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Numerical investigation of electrostatic interactions in nanoscale substances based on finite-size particle simulation

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ABSTRACT

We use the optimized finite-size particle techniques derived from plasma simulations to investigate the electrostatic interactions in nanoscale substances. In conjunction with electron tunneling, the substance surface is modeled as a potential well that confines simulated electrons for reaching equilibrium in an electrostatic system governed by Poisson's equation. This scheme avoids the mathematical difficulty of handling sophisticated boundary conditions at the interface and easily treats complicated shapes. We demonstrate the performance of the proposed method by simulating millions of electrons propagating in isolated substances at nanoscale. Numerical results are consistent with theoretical predictions of electrostatic properties in equilibrium.

Nanoparticles and nanostructures have gained increasing attention in recent years due to their success in the fields of medicine, metrology, biotechnology, and applied physics [1–4]. Electrical transport is of fundamental importance as well as of scientific interest due to practical applications such as the modeling of electrochemical interfaces, measuring of conductivity with electron and ion holes, and studying of domain structures in nanoferroelectrics [5–8]. Charged nanoparticles have been modeled using a hard-sphere approach [9] and deposited onto a patterned surface in the presence of an applied electric field [10]. Nevertheless, the fabrication of conducting nanostructures, say carbon nanotube superconducting devices [11], requires the understanding of the electrostatic properties of isolated nanoscale systems [12].

To study the electrostatic behavior of physical systems at nanoscale, a variety of approaches have been proposed both experimentally [13–15] and analytically [16,17]. Indeed, scanned capacitance microscopy (SCM), atomic force microscopy (AFM), and electrostatic force microscopy (EFM) techniques have been extensively used to detect single charge motion in nanoscale devices [5,18]. In the case of a large number of electrons, however, one soon realizes the total impracticality of such approaches. Moreover, the interaction between two isolated point charges described by the bare Coulomb potential needs to be modified as a result of collective effects between each other in a many-body system [19,15]. Fortunately, thanks to the advancement of modern high-speed computers investigating the simultaneous interaction of a large number of electrons has become possible through computer modeling [20].

In this Letter, we develop a theoretical model in an attempt to investigate the electrostatic interactions in nanoscale substances through computer simulations. A computationally efficient framework based on the optimized finite-size particle techniques is adopted to solve Poisson's equation that governs the electrostatic system in nanosubstances. In conjunction with electron tunneling, substance surfaces are modeled as potential wells that confine simulated electrons for reaching equilibrium. In particular, charged conductors that have reached electrostatic equilibrium share a variety of unique characteristics [21] as summarized in Table 1. Balancing between electric and reacting forces, the electrons advance in such a way to minimize the electrostatic energy as consistent with the theory of electrostatics. Excellent agreement between the theoretical predictions and simulated results is obtained. While characteristics of electrostatic equilibrium in conductors are studied, the methods developed appear promising for applications to other materials [14] exhibiting the same phenomena and to sophisticated computer simulations based upon electrostatics [20,17].

Considering a large set of electrons uniformly distributed in a nanoscale substance, the force $\mathbf{F}_i$ exerted on an arbitrary electron i arises from the interaction of two different sources:

$$\mathbf{F}_i = \mathbf{F}_{ele} + \mathbf{F}_{ssr}, \tag{1}$$

where $\mathbf{F}_{ele}$ represents the electric force due to all other electrons and it can be computed in terms of the electric field $\mathbf{E}$,

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Table 1
Essential properties of isolated conductors in electrostatic equilibrium.

Quantity	Property
Electric filed	1. The field anywhere inside the conductor is zero 2. The field just outside the conductor surface is perpendicular to the surface and its magnitude is proportional to the local charge density and curvature
Electric potential	1. Every point on the surface of the conductor is at the same potential, i.e., the surface is an equipotential

Table 2
Parameters for the investigation of electrostatic interaction in nanosubstances.

Parameter	Setting
Electron mass (m_e)	9.10938×10^{-31} kg
Electron charge (q)	-1.60218×10^{-19} C
Electron density	1.40×10^{28} electrons/m^3
Electron energy (E)	7 eV
Potential energy (U)	10 eV
Insulator thickness (L)	1 nm
Simulation dimension	$128 \times 128 \times 128$ nm^3
Equilibrium condition (γ)	0.01%
Time interval	0.0001 ms
Sphere substance size	$R = 32$ nm
Cylinder substance size	$R = 32$ nm, $H = 64$ nm

$$\mathbf{F}_{ele} = q\mathbf{E}, \tag{2}$$

where q is the electron charge and the electric field can be computed through the electric potential Φ,

$$\mathbf{E} = -\nabla\Phi. \tag{3}$$

The potential can be further computed from Poisson's equation as

$$\nabla^2\Phi = -4\pi\rho, \tag{4}$$

where ρ is the electron density. In Eq. (1), $\mathbf{F}_{ssr}$ represents the substance surface restraint force used to confine electrons moving inside the substance,

$$\mathbf{F}_{ssr} = -\alpha\nabla G_\sigma * (U - E), \tag{5}$$

where α is a weight for balancing, G_σ is a Gaussian filter with standard deviation σ, $*$ represents convolution, U represents the surface potential energy used to construct a potential well to enclose the electrons, and E represents the energy of an electron. By solving the Schrödinger's equation with continuous boundary conditions, the approximate transmission probability T is obtained [22],

$$T = \exp -2\sqrt{2m_e(U - E)}\frac{L}{\hbar}, \tag{6}$$

where m_e is the electron mass, L is the thickness of the surrounding insulator, and $\hbar$ is the reduced Planck's constant. Accordingly, the number of electrons passing through the potential well is the multiplication of the transmission probability and the count of the electron movement. As such, the number of remaining electrons at iteration i is computed using

$$N_i = N_0(1 - iT), \tag{7}$$

where N_0 is the initial number of electrons inside the nanoscale conductor.

