Physica A 406 (2014) 185–190

Contents lists available at ScienceDirect

Physica A

journal homepage: www.elsevier.com/locate/physa

A Wigner approach to the study of wave packets in ordered and disordered arrays of dopants

J.M. Sellier*, I. Dimov

IICT, Bulgarian Academy of Sciences, Acad. G. Bontchev str. Bl25A, 1113 Sofia, Bulgaria

HIGHLIGHTS

- We study the dynamics of a wave packet in the presence of the ordered and disordered arrays of dopants.
- We utilize the signed particle Wigner Monte Carlo method.
- We show how the particle current is affected by the disorder in the dopant positions.

ARTICLE INFO

Article history:
Received 17 January 2014
Available online 24 March 2014

Keywords:
Wigner equation
Monte Carlo methods
Arrays of dopants
Quantum electron transport

ABSTRACT

We study the evolution of a Gaussian wave packet in the presence of the ordered and disordered arrays of dopants, described by means of Coulombic potentials. As a first step, we investigate the dynamics of the packet in three different ordered configurations consisting of two, three and four-columns arrays. Then, random but controlled disorder is introduced and increased constantly by perturbing the initial position of the dopants by a given amount of noise. The effects over the dynamics of an electron wave packet are clearly observable in the simulation results. After a detailed investigation for different values of perturbation, 20%, 40% and 60%, on three different dopant arrays, one concludes that the best performance, in terms of conductance and current, is achieved for ordered arrays of dopants, in perfect agreement with the available experimental results.

1. Introduction

Semiconductor device active lengths are now of the order of only several tens of nanometers due to the continuous process of miniaturization. At that scale, many of the common assumptions such as classical particles, and homogeneous dopant distribution, are not justifiable any longer. Furthermore, quantum effects are now dominant and classically designed transistors do not operate reliably in that regime. We are now in the so-called post-CMOS (complementary metal-oxide-semiconductor) era. This opens opportunities for the development of novel device architectures, most likely to be drastically different from what we have seen in CMOS technologies. It is highly plausible that, in order to be successful, a new design paradigm will be required which exploits in some way typical phenomena of quantum mechanics.

Among the new post-CMOS devices recently proposed, the Silicon based devices exploiting single buried dopants seem to be in a very promising direction [1]. Such class of devices are also considered to be good candidates for realistic quantum computing building blocks [2,3]. It is now possible to build prototypes of such devices in laboratories, experiments are advancing quickly [4–6] and, today, single dopants can be placed even with atomistic precision [7]. While the experiments

* Corresponding author.
E-mail address: jeanmichel.sellier@gmail.com (J.M. Sellier).

http://dx.doi.org/10.1016/j.physa.2014.03.065
0378-4371/

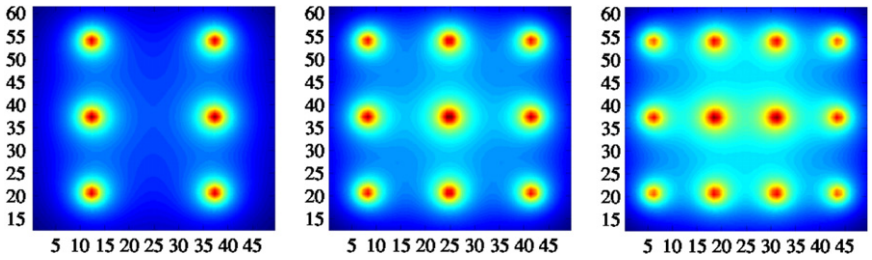

Fig. 1. Ordered arrays of dopants consisting of, respectively, 3×2, 3×3 and 3×4 matrices of Phosphorus atoms buried in Silicon.

