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Computational algorithms for fast-building 3D carbon nanotube models with defects

M. Leonor Contreras[a], Diego Ávila[b], José Alvarez[b], Roberto Rozas[a,*]

[a] Environmental Sciences Department, Faculty of Chemistry and Biology, University of Santiago de Chile, Usach, Avda. L. B. O'Higgins 3363, Santiago, Chile
[b] Informatics Department, Faculty of Engineering, University of Santiago de Chile, Usach, Avda. Ecuador 3659, Santiago, Chile

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ABSTRACT

Algorithms for generating defective carbon nanotubes have been developed and implemented in software. The algorithms were designed to create arrays of carbon atoms that form layers and interconnect. The parameters for construction were the following: Hamada indices that respond to topology (armchair, zigzag or chiral nanotubes) and diameter, the saturated or unsaturated nature of the nanotube, the length and, most importantly, the presence of defects that can be built individually or repetitively by rotating bonds, removing atoms, or adding additional carbon atoms. The output was written in a standard, exportable file format that contained atomic coordinates useful for further computational chemistry work.

1. Introduction

Carbon nanotubes (CNTs) have been recognized as one of the most important materials of the future [1] due to their remarkable properties. They have potential uses in a wide variety of applications, from molecular electronics devices to mechanical, biomedical, medicine, and analytical fields [2–6]. In particular, single-walled CNTs have interesting electronic properties that depend upon factors [7–11] such as chemical constitution, configuration, diameter, and length.

The properties of these nanostructures are drastically modified in the presence of defects such as pentagons, heptagons, rehybridization, vacancies, or dopants. The presence of one or more 5–7 defects (pentagon–heptagon pair) in CNTs has been shown to produce changes in topology that affect the electronic structure [12–14] and mechanical properties of nanotubes, inducing plastic transformations in an otherwise a brittle material [15]. Furthermore, the presence of pentagon–heptagon defects allowed for the heterojunction of nanotubes with different helicities [16,17] that had particular electronic properties that are potentially useful for designing new microelectronic devices [11]. Defects have also been shown to modify the hydrogen adsorption behavior of nanotubes.

Molecular dynamics simulations and density functional theory calculations indicated that defects created on the exterior wall of a (10,10) carbon nanotube enhanced hydrogen adsorption potential. The physisorbed hydrogen molecules remained on the defected nanotube at 300 K, while the hydrogen molecules adsorbed on a perfect nanotube were desorbed [18]. The use of defective nanotubes as an environmental protective agent has been studied using the B3LYP/6-31G(d) method [19]. An interesting application of CNTs with defects involved nitrogen-doped carbon nanotubes used for C—H activation [20,21]. Functionalized [22,23], or doped, nanotubes with a particular distribution of dopants can be useful in many fields and need to be further researched. DFT (density functional theory) calculations of small diameter (∼0.3 nm) nitrogen-containing carbon nanotubes suggested that they could possibly be used as a conducting material for electronic nanodevices [24].

How are these defects produced? It has been observed that when CNTs are formed they are under great tension. One way they released this strain was by a 90° rotation of a C—C bond around its center, creating a Stone–Wales (SW, 5-7-7-5) defect [15]. That defect behaved as a nucleation center for the formation of other defects. Carbon dimers have also been incorporated into nanotubes and formed a new set of defects involving pentagons and heptagons or pentagons and octagons [5,13–15].

* Corresponding author at: Computational Chemistry & Intellectual Property Laboratory, University of Santiago de Chile, Usach, Casilla 40, Correo 33, Santiago 71772-K, Chile. Tel.: +56 2 718 1151; fax: +56 2 681 2108.
E-mail addresses: leonor.contreras@usach.cl (M. Leonor Contreras), diego.avila.o@gmail.com (D. Ávila), jose.alvarez@usach.cl (J. Alvarez), roberto.rozas@usach.cl (R. Rozas).

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Although many advances in nanotube synthetic methods have been published [25,26], it has always been more convenient to model these new nanostructures to predict their properties before synthesizing them in the laboratory. Molecular modeling offers a practical way to evaluate the potential properties of new materials, such as CNTs, before they are synthesized.

