was carried out in Geant4 using cross section of a specific physics process and density of atoms. In a simple material, it shows that the number of atoms per volume is [5]:

$$n = \frac{N\rho}{A} \tag{3}$$

where N is the Avogadro's number, ρ the density of the medium and A the molar mass.
For a compound material the number of atoms per volume of the i^{th} element is:

$$n_i = \frac{N\rho w_i}{A_i} \tag{4}$$

Where w_i is the proportion by mass of the i^{th} element and A_i mass of a mole of the i^{th} element.
The mean free path of a process, λ, also called the interaction length, can be given in terms of the total cross section [5]:

$$\lambda(E) = (\sum_i [n_i . \sigma(z_i, E)])^{-1} \tag{5}$$

where $\sigma(z_i, E)$ is the total cross section per atom of the process and the summation runs over all elements making up the material. $\sum_i [n_i . \sigma(z_i, E)]$ is also called the macroscopic cross section. The mean free path is the inverse of the macroscopic cross section. Cross sections per atom and mean free path values may be calculated during initialisation [8].

2.3 Updating the Particle Time

After each step, the laboratory time of a particle should be updated using the equation [6]:

$$\Delta t_{lab} = 0.5\ \Delta x \left(\frac{1}{v_1} + \frac{1}{v_2}\right) \tag{6}$$

where Δx is a true step length covered by the particle, v_1 and v_2 are particle velocities at the onset and at the end of the step correspondingly. This is done in order to establish additional step limitation.

2.4 Transportation

In order to determine the geometrical limits of a step, the transportation process is undertaken [2]. All six surfaces are assigned reflecting boundary conditions [9].We also modeled one-speed phonons and isotropic scattering. There are no survival biasing or other variance reduction methods as the Monte Carlo algorithm is only analog. The number of phonons per propagation is sustained and designated by N.

An equation can be given by Geant4, for the case a magnetic or electromagnetic field, or can be given for other fields [10].

$$\frac{d\vec{p}}{ds} = \frac{1}{v}\vec{F} = \frac{q}{v}\left(\vec{E} + \vec{v} \times \vec{B}\right) \tag{7}$$

Where $\frac{d\vec{p}}{ds}$ is the change in density with distance, $\vec{F}$ is the force, $\vec{E}$ is the electric field, $\vec{v}$ is the velocity of particles, q is the electric charge and $\vec{B}$ is the magnetic field.

Extensions are provided for the propagation of the polarization, and the effect of a gravitational field, of potential interest for cases of slow neutral particles. Because of the convolution of the integral at the exponent, generation of stochastic free flights with the distribution of the equation above is not feasible in practice. Simulators use a fictitious "self-scattering" scheme [8]in order to overcome this difficulty. When simulators do these, the total scattering rate, including this self-scattering is continuous by random selection, which means if self-scattering is selected, k′ after the collision is the same as k. The simulation time used for self-scattering is more than covered for by the elimination of superfluous details in the calculation of the free-flight duration [2]. To increase the speed of free flight time calculation, several schemes such as "Constant Technique", and "Piecewise Technique" are used to

reduce the self-scattering events [4].

A propound step is correct if the magnitude of the location components of the error is below a tolerated fraction ε of the step length s [5].

$$|\Delta x| = |x_{error}| < \varepsilon * s \tag{8}$$

and the relative momentum error is also below ε:

$$|\Delta p| = |p_{error}| < \varepsilon \tag{9}$$

The ballistic conduction also updates the time of flight of a particle [2]. It uses the average inverse velocity (average of the onset and end value of the inverse velocity) in the case of a neutral particle or of a charged particle in a pure magnetic field [4]. Likewise, an explicit integration of time along the track is used in the case of a charged particle in an electric field or other field which does not preserve the energy [5]. Integrating the inverse velocity along the track, we have [8]:

$$t_1 = t_0 + \int_{s_0}^{s_1} \frac{1}{v} ds \tag{10}$$

3. Results and discussions

Figure 1 shows the temperature profile in the mid plane of the central cross section (Y=100 nm) in the computation domain after 1 nanosecond. Figure 2 shows accumulation of phonons at the nanowire interface. Figure 3 shows the log scale variation of energy with time in the domain.

