Simulation of nanofractal dynamics with MBN Explorer

Ilia A. Solov’yov\textsuperscript{1,2,3}, and Andrey V. Solov’yov\textsuperscript{1,3,4}

\textsuperscript{1} Virtual Institute on Nano Films (VINF), Allée des Noisetiers, 2 bte 30 Angleur, Belgium
\textsuperscript{2} Beckman Institute for Advanced Science and Technology, University of Illinois at Urbana-Champaign, 405 N. Mathews Ave, Urbana Illinois 61801, USA
\textsuperscript{3} On leave from A.F. Ioffe Physical-Technical Institute, Politechnicheskaya Str. 26, 194021 St. Petersburg, Russia
\textsuperscript{4} Frankfurt Institute for Advanced Studies, Ruth-Moufang-Str. 1, 60438 Frankfurt am Main, Germany

E-mail: illia@illinois.edu

Abstract. One of the goals of nanotechnology is the development of controlled, reproducible, and industrially transposable nanostructured materials. In this context, controlling of the final architecture of such materials by tuneable parameters is one of the fundamental problems. Post-growth processes occurring in patterns grown on a surface were studied using a multi-purpose computer code MBN Explorer introduced in the present paper. The package allows to model molecular systems of varied level of complexity, and in the present paper was used, in particular, to study dynamics of silver nanofractal formation and fragmentation on graphite surface. We demonstrate that the detachment of particles from the fractal and their diffusion within the fractal and over the surface determines the shape of the islands remaining on a surface after the fractal fragmentation.

1. Introduction

In recent years, numerous nanosystems possessing unique structural, optical, electric and magnetic properties have been discovered [1–11]. The aggregation of atoms and small molecules into clusters, nanoparticles, micro-droplets is a process in which a wide range of complex bio-, nano- and mesoscopic objects can be created. Often, such systems are seen as building blocks for new nanostructured materials with specific tailored properties, and many of these systems have become a subject of intensive investigations because of the variety of potentially important applications [5,8,12–18].

The present paper features a multi-purpose computer package, MesoBioNano Explorer (MBN EXPLORER), which can be used for advanced theoretical characterization and analysis of a variety of bio- nano systems [1]. The package has been specifically developed to enable a unified approach for simulating of complex molecular structure and dynamics on different temporal and spatial scales, ranging from atoms to clusters, macromolecules, crystals and surface patterns. \textsuperscript{1} The ultimate goal of MBN EXPLORER is to expand the understanding of mechanisms of stability,

\textsuperscript{1} The binary files of MBN EXPLORER, the user’s guide and a number of representative examples are available upon registration online at http://www.mbnexplorer.com/.
Figure 1. Variety of molecular systems which can be simulated using MBN EXPLORER: (a) encapsulated clusters, (b) nanoindentation of titanium crystal, (c) nanofractals, (e) proteins, (f) biomolecules, e.g., DNA on the histone. Structure and properties of any of these objects or any of their combinations can be studied using MBN EXPLORER. The figure has been adapted from Ref. [19].

self-organization and growth, as well as the ways of manipulation and control of bio-nano systems with potential applications in nanotechnology, microelectronics and medicine.

Figure 1 highlights a variety of molecular systems, which can be simulated using MBN EXPLORER. In particular, MBN EXPLORER is suited to compute the system's energy, to optimize molecular structures, as well as to explore the molecular and random walk dynamics. MBN EXPLORER allows to use a broad variety of interatomic potentials, to model different molecular systems, such as atomic clusters [20–23], fullerenes, nanotubes [24], polypeptides, proteins [25], composite systems [26–29], nanofractals [30–32], etc.

In this paper we overview the key functionality of the present version of MBN EXPLORER. Then we utilize the program for a concrete case-study. In particular, the investigation of the dendritic structures (fractals) has recently raised an increased interest [10, 33–40] and, therefore, is in the focus of the present investigation. The formation of fractals provides a natural framework for studying disordered structures on a surface because fractals are generally observed in far-from-equilibrium growth regime.