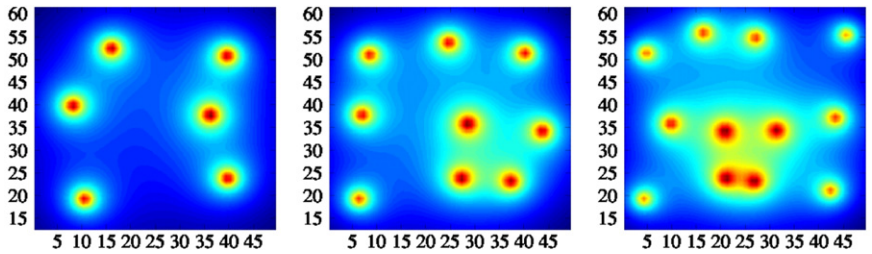

Fig. 2. Disordered arrays of dopants (40%).

are already advancing quickly, the theoretical comprehension of the experimental results is still very basic. Indeed, from a theoretical perspective, this new design paradigm comes with incredible challenges.

In order to achieve reliable and predictive simulations, the new models have to be full quantum and time dependent. Indeed, in nanometer scaled devices the wave-particle duality is a well pronounced phenomenon that cannot be simulated by first-order quantum corrections. Furthermore, in these novel devices, it is not known if a stationary regime eventually can be reached or even exists. Finally, the doping as a continuum is not a realistic hypothesis anymore. It now consists of a discrete number of dopants scattered in some area of the device. A very promising model that seems to cope with the mentioned (and necessary) above requirements is the Wigner equation, an intuitive formulation of quantum mechanics in terms of a phase–space. This approach is equivalent to the Schrödinger equation but has some advantage over it. For example, it allows the inclusion of absorbing (open) boundary conditions in a natural way, allowing the presence of leads attached to the device.

In this work we apply the signed particle Wigner MC method [8–11] to simulate the two-dimensional and time dependent evolution of an electron wave packet in the presence of arrays of dopants in different configurations and absorbing only boundary conditions. For simplicity, we restrict ourselves to the ballistic regime and no injecting boundaries are taken into account in this paper, thus avoiding the problems mentioned in Ref. [12].

We start with ordered configurations consisting of 3×2, 3×3 and 3×4 matrices of dopants (Coulombic potentials) reported in Fig. 1. Leads are attached to the bottom and the top of the devices, i.e. wave packets are free to eventually leave. We then proceed with introducing noise in the position of the dopants by a given amount, i.e. 20%, 40% and 60%. As an example, Fig. 2 reports the distribution of dopants in the case of 40% noise around the initial configuration. We observe how the dynamics of the wave packet is affected by the increasing disorder. From these numerical experiments, by comparing ordered against disordered array results, it is clear that the best performances, in terms of conductance and current, are reached for highly ordered arrays, in accordance with available physical experiments [13]. This shows how the Wigner MC method is reliable and can be used to support, if not to predict, experimental results.

2. The Wigner Monte Carlo method

The Wigner equation is an intuitive formulation of quantum mechanics in terms of a phase–space [14]. It is equivalent to the Schrödinger equation. Indeed a transform, known as the Wigner–Weyl transform, and its inverse operator exist that convert a solution from one formalism to the other (under the mathematical condition that the operator is non-singular) [14, 15]. In a two-dimensional space (2D), in ballistic regime and parabolic energy band, with $\mathbf{x} = (x, y)$ and $\mathbf{k} = (k_x, k_y)$, the model reads

$$\frac{\partial f_W}{\partial t} + \frac{\hbar}{m^*}\mathbf{k} \cdot \nabla_{\mathbf{x}} f_W = \int \mathrm{d}\mathbf{k}' V_W(\mathbf{x}, \mathbf{k} - \mathbf{k}', t) f_W(\mathbf{x}, \mathbf{k}', t). \tag{1}$$