Nanotube molecular design requires structural visualization, information on the atomic coordinates, and consideration of the presence of different nanostructure topologies and geometries. Having appropriate atomic coordinates necessary for computational chemistry work is a challenge, especially for structures with a large number of atoms (i.e., over 300 atoms) bonded with a particular topology, such as defective CNTs. Clearly, an automated computational tool specific, with appropriate user control, for these kind of molecules would be advantageous.

Algorithms for the automated generation of CNTs with a regular hexagonal wall and without any defects are not very complex and have been solved using various tools and software. Most of the solutions [27,28] started with specified (n,m) Hamada indices [10] and utilized a graphene sheet roll-up algorithm to generate single-walled CNTs.

In a related problem, Melchor and Dobado [29] developed software, CoNTub, to solve the problem of joining two arbitrary CNTs. Their nanotube generation algorithm connects both tubes based on a topological algebra. This algebra takes into account a number of combinations and relative orientations between a minimum number of defects using a continuous strip of hexagons containing pentagon and heptagon cycles. However, that software is useful for regular nanotubes, not defective ones.

Stenberg et al. [5,13], using computer simulation tools, inserted molecular moieties of two carbons into a single-walled carbon nanotube to generation bumpy or zipper nanotubes. That approach applied modifications to a previously created nanotube structure; it is not a piece of software that builds defective carbon nanotubes from atomic units.

The algorithms developed in this work were capable of building defect-containing nanotubes, atom by atom, of various topologies and defects. The procedure was implemented as scripts written in the Tcl/Tk language, making it portable to other modeling systems for further property calculations.

2. Computational methods

Instead of using an algorithm oriented towards cutting and rolling up a previously constructed graphene sheet for tube creation, we have created algorithms for nanotube construction by "stacking up" layers or rings, as shown in Fig. 1. A layer is the shorter closed path that begins and ends with the same atom. The number of layers defines the length of the tube, and the number of atoms included in each layer defines its diameter. Nanotube chirality is defined by the particular interconnections between layers. In a single layer, each atom is bound to the previous atom and to the next one. At the same time, each atom has two free valences to connect to both carbon atoms in neighboring layers and hydrogen, if applicable.

Table 1
Relationship between Hamada indices and the number of atoms per layer.

Nanotube configuration	Hamada indexes	x
Zigzag	(n,0)	$2{\cdot}n$
Chiral	(n,m)	$2{\cdot}n+m$
Armchair	(n,n)	$4{\cdot}n$

2.1. Generation of the base layer

Let us consider atoms placed in a two dimensional matrix, R (see Fig. 2) whose size, as expected, depends on the tube length and chirality. Each row, $R[i]$, represents the i layer for the zigzag and armchair topologies, with $R[0]$ being the first row. The number of atoms constituting each layer, x, is related to the Hamada indices, as shown in Table 1. Atoms are consecutively numbered from 1 to x for the first layer. The layers increase in such a way that second layer starts with $x+1$, the third layer starts with $2x+1$ and so on. The first layer is finished when the atom in column x is bound to the atom in column 1. The same is true for the second layer, the atom numbered $3x$ (i.e., $2x+x$) is bound to atom $2x+1$ and so on. Atom numbering is an important factor when writing scripts to define the interconnections between layers as they are built.

2.2. Layer interconnection

Layers were connected in a specific way to generate spatially ordered hexagons of a particular topology according to the following rules:

1. *Zigzag nanotubes*. (i) Odd atoms of an odd row were connected to odd atoms of an anterior row; (ii) even atoms of an even row were connected to even atoms of an anterior row, as is shown in Fig. 2a.
2. *Armchair nanotubes*. For each atom, starting with the first atom of the second row, the corresponding atom identifier number was divided by 4. If the remainder of that division was 0 or 1, a connection with an anterior row was produced in the following way: (i) if the remainder was 1, the atom was connected to an atom of an anterior row having the "same column" plus 1 in matrix R; (ii) if the remainder was 0, connection was made to an atom in an anterior row having the "same column" minus 1 in matrix R, as shown in Fig. 2c.
3. *Chiral nanotubes*. The general procedure was similar to that of zigzag nanotubes except for the closure of the base layer. For a (n,m) tube with a length of l, the size of matrix R was $2n^*(l+m)$, and first atom in row $R[0]$ was bonded with the last atom in row $R[m]$. In general, the last atom in row $R[i+m]$ was bonded with first atom in row $R[i]$. Finally, a cutting away (or atom deletion) step in the initial (top right) and final (bottom left) left-over triangular sections of the nanotube matrix was performed (see Fig. 2b).