Here we make an important step towards understanding of the nanofractal stability. Using MBN EXPLORER we perform analysis of the post-growth processes occurring in a nanofractal on a surface. We demonstrate that the detachment of particles from the fractal and their diffusion within the fractal and over the surface determines the shape of the islands remaining on a surface after the fractal fragmentation. Additionally we advocate MBN EXPLORER as a universal tool for studying structure and dynamics, as it has also been successfully used for studying such processes as nanoindentation of titanium alloys [41], conventional molecular dynamics [19], and
other problems in bio-nano science [42].

2. MBN Explorer functionality
MBN EXPLORER is a multi-purpose computer code [1] available for download at http://www.mbnexplorer.com/. The essential functionality modules of MBN EXPLORER are summarized below, subdivided into several categories. In particular, MBN EXPLORER allows to perform the following computational tasks:

- Single point energy calculation;
- Molecular structure optimization;
- Classical molecular dynamics simulation;
- Relativistic molecular dynamics simulation;
- Random walk dynamics;

MBN EXPLORER has a rapidly expanding list of interaction potentials, that include

- Power potential;
- Exponential potential;
- Coulomb potential;
- Yukawa potential;
- Moliere potential;
- Pacios potential;
- Lennard-Jones potential;
- Morse potential;
- Girifalco potential;
- Dzugutov potential;
- Quasi Sutton-Chen potential;
- Sutton-Chen potential;
- Gupta potential;
- Brenner potential;
- Tersoff potential;
- Finnis-Sinclair potential;
- CHARMM molecular mechanics potential;
- Dissociative CHARMM molecular mechanics potential;
- External electric fields;
- External viscous fields;

The program is developed based on the following basic algorithms

- OpenMP parallelization for shared memory computers;
- Velocity Verlet and Leapfrog integrators;
- Velocity quenching and conjugate gradient optimization methods;
- Linked Cell algorithm;
- Periodic and reflective boundary conditions;
- Langevin and Berendsen thermostats;
- Ewald summation for long-range interactions;
– Rigid body Euler dynamics;
– Adaptive 4th order Runge-Kutta integrator for relativistic dynamics;
– External forces and user-defined particle manipulation;
– Momentum and angular momentum control;

MBN EXPLORER supports different standards of input and output formats, in particular:

– Cartesian XYZ;
– Binary DCD;
– Protein data bank, PDB;
– X-PLOR PSF;

More detailed description of algorithms and methods implemented in MBN EXPLORER is available in the key publication [1] and also on the website http://www.mbnexplorer.com/.

3. Stochastic Monte-Carlo-based dynamics in MBN EXPLORER

This section describes the basics of the stochastic Monte-Carlo-based dynamics algorithm implemented in MBN EXPLORER. In this case, the time-evolution of a coarse-grained molecular system is modeled stepwise in time, where at each step of the simulation, the system undergoes a structural transformation with a certain probability. The new configuration of the system is then used as the starting point for the next simulation step. The transformation of the system is governed by predefined kinetic rates which are determined by interparticle interactions. Due to its probabilistic nature, stochastic Monte-Carlo-based dynamics allows to study processes on time scales significantly exceeding time scales of conventional molecular dynamics and is ideally suited for simulations where details of individual kinetic processes are not important, and can be parameterized by a few kinetic rates.

MBN EXPLORER allows to study random walk dynamics in open molecular systems. The implemented algorithm is illustrated in Fig. 2. Consider a molecular system at time t = 0 which evolves in time. At periodic time intervals new particles are added to the system with a certain probability. At each step of the simulation the list of mobile particles is constructed, and these particles are then displaced in a random direction with a certain probability. The algorithm is repeated until the necessary number of simulation steps is performed.

To simplify calculations, the random walk motion of particles is simulated on a grid. A grid represents an artificial subdivision of the simulation space into cells which accommodate particles of the system. A particle in the grid occupies a single cell and can move from this cell only to a neighboring non-occupied cell. The number of possible directions for a particle displacement depends on the grid packing and on the number of occupied neighbor cells. The present version of MBN EXPLORER considers interaction between neighboring particles in Arrhenius approximation. Thus, two coarse-grained particles being in the stochastic Monte-Carlo-based dynamics are assumed to have a bond if they occupy two neighboring grid cells.