The function $V_W = V_W(\mathbf{x}, \mathbf{k}, t)$ is known as the Wigner potential and defined as

$$V_W(\mathbf{x}, \mathbf{k}, t) = \frac{1}{i\hbar(2\pi)^2} \int \mathrm{d}\mathbf{x}' \mathrm{e}^{-i\mathbf{k}\cdot\mathbf{x}'} \left(V\left(\mathbf{x} + \frac{\mathbf{x}'}{2}, t\right) - V\left(\mathbf{x} - \frac{\mathbf{x}'}{2}, t\right)\right) \tag{2}$$

where $V = V(\mathbf{x}, t)$ is the (eventually time dependent) potential involved in the problem and m^* is the effective mass. By exploiting the semi-discrete nature of the phase–space, in accordance to the principles of quantum mechanics [9], it is possible to rewrite the Wigner equation in a semi-discrete form

$$\frac{\partial f_W}{\partial t}(\mathbf{x}, \mathbf{M}) + \frac{\hbar}{m^*}\mathbf{M}\Delta\mathbf{k} \cdot \nabla_{\mathbf{x}} f_W(\mathbf{x}, \mathbf{M}) = \sum_{\mathbf{N}=-\infty}^{+\infty} V_W(\mathbf{x}, (\mathbf{M}-\mathbf{N}))\, f_W(\mathbf{x}, \mathbf{N}) \tag{3}$$

and the Wigner potential is reformulated accordingly

$$V_W(\mathbf{x}, \mathbf{M}, t) = \frac{1}{i\hbar\mathbf{L}_C} \int_{-\mathbf{L}_C/2}^{+\mathbf{L}_C/2} \mathrm{d}\mathbf{x}' \mathrm{e}^{-i2\mathbf{M}\Delta\mathbf{k}} \left(V(\mathbf{x}+\mathbf{x}', t) - V(\mathbf{x}-\mathbf{x}', t)\right) \tag{4}$$

where $\mathbf{L}_C = (L_C^x, L_C^y)$ is the coherence length [9], $\mathbf{M} = (M_x, M_y)$ and $\mathbf{N} = (N_x, N_y)$ are two couples of integers (pseudo-wave vectors can be described in terms of integers in a semi-discrete phase–space), and $\Delta\mathbf{k} = \left(\frac{\pi}{L_C^x}, \frac{\pi}{L_C^y}\right)$.

The semi-discrete reformulation of Wigner equation (3) allows the development of a Monte Carlo algorithm [8–11]. Indeed, this equation can be rewritten in terms of a Fredholm integral equation of second kind [8,10]

$$f_W(\mathbf{x}, \mathbf{M}, t) = f_W^0(\mathbf{x}, \mathbf{M}) + \int\int\int \mathrm{d}t' \mathrm{d}\mathbf{M}' \mathrm{d}\mathbf{x}' K(\mathbf{x}, \mathbf{M}, t, \mathbf{x}', \mathbf{M}', t') f_W(\mathbf{x}', \mathbf{M}', t') \tag{5}$$

where $f_W^0(\mathbf{x}, \mathbf{M})$ is the initial conditions of the problem and the unknown is the Wigner quasi-distribution function $f_W = f_W(\mathbf{x}, \mathbf{M}, t)$. The solution of problem (5) can be expressed in terms of a Liouville–Neumann series [10] which can be used to calculate the expectation value $\langle A \rangle(t)$ of a macroscopic variable $A = A(\mathbf{x}, \mathbf{M})$ expressed as an iterative series [9]

$$\langle A \rangle = \int_0^\infty \mathrm{d}t' \int d\mathbf{x}_i \sum_{\mathbf{M}'=-\infty}^{\infty} f_W^0(\mathbf{x}_i, \mathbf{M}') \mathrm{e}^{-\int_0^{t'} \gamma(\mathbf{x}_i(y))\mathrm{d}y} g_W(\mathbf{x}_i(t'), \mathbf{M}', t') \tag{6}$$

with

$$\mathbf{x}'(y) = \mathbf{x}_i(y) = \mathbf{x}_i + \frac{\hbar\mathbf{M}'\Delta\mathbf{k}}{m^*} y; \qquad \mathbf{x}' = \mathbf{x}'(t') = \mathbf{x}_i(t'); \quad \mathrm{d}\mathbf{x}' = \mathrm{d}\mathbf{x}_i.$$

The function $g_W = g_W(\mathbf{x}, \mathbf{M}, t)$ is the solution of the adjoint equation [8] and the quantity $\gamma = \gamma(\mathbf{x})$ is defined as

$$\gamma(\mathbf{x}) = \sum_{\mathbf{M}=-\infty}^{\infty} V_w^+(\mathbf{x}, \mathbf{M}) \tag{7}$$

where V_w^+ takes the values of V_w if $V_w > 0$ and 0 otherwise. The technical details of the analytical calculations are given in Ref. [10] as well as in Ref. [11].