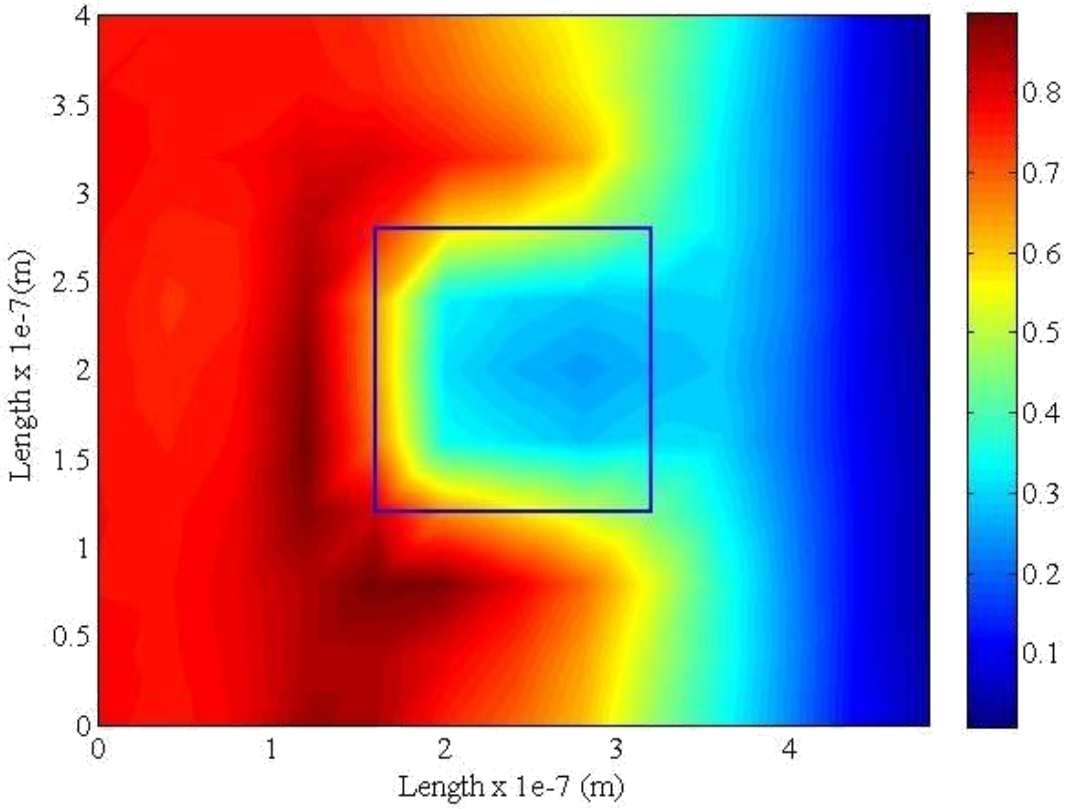

Figure 1: Temperature profile in the mid plane along the length of transport domain