Monte-carlo-based dynamics module of MBN EXPLORER allows to study self-assembly, pattern formation and pattern fragmentation on a surface. in this case the diffusion rate of a free particle \( \Gamma_d \) is determined by the diffusivity of a particle on the surface. If a particle is bound to periphery of a group of particles (an island) it can experience diffusion along the periphery, thereby maintaining some of its bonds with neighboring particles, or detach from the island. The probability of particle detachment in MBN EXPLORER is given by:

\[
\Gamma_{de} = \Gamma_d \exp \left( \frac{-lE_b}{k_B T} - \frac{\Delta \mu}{k_B T} \right),
\]

where \( l \) is the number of bonds broken after particle detachment, \( E_b \) is the binding energy of two particles, \( \Delta \mu \) is the chemical potential of particle detachment [36, 43–45], \( T \) is the temperature
of the system and $k_B$ is the Boltzmann constant. The peripheral diffusion of a particle is parameterized as

$$\Gamma_{pd} = \Gamma_d \exp \left[ -\frac{mE_b}{k_B T} - \frac{n\Delta \epsilon}{k_B T} \right], \quad (2)$$

where $m$ is the number of bonds that are broken due to particle motion, $n$ is the number of maintained neighbor bonds between two particles and $\Delta \epsilon$ is the diffusion energy barrier.

4. Results
Using the method outlined above we have performed analysis of the silver cluster fractal post-growth relaxation on a graphite surface. The fractal structure shown in Fig. 3 has been chosen for the further investigation of the post-growth relaxation processes. The diameter of the fractal in the considered example is 1.2 $\mu$m, which corresponds to the diameter of the experimentally grown structures [10,36,37], and consist of 38,012 $A_{500}$ particles.

An important quantity in the stochastic Monte-Carlo-based dynamics method is the

---

Figure 2. The principal scheme of stochastic Monte-Carlo algorithm implemented in MBN EXPLORER and used for random walk dynamics simulations. The figure has been adapted from Ref. [1].
simulation time step, $\Delta t$, which defines the characteristic time for particle diffusion over a surface as \cite{30–32,46,47}

$$\Delta t(T) = \frac{d_0^2}{4D(T)}.$$  \hspace{1cm} (3)

Here $d_0$ is the diameter of a particle and $D(T)$ is the diffusion coefficient of the particle at a given temperature, $T$.

Stability of the silver cluster fractals on graphite surface has been studied earlier in detail \cite{30–32} using a prototype version of MBN EXPLORER for a smaller system, and here we illustrate it for a $\mu$m-large fractal which evolves on the timescale of seconds. Stability of silver cluster fractals on graphite surface is of great relevance to experiment, as the post-growth relaxation of silver fractals has been extensively studied over the last decade \cite{10,36,37}. To make our simulations consistent with experimental observations we thus have used the model parameters derived from the experiment: the diameter of a particle has been taken equal to 2.5 nm, and the diffusion coefficient of a silver cluster on graphite at room temperature was reported \cite{37} to be equal to $2 \cdot 10^{-7}$ cm$^2$/s. Substituting this value into Eq. (3), one obtains $\Delta t(300 \text{ K}) = 78$ ns, which allows one to simulate the process during the time period

$$t = N_{\text{step}}\Delta t,$$  \hspace{1cm} (4)

where $N_{\text{step}}$ is the number of simulation steps. The simulation stepsized $\Delta t$ in stochastic Monte-Carlo-based dynamics is significantly larger than the stepsize of conventional molecular dynamics (where it is typically taken as 1-2 fs), and, therefore, allows to perform simulations on significantly larger time scales. In the present example we analyze several paths of fractal fragmentation. The rate of fractal decay depends on the interparticle interaction, and it defines the morphology of the fragments that are formed during the process. Snapshots of the structures arising at different stages of the fragmentation process simulated at different parameters of interparticle interactions are shown in Fig. 4. This example shows that fragmentation paths and the fragments morphology depends on the interparticle interaction energies. In particular we analyze the post-growth evolution of the fractal on surface depending on the particle interaction energy $E_b$ and peripheral diffusion barrier $\Delta \epsilon$, see Eq. (1)-(2) for the definition of $E_b$ and $\Delta \epsilon$. 