Now, a physical interpretation can be given. The quantity $\gamma = \gamma(\mathbf{x})$ can be considered as a normalization factor and a generation process is introduced. An initial signed particle creates a pair of new particles, one positive and the other negative. If, initially, the parent particle has a sign s and a wave-vector $\mathbf{M}$, it generates, with a rate $V^+(\mathbf{N})$, a pair of new particles with signs s, $-s$ and momenta $\mathbf{M}' = \mathbf{M}+\mathbf{N}, \mathbf{M}' = \mathbf{M}-\mathbf{N}$, respectively. Then, the original particle continues its free flight evolution until a given time T. The new pair of particles is evolved in the same way. The signed particles evolve over field-less Newton trajectories and contribute to the values of the physical averages only by their sign. The action of the Wigner potential on a signed particle happens only by generation of particles with opposite sign, in the same position of the parent particle, and following certain rules in the momentum component of the phase space. Thus, the time-dependent evolution of the Wigner quasi-distribution happens only by creation and annihilation of particles which replace the acceleration due to Newtonian forces [9].

This Monte Carlo technique is relatively easy to include in already existing semi-classical MC device simulators as it is shown in the GNU package Archimedes [16] and its quantum counter-part [17].

3. Simulation results

In this section we report the results of several numerical experiments aiming to explain the dynamics of an electron wave packet in the presence of arrays of dopants (ionized Phosphorus atoms) buried in a Silicon box. The spatial domain consists of a 2D Silicon box with dimensions $L_x = 50$ nm $\times$ $L_y = 50$ nm. The boundaries at the top and the bottom are absorbing, while the left and right boundaries are reflective. The wave packet is initially Gaussian and has only a longitudinal component in its wave-vector (i.e. directed from the bottom to the top of the domain). The system is evolved from its initial conditions till 200 fs when the packet starts to leave the device through the top lead. We explore several type of arrays of dopants. The first ones are highly ordered arrays (or matrices) of dopants of which dimensions are, respectively, 3×2, 3×3 and 3×4 (see Fig. 1). We then introduce some noise to perturb the initial position of the dopants. This introduces some level of chaos