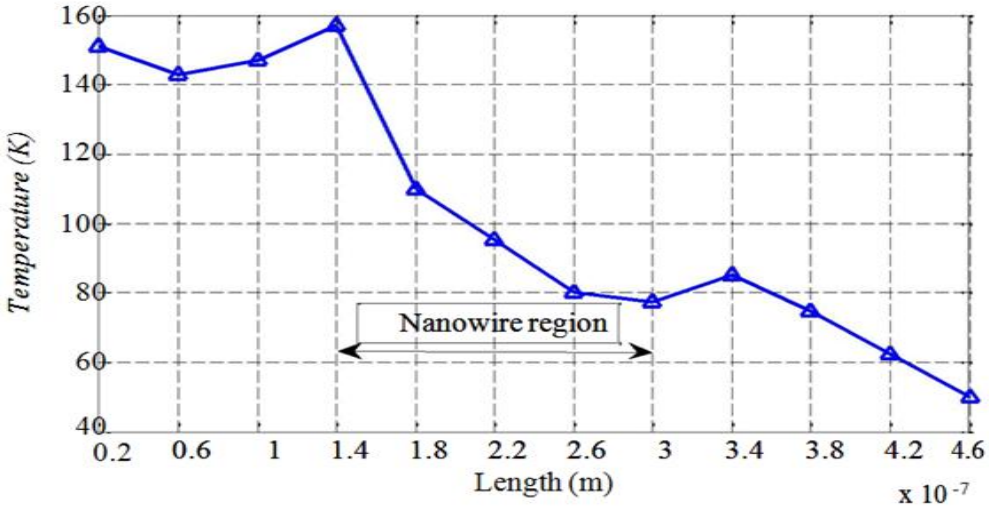

Figure 2: Accumulation of phonons at the nanowire interface

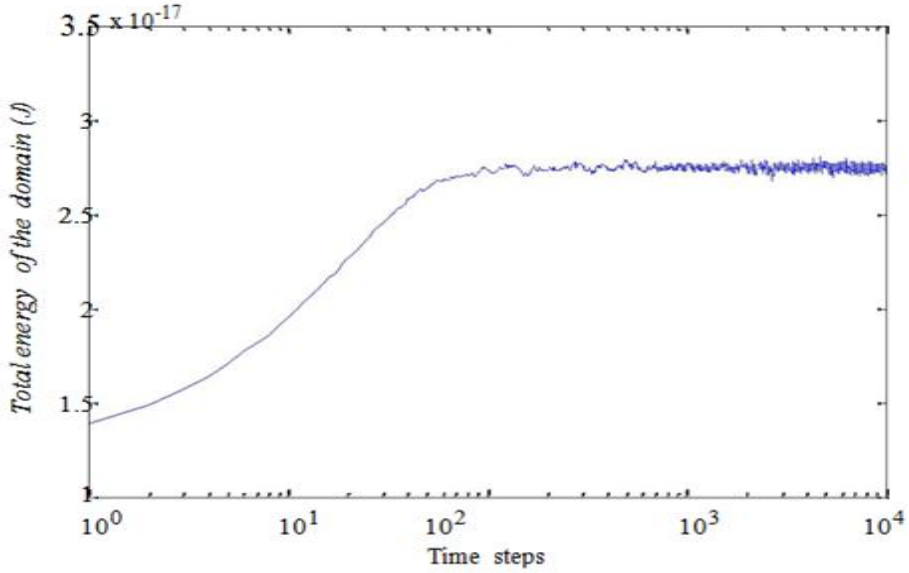

Figure 3: Log scale variation of total energy of the computation domain with time.

For the thermal profile simulations reported in Figure 1, the length of the simulated nanowire met the requirements reported by Succi [10], whose study reported that the temperature profile remains linear and that no temperature jumps appear in the two ends. For the thermal profile simulations reported here (Figure 1), the values of the temperature in each cell were all within ten percent of the average temperature and the temperature profiles were essentially linear at the two ends of 150 and 50 K, just as reported by Succi [8]. An explanation for this anisotropy is offered based on *a* detailed examination of ballistic conduction carried on SiSn at cryogenic temperatures [10]. However, there were slight jumps at the nanowire region with temperature increases from 80 to 90 K and then, a drop to 70 K at length 2.2 nm, 2.3 nm and 3 nm, respectively. This is due to resistance provided by the silicon nanowire at the center of the domain to the heat transfer process.

In the center of Figure 2, where the nanowire is placed, a lighter shade than the boundaries indicate an accumulation of phonons at the nanowire interface, suggesting the resistance being provided by the nanowire to the heat flow. The maximum temperature was now at the nanowire interface not at the boundary and this affirms the findings of Mazmudar and Majumdar (2010) that reported the resistance of silicon nanowire due to phonon accumulation at the nanowire region of a small domain length in their Monte Carlo simulation of phonon conduction of solid films. The value of the times steps is 100.

A study on the influence of the value of the time step on the results previously reported showed that the “noise” observed after more than 100 steps is not entirely a numerical

problem but of a white *noise* process *over* an interval and is thus well defined, even when intermittently observed [3]. The log scale variation (Figure 3) indicates that the total energy of the domain stabilizes, approximately at the 100 time step after which it fluctuates around a constant value which is in agreement with the findings of Singh *et al.* [8], in his analysis of phonon transport in nanocomposites. The result suggests that the system attained a steady state after 100 time steps as energy no longer varied with time. At this point, the thermal conductivity of the composite structure can be calculated, and the effectiveness of the simulation evaluated.

4. Conclusions

We have explored a low cost Geant4 Monte Carlo simulation of phonon conduction by simulating phonon conduction in Sn Host with Si Nanowire Interface to study the effectiveness of Geant4 simulation package. Geant4 simulation effectively predicts the thermal profile simulations of the values of the temperature in each cell were all within 10% of the average temperature and the temperature profiles were essentially linear at the two ends of the domain, therefore, confirming Geant4 package results in smaller approximation error.

This study also found out that improvements to the Geant4 package could be made to enhance its reading at nanowire region beyond 70K.This study also opens up further exploration opportunity for Geant4 software package for simulating phonons as well as electrons in semiconducting nano sized materials.

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