\textbf{Figure 3.} The fractal structure chosen for the further investigation of the post-growth relaxation processes in fractals. The figure has been adapted from Ref. \cite{1}. 

$\text{500 nm}$
Figure 4. Evolution of a fractal structure on a $4.3 \times 5.0 \, \mu m^2$ substrate with periodic boundary conditions at temperature $T = 300$ K. The initial fractal structure, consisting of 38,012 particles (shown in Fig. 3) undergoes fragmentation in different final states depending on the interparticle interactions in the system (shown right). Numbers above the images indicate the simulation time $t$, see Eq. (4), at which the corresponding snapshots were rendered. The figure has been adapted from Ref. [1].
Figure 5. Time evolution of the number of fragments $N_{fr}$, normalized maximal island size $N_{max}/N_0$ (where $N_0 = 38,012$ is the number of particles in the initial fractal structure), maximal radius of an island $R_{max}$, and area to perimeter ratio for the largest island $S_{max}/P_{max}$ calculated for the fractal structure shown in Fig. 4. The fractal fragmentation has been analyzed for different values of the binding energy $E_b$ and the barrier energy $\Delta \epsilon$, as indicated in the figure legend. The figure has been adapted from Ref. [1].

Figure 4 shows that for $E_b = 0.051$ eV, $\Delta \epsilon = 0.005$ eV the entire fractal structure melts and forms a large compact droplet, while two additional smaller droplet are seen for $E_b = 0.051$ eV, $\Delta \epsilon = 0.051$ eV after 18.29 s of simulation. In both cases the binding energy $E_b$ between the particles is small, allowing an easy detachment of particles, but at the same time it is large enough to make the characteristic particle detachment time comparable with the characteristic particle nucleation time, thereby preventing the system from entire defragmentation. Thus, the fragmentation path at $E_b = 0.051$ eV goes via the rearrangement of the entire system and results in the formation of large stable droplets.

An increase of the interparticle interaction energy leads to the change of the fractal fragmentation pattern. As seen in Fig. 4 at $E_b = 0.08 - 0.1$ eV the fractal fragments into several compact droplets, while the overall profile of the initial fractal structure is preserved even after $t = 18.29$ s. The analysis of morphology of the created patterns leads us to the following main conclusions: (i) the growth of $E_b$ leads to the decrease of the average fractal-core branch width during the fragmentation process. This happens because the detachment of particles from the fractal becomes energetically unfavorable process, and the fractal fragments slower. (ii) The increase of the peripheral diffusion barrier energy $\Delta \epsilon$ suppresses the diffusion of particles, resulting in a slower evolution and fragmentation of the fractal shape.
An important characteristic of the fractal fragmentation process is the number of fragments at a given time, \( N_{fr} \). The smallest fragment is a single particle. The time evolution of the number of fragments calculated for different sets of model parameters is shown in Fig. 5. The figure shows that the number of fragments in the six considered cases rapidly approaches an asymptotic value which decreases with increasing the \( E_b \) value. It is interesting to note that at \( E_b = 0.051, 0.077 \) and 0.102 eV there are \(~1000, 100, \) and 10 fragments on the surface, respectively, i.e., increasing the binding energy between particles in the fractal on \( k_B T \) leads to an order of magnitude change of the number of fragments on the surface. For the largest island on the surface we have calculated the normalized maximal island size \( N_{max}/N_0 \), see Fig. 5, where \( N_0 \) is the number of particles in the initial fractal structure. This characteristic is useful to illustrate the dispersion of island sizes on the surface and demonstrates that except the \( E_b = 0.1 \) eV the largest fragment on the surface still continues to nucleate individual particles dispersed on the surface.