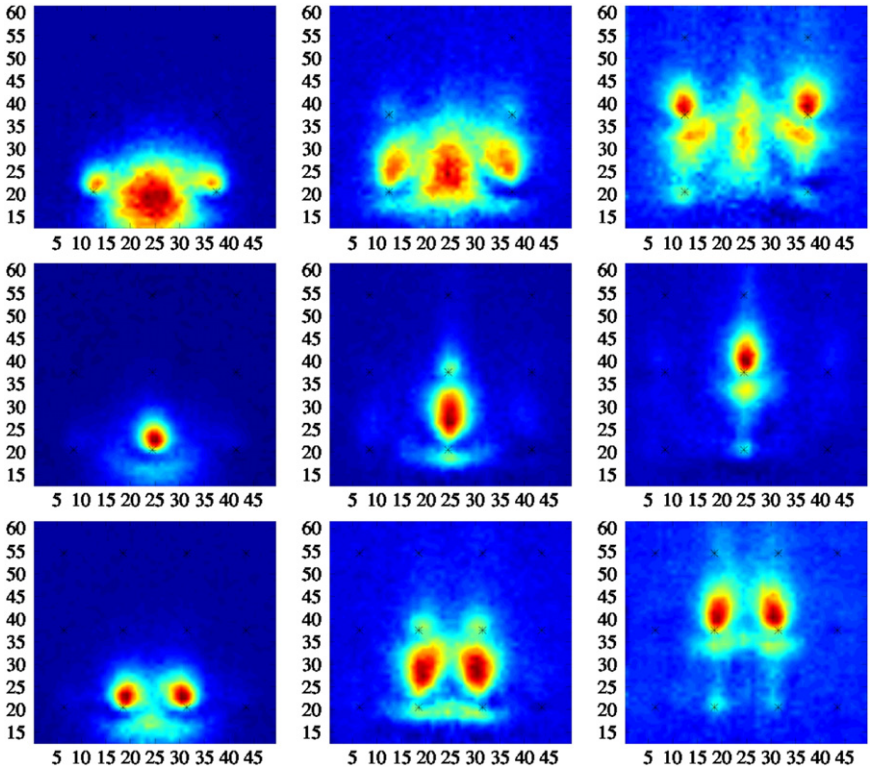

Fig. 3. Evolution of a wave packet in ordered arrays of dopants consisting of, respectively, 3×2 (top row), 3×3 (middle row) and 3×4 (bottom row) matrices of dopants buried in a Silicon substrate. The times reported are, respectively 50 fs (left column), 100 fs (middle column) and 150 fs (right column). The (black) $\times$ symbols represent the position of the dopants.

and the dynamics of the wave packet is affected accordingly. We utilize a homogeneous random generator and perturb the initial position in a box of which dimensions are $[-L_x/2; +L_x/2] \times [-L_y/3; +L_y/3]$, $[-L_x/3; +L_x/3] \times [-L_y/3; +L_y/3]$ and $[-L_x/4; +L_x/4] \times [-L_y/3; +L_y/3]$, depending on the dimensions of the dopant matrix involved in the problem. The noise introduced in our numerical experiments is of an amount of 20%, 40% and 60%. The case for 40% of noise, as an example, is reported in Fig. 2. The Coulombic potential, representing the presence of the ith dopant, is of the following shape:

$$V_i(\mathbf{x}) = \frac{q}{4\pi\epsilon_0\epsilon_r \left((\mathbf{x} - \mathbf{x}_i)^2 + \frac{1}{2}a_0^2\right)^{\frac{1}{2}}}, \tag{8}$$

where a_0 is the Bohr radius in Silicon $a_0 = \frac{4\pi\epsilon_0\epsilon_r \hbar^2}{m^* e^2}$ [18] and $\mathbf{x}_i$ is the position of the center of the ith dopant. This model has been extensively validated against Boltzmann MC benchmark tests [18] and is extended to the Wigner MC method based on particle signs (since both methods utilize Newtonian particles). One should note that the choice of this truncated Coulombic potential does not represent a restriction for the method.

Figs. 3 and 4 report the results of our simulations by means of the Wigner MC method based on signed particles. Both figures show the evolution of a wave packet in arrays of dopants consisting of, respectively, 3×2 (top row), 3×3 (middle row) and 3×4 (bottom row) matrices of dopants buried in a Silicon substrate. The times reported are, respectively 50 fs (left column), 100 fs (middle column) and 150 fs (right column). For clarity the position of dopants are shown in (black) $\times$ symbols.

It is clear from these figures that the dynamics of the wave-packet is profoundly affected by the position and number of dopants. Indeed, in the case of perfectly ordered arrays the evolution is axially symmetric. In the case of 3×2 array (top part of Fig. 3) one can observe how the initially Gaussian wave packet splits eventually into three parts. This splitting appears as soon as the first encounter with the first row of dopants happens. It occurs before the direct contact with the dopants, a clear signature of non-locality, typical of quantum mechanical effects. Once splitted, highest probability of finding an electron travels along three longitudinal directions, i.e. along the 2 columns of dopants and their middle axis. In a similar way, the symmetry is maintained in the 2 remaining highly ordered configurations (middle and bottom of Fig. 1). In particular, the wave packet collapses in the energy valley created by the first Coulombic potential encountered (in the middle) and proceeds along that column *jumping* from one dopant to the next one. One should note, finally, how for all ordered arrays of dopants the parts of the wave packet are always traveling in longitudinal direction, which, in other words, maximizes the current through the top contact (the Ramo–Shockley formula applied to the Newtonian signed particles). In the case of the