Although this scheme sounds straightforward, practical computational limitations require the use of more sophisticated techniques that increase the difficulties of simulation in nanoscale for any appreciable length of time. Throughout the simulation process there are two different forces exerted on each electron. Inside the simulated substance, the electrons are advanced mainly according to $\mathbf{F}_{ele}$ since $\nabla(U - E) = 0$. However, there are salient $\mathbf{F}_{ssr}$ at simulated surfaces that are able to cancel out $\mathbf{F}_{ele}$ in the surface normal direction and to change the motion of the electrons toward equilibrium. Further applying Gauss's law to evaluate the force equilibrium condition between $\mathbf{F}_{ele}$ and $\mathbf{F}_{ssr}$, we obtain the condition for α in Eq. (5) as $\alpha \geqslant 4N_iq^2/|\nabla(U - E)|D^2$, where D is the effective diameter of the simulated substance in 3-D and $|\nabla(U - E)|$ is the modulus of energy gradients.

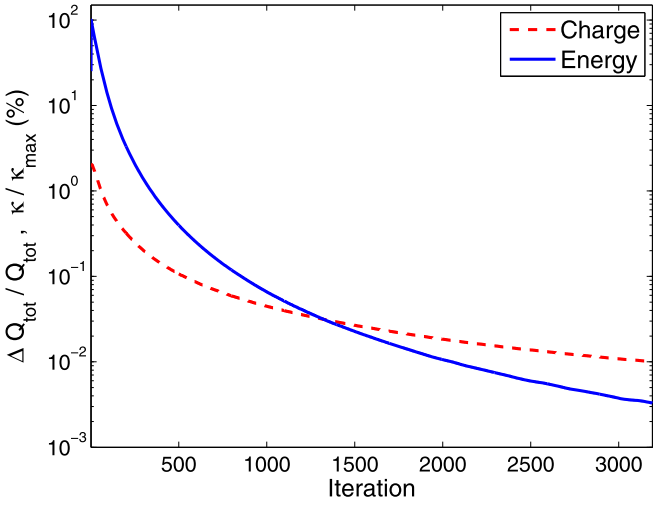

Fig. 1. Plots of the charge difference ratio [the (red) dashed curve] and normalized kinetic energy [the (blue) solid curve] in a sphere nanosubstance with respect to the number of iterations. (For interpretation of colors in this figure, the reader is referred to the web version of this Letter.)

The remaining challenge for the simulation is to efficiently solve Poisson's equation in Eq. (4) to compute Φ for the corresponding field and force in nanoscale. In light of employing the finite-size particle (FSP) method [23], the computation is greatly accelerated by approximating the charge density ρ as

$$\begin{aligned}\rho(x, y, z) &\equiv \sum_{i=1}^{N_i} qS\big(|\mathbf{r} - \mathbf{r}_i|\big) \\ &\cong \sum_{m=1}^{L_m}\sum_{n=1}^{L_n}\sum_{p=1}^{L_p} Q(m, n, p)S\big(\big|\mathbf{r} - \mathbf{r}(m, n, p)\big|\big),\end{aligned} \tag{8}$$

where L_m, L_n, and L_p are the lengths of grid points along the m, n, and p axes, respectively. Interpolating the electron charge q into lattice using the clouds-in-cells (CIC) method [24], we replace the sum over electrons by a sum over grid points with respect to Q. In Eq. (8), S is the shape factor giving the way an electron is distributed about its center,

$$\begin{aligned}S(r) &\equiv \frac{1}{(2\pi)^{\frac{3}{2}}}\exp\left(-\frac{r^2}{2}\right) \\ &= \frac{1}{(2\pi)^{\frac{3}{2}}}\exp -\frac{1}{2}\big[(x - x_i)^2 + (y - y_i)^2 + (z - z_i)^2\big],\end{aligned} \tag{9}$$

where $S(r)$ is the Gaussian shape factor in terms of distance $r = [(x - x_i)^2 + (y - y_i)^2 + (z - z_i)^2]^{\frac{1}{2}}$ and its integration over the entire space is normalized to unity through the factor $(2\pi)^{\frac{3}{2}}$, i.e., $\int\int\int S\,dx\,dy\,dz = 1$.

By introducing the shape function to electrons, the FSP enables the new electrons, which have a spread-out charge distribution, to interact simultaneously due to the Coulombic force at large distances but to cross each other easily due to the dropping force