Useful quantity for the characterization of patterns on a surface are: (i) the ratio between the area and perimeter of the structures (\( S/P \) ratio) as this ratio characterizes the branch width of the fragmenting structures [10], and (ii) the maximal radius of a structure \( R_{max} \). Figure 5 shows the area to perimeter ratio for the largest island on the surface, \( S_{max}/P_{max} \). The dependencies calculated for all studied energies show a monotonous increase with slight fluctuations due to structural rearrangements in the system. Note that the smallest asymptotic value of \( S_{max}/P_{max} \) is observed for \( E_b = 0.102 \) eV and \( \Delta \epsilon = 0.102 \) eV, because the width of the fractal branches after 20 s of fragmentation are the smallest in this case.

Figure 6 shows the probability density functions of the \( S/P \) ratio calculated for the morphology on surface after \( t = 18.29 \) s of the fractal post-growth relaxation. The distributions plotted in Fig. 6 have been obtained with the model parameters \( E_b = 0.05 - 0.1 \) eV, \( \Delta \epsilon = 0.1E_b \)
and $\Delta \epsilon = 1.0 E_b$ and correspond to the final patterns shown in Fig. 4. The position of the maxima in these distribution functions allows to determine the branch width of the probable fragments on the surface. Thus, for $E_b = 0.05$ eV fragments of smaller size appear on the surface with increased probability together with one large fragment having $S/P \sim 30$ nm. Contrary, for $E_b = 0.1$ eV, $\Delta \epsilon = 0.1$ eV the probability distribution of the $S/P$ ratio appears to be symmetric, centered at $S/P = 11$ nm. Note that Fig. 6 did not account for the area to perimeter ratio of individual particles and particle dimers on surface, as such configurations are typically not visible in experiment [10,36,37].

In this example we have performed analysis of the post-growth processes occurring in a nanofractal on a surface using the method implemented in MBN EXPLORER, which models the internal dynamics of particles in a fractal and accounts for their diffusion and detachment. We have demonstrated that these kinetic processes are responsible for the shape of the islands created on a surface after the post-growth relaxation. In the present example we have studied particle dynamics in 2D, while MBN EXPLORER allows to perform stochastic Monte-Carlo-based dynamics in 3D. This is especially interesting to do, because there are many examples of three dimensional fractal systems in biology [48, 49], where the dendritic shapes are rather common.

5. Conclusion

MBN EXPLORER is a program with several important features, which make it potentially interesting to diverse communities including physicists, chemists, biologists and material scientists. MBN EXPLORER permits energy calculation, structure optimization, molecular and random walk dynamics simulations. The development of a new program for studying molecular structures and dynamics is motivated by the need of a universal extendable code, which would permit investigation of molecular processes on the nano- and meso-scales. Through the combination of advanced MD techniques and simplified coarse-grained models, MBN EXPLORER is suitable for the description of molecular systems on the basis of a multiscale approach, which is not provided by the most of existing standard molecular dynamics codes: the standard codes would require additional input, involving either plugin or module development, to permit the multiscale calculations, while MBN EXPLORER supports it intrinsically.

As an example of MBN EXPLORER extended functionality, the program allows for straightforward simulations using Monte-Carlo-based dynamics, classical molecular dynamics involving a large number of rigid molecules of arbitrary shapes, molecular dynamics simulations of bio-nano systems modeled through a combination of pairwise and many-body potentials (e.g., a gold nanoparticle marker linked to a DNA molecule). In the paper we have considered only one illustrative example, which outline the key features of MBN EXPLORER, but, of course, do not describe all of them, since MBN EXPLORER allows to combine most of its features in a user-friendly manner, permitting simulations of various molecular assemblies in special environments. It is worth noting that although most of the computational features of MBN EXPLORER can be found in other computer packages, MBN EXPLORER is unique because it combines a vast majority of these features into one computationally efficient code. The current version of MBN EXPLORER supports calculations on the multiple CPU cores with sheared memory by means of OpenMP parallelization technique.