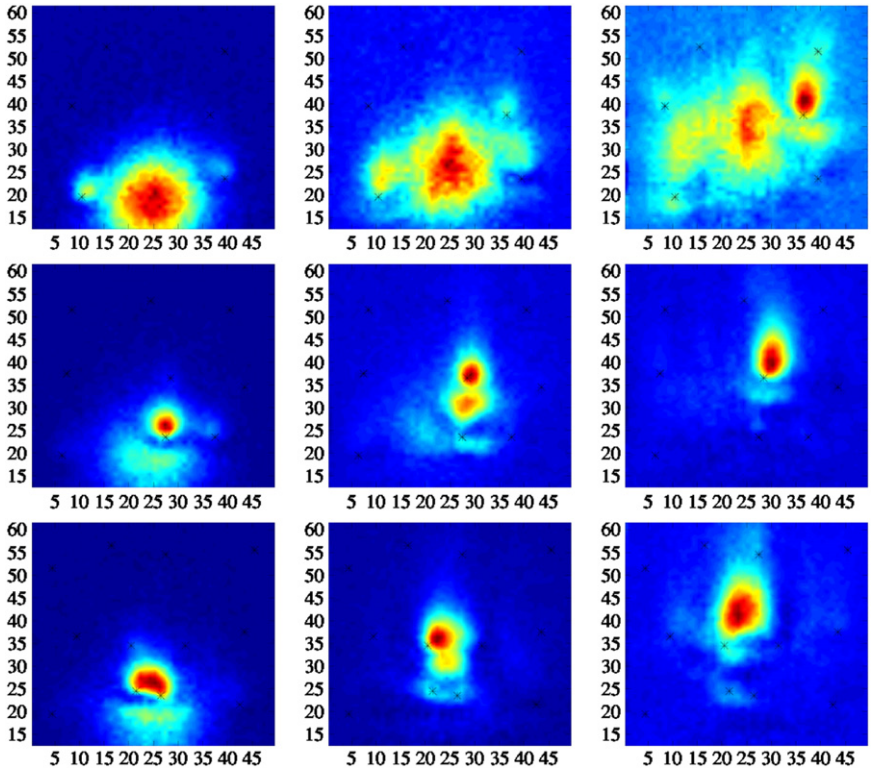

Fig. 4. Evolution of a wave packet in disordered arrays of dopants (40%) consisting of, respectively, 3×2 (top row), 3×3 (middle row) and 3×4 (bottom row) matrices of dopants buried in a Silicon substrate. The times reported are, respectively 50 fs (left column), 100 fs (middle column) and 150 fs (right column). The (black) $\times$ symbols represent the position of the dopants.

introduction of 20% of noise, things are very similar to the ordered cases. Indeed the position is not very much perturbed and the wave-packet dynamics continues to be almost symmetric. In the case of highly disordered arrays (40% and 60%), the evolution is drastically modified. The symmetry is broken and the velocity component of the packet is not purely longitudinal any longer. This can be clearly seen in Fig. 4 for the case 40%. This minimizes the current eventually measured at the top contact (the current is directly proportional to the perpendicular direction of the velocity with respect to a given surface). This is in accordance with the experiments performed in Ref. [13].

4. Conclusions

In this paper we reported the study of the dynamics of an initially Gaussian wave-packet in the presence of several dopant arrays by means of the full quantum, time dependent and multi-dimensional Wigner MC method based on signed particles. We studied three different ordered configurations (see Fig. 1), with dimensions 3×2 (top row), 3×3 (middle row) and 3×4 (bottom row), respectively. We have, then, introduced some noise in the initial position of the dopants by an amount of 20%, 40% and 60%. The results for several numerical experiments are reported in Figs. 3 and 4. One observes that while in the ordered case (Fig. 3) the wave packet develops an axial symmetry, this does not happen in the disordered arrays (Fig. 4 for example). Eventually, the packet gets an additional transversal component which reduces the performances of the device in terms of measured current and conductance at the top (absorbing) contact, in agreement with the experimental results reported in Ref. [13].