MBN Explorer is made compatible with the popular molecular dynamics programs NAMD [50], CHARMM [51] and visualization program VMD [52]. This permits to easily swap files between the programs and prepare molecular systems for simulations in a straightforward way. The visualization support through the VMD program is necessary for analysis of MBN EXPLORER output and the build-in Tcl scripting language in VMD allows to develop specialized plugins to perform the extended analysis of the calculations results.
Acknowledgments

We acknowledge the Frankfurt Center for Scientific Computing for providing computer resources that have contributed to the research results reported within this paper. I.S. acknowledges support as a Beckman Fellow.

References

[1] Solov'yov I A, Yakubovich A V, Nikolaev P V, Volkovets I and Solov'yov A V 2012 Journal of Computational Chemistry 33 2412–2439
[2] Neto A H C, Guinea F, Peres N M R, Novoselov K S and Geim A K 2009 Rev. Mod. Phys. 81 109–162
[3] Ohkoshi S, Imoto K, Tsunobuchi Y, Takano S and Tokoro H 2011 Nat. Chem. doi:10.1038/nchem.1067
[4] Tan S J, Campolongo M J, Luo D and Cheng W 2011 Nat. Nanotech. 6 268–276
[5] Nie Z, Petukhova A and Kumacheva E 2010 Nat. Nanotech. 5 15–25
[6] Adler-Abramovich L, Aronov D, Becker P, Yevnin M, Stemppler B, Buzhansky L, Rosenman G and Gazit E 2009 Nat. Nanotech. 4 849–854
[7] Yan R, Gargas D and Yang P 2009 Nat. Photon. 3 569–576
[8] Mann S 2009 Nat. Mat. 8 781–792
[9] Withers N 2009 Nat. Mat. doi:10.1038/nchem.476
[10] Lando A, Kébaïli N, Cahuzac P, Masson A and Bréchignac C 2006 Phys. Rev. Lett. 97 133402
[11] Carlier F, Benrezzaak S, Cahuzac P, Kébaïli N, Masson A, Srivasta A K, Colliec C, de Frutos M and Bréchignac C 2006 Nanoletters 6 1875–1879
[12] Stuart M A C, Huck W T S, Genzer J, Ober C, Stamm M, Sukhorukov G B, Szeleifer I, Tsukruk V V, Urban M, Winnik F, Zauscher S, Luzinov I and Minko S 2010 Nat. Mat. 9 101–113
[13] Nie Z and Kumacheva E 2008 Nat. Mat. 7 277–290
[14] Ciofani G 2010 Expert Opinion on Drug Delivery 7 889–893
[15] Yang P, Yan R and Fardy M 2010 Nano Lett. 10 1529–1536
[16] Schneider G F, Kowalczyk S W, Calado V E, Pandraug D, Zandbergen H W, Vandersypen L M K and Dekker C 2010 Nano Lett. 10 3136–3167
[17] Garaj S, Hubbard W, Reina A, Kong J, Brantong D and Golovchenko J A 2010 Nature 467 190–194
[18] Yakubovich A, Solov’yov I and Solov’yov A 2013 Physics Procedia 40 93 – 99
[19] Solov’yov I A, Solov’yov A V and Greiner W 2003 Int. J. Mod. Phys. E 13 697–736
[20] Obolensky O I, Solov’yov I A, Solov’yov A V and Greiner W 2005 Comp. Lett. 1 313–318
[21] Koshelev A, Shutoyev A, Solov’yov I A, Solov’yov A V and Greiner W 2003 Proceedings of International Workshop “From Atomic to Nano-scale”, Old Dominion University 184–194
[22] Solov’yov I A, Solov’yov A V, Greiner W, Koshelev A and Shutoyev A 2003 Phys. Rev. Lett. 90 053401–(1–4)
[23] Solov’yov I A, Mathew M, Solov’yov A V and Greiner W 2008 Phys. Rev. E 78 051601–(1–13)
[24] Solov’yov I A, Yakubovich A, Solov’yov A V and Greiner W 2010 Phys. Rev. E 75 051912–(1–9)
[25] Geng J, Solov’yov I A, Zhou W, Solov’yov A V and Johnson B F G 2009 J. Phys. Chem. C 113 6390–6397
[26] Solov’yov I A, Geng J, Solov’yov A V and Johnson B F G 2009 AIP Conf. Proc. 1197 89–102
[27] Solov’yov I A, Geng J, Solov’yov A V and Johnson B F G 2009 Chem. Phys. Lett. 472 166–170
[28] Geng J, Solov’yov I A, Reid D G, Skelton P, Wheatley A E H, Solov’yov A V and Johnson B F G 2010 Phys. Rev. B 81 214114–(1–13)
[29] Dick V V, Solov’yov I A and Solov’yov A V 2009 AIP Conf. Proc. 1197 76–88
[30] Dick V V, Solov’yov I A and Solov’yov A V 2010 J. Phys.: Conf. Ser. 248 012025–(1–11)
[31] Dick V V, Solov’yov I A and Solov’yov A V 2011 Phys. Rev. B 84 115408–(1–14)
[32] Coatiri, Meerson B and Sasorov P V 1998 Phys. Rev. Lett. 80 4693
[33] Sharon E, Moore M G, McCormick W D and Swinney H L 2003 Phys. Rev. Lett. 91 205504
[34] Semépère R, Gourret D, Wagnier T, Philippou J and Jullien R 1993 Phys. Rev. Lett. 71 3307
[35] Bréchignac C, Cahuzac P, Carlier F, Colliex C, de Frutos M, Kébaïli N, Roux J L, Masson A and Yoon B 2003 Eur. Phys. J. B 24 265–268
[36] Lando A, Kébaïli N, Cahuzac P, Colliec C, Couillard M, Masson A, Schmidt M and Bréchignac C 2007 Eur. Phys. J. D 43 151–154
[37] Li W, Zheng X and Fei W 2009 Vacuum 83 949
[38] Jensen P, Barabási A L, Larralde H, Havlin S and Stanley H E 1994 Phys. Rev. B 50 15316
[39] Neto A H C, Guinea F, Peres N M R, Novoselov K S and Geim A K 2009 Rev. Mod. Phys. 81 109–162
[40] Yakubovich A V, Verkhovtsev A V, Hanauske M and Solov’yov A V 2013 Computational Materials Science – ISSN 0927-0256 URL http://www.sciencedirect.com/science/article/pii/S0927025613000037
[41] Surfutovich E, Yakubovich A V and Solov’yov A V 2013 Sci. Rep. 3 1289
[43] Irisawa T, Uwaha M and Saito Y 1995 *Europhys. Lett.*, **30** 139–144
[44] Bréchignac C, Houdy P and Lahmani M (eds) 2007 *Nanometerials and Nanochemistry* (Cambridge University Press)
[45] Frenkel J (ed) 1955 *Kinetic Theory of Liquids* (Dover)
[46] Einstein A 1956 *Investigations on the Theory of Brownian Movement* (New York: Dover)
[47] Landau L D and Lifshitz E M 1987 *Fluid Mechanics* (Elsevier, Butterworth-Heinemann, Oxford)
[48] Mashiah A, Wolach O, Sandbank J, Uziel O, Raanani P and Lahav M 2008 *Acta Haematol.* **119** 142–150
[49] Baish J W and Jain R K 2000 *Cancer Resarch* **60** 3683–3688
[50] Phillips J C, Braun R, Wang W and *et al* 2005 *J. Comp. Chem.* **26** 1781–1802
[51] Brooks B, Bruccoleri R, Olafson B, States D, Swaminathan S and Karplus M 1983 *J. Comp. Chem.* **4** 187–217
[52] Humphrey W, Dalke A and Schulten K 1996 *J. Molec. Graphics* **14** 33–38