Acknowledgment

The research activities leading to this work have been partially supported by the FP7 project AComIn (FP7 REGPOT-2012-2013-1).

References

[1] P.M. Koenraad, M.E. Flatte, Single dopants in semiconductors, Nature Mater. 10 (2011) 91–100.
[2] B.E. Kane, A silicon-based nuclear spin quantum computer, Nature 393 (1998) 133–137.

[3] L.C.L. Hollenberg, A.S. Dzurak, C. Wellard, A.R. Hamilton, D.J. Reilly, G.J. Milburn, R.G. Clark, Charged-based quantum computing using single donors in semiconductors, Phys. Rev. B 69 (2004) 113301.
[4] K. Yokoi, D. Moraru, M. Ligowski, M. Tabe, Single-gated single-electron transfer in nonuniform arrays of quantum dots, Japan. J. Appl. Phys. 48 (2009) 024503.
[5] E. Hamid, D. Moraru, J.C. Tarido, S. Miki, T. Mizuno, M. Tabe, Single-electron transfer between two donors in nanoscale thin silicon-on-insulator field-effect transistors, Appl. Phys. Lett. 97 (2010) 262101.
[6] D. Moraru, A. Udhiarto, M. Anwar, R. Nowak, R. Jablonski, E. Hamid, J.C. Tarido, T. Mizuno, M. Tabe, Atom devices based on single dopants in silicon nanostructures, Nanoscale Res. Lett. 6 (2011) 479.
[7] M. Simmons, S. Schofield, J. Obrien, N. Curson, L. Oberbeck, T. Hallam, R. Clark, Towards the atomic-scale fabrication of a silicon-based solid state quantum computer, Surf. Sci. (2003) 1209–1218.
[8] M. Nedjalkov, H. Kosina, S. Selberherr, Ch. Ringhofer, D.K. Ferry, Unified particle approach to Wigner–Boltzmann transport in small semiconductor devices, Phys. Rev. B 70 (2004) 115319–115335.
[9] M. Nedjalkov, P. Schwaha, S. Selberherr, J.M. Sellier, D. Vasileska, Wigner quasi-particle attributes: an asymptotic perspective, Appl. Phys. Lett. 102 (2013) 163113.
[10] I. Dimov, Monte Carlo Methods for Applied Scientists, World Scientific, New Jersey, London, 2008, p. 291. ISBN: 13 978-981-02-2329-8, ISBN: 10 981-02-2329-3.
[11] M. Nedjalkov, D. Vasileska, I.T. Dimov, G. Arsov, Mixed initial–boundary value problem in particle modeling of microelectronic devices, Monte Carlo Methods Appl. 13 (4) (2007) 299–331.
[12] R. Rosati, F. Dolcini, R.C. Iotti, F. Rossi, Wigner-function formalism applied to semiconductor quantum devices: failure of the conventional boundary condition scheme, Phys. Rev. B 88 (2013) 035401.
[13] T. Shinada, S. Okamato, T. Kobayashi, I. Ohdomari, Enhancing semiconductor device performance using ordered dopant arrays, Nature 437 (2005) 1128–1131.
[14] E. Wigner, On the quantum correction for thermodynamic equilibrium, Phys. Rev. 40 (1932) 749.
[15] D. Querlioz, P. Dollfus, The Wigner Monte Carlo Method for Nanoelectronic Devices—A Particle Description of Quantum Transport and Decoherence, ISTE-Wiley, 2010.
[16] www.gnu.org/software/archimedes.
[17] www.nano-archimedes.com.
[18] A. Goldberg, H.M. Schey, Computer-generated motion pictures of one-dimensional quantum-mechanical transmission and reflection phenomena, Amer. J. Phys. 35 (1967) 177.