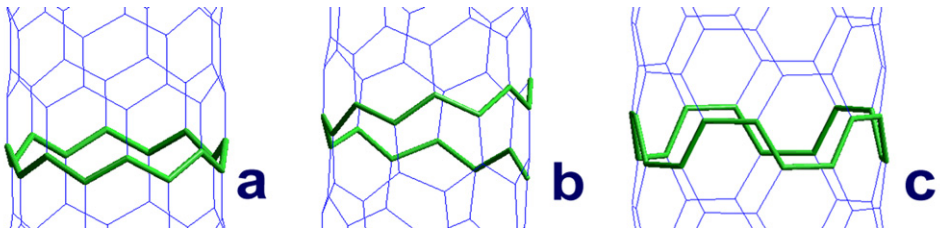

Fig. 1. Base layers (highlighted) for the: (a) zigzag, (b) chiral, and (c) armchair nanotubes.

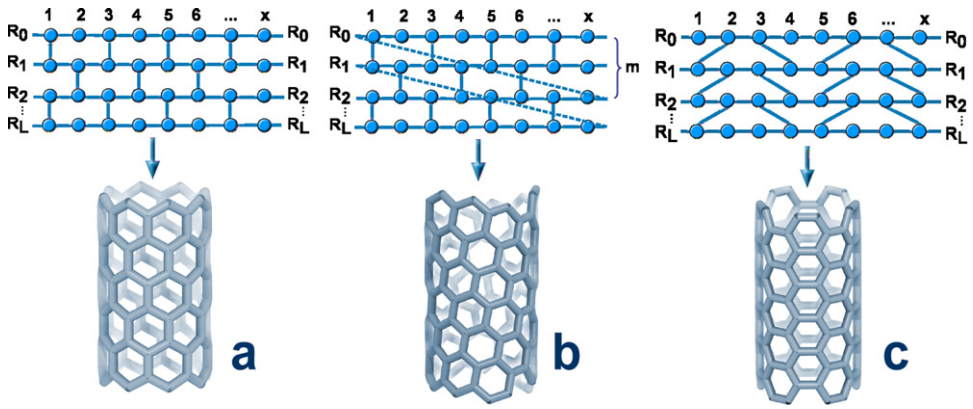

Fig. 2. Layer interconnections for: (a) zigzag, (b) chiral, and (c) armchair nanotubes.

The algorithm for generation of a (*n*,0) zigzag nanotube is shown below. The algorithms for armchair, chiral and defective nanotube generation are shown in Supplementary Information.

Algorithm 1. Zigzag nanotube construction

```
Procedure GenerateZigzag (size n, length l)
x = n * 2                          // size of layer
Matrix Tube[x,l] of Carbon         // tube is a matrix of carbon atoms
atom_id = 1                        // the current atom id
CreateAtom(Carbon)                 // create first carbon atom
// generation of the base (0) or first  layer
for  atom_id from 2 to x
        CreateAtom(Carbon)             //create a carbon atom and put it in Tube[0,atom_id] matrix
        BondAtoms(atom_id, atom_id-1)// make a bond between atoms atom_id  and atom_id-1
        atom_id++
BondAtoms (x, 1)                   // the layer is closed
// further layer generation
for   layer from 1 to  l
        CreateAtom(Carbon)             // first atom in layer
        for  col from 0 to  x
                CreateAtom(Carbon)     // next atom in layer
                atom_id ++
                BondAtoms(atom_id, atom_id-1)          // bond with previous atom in same layer
                if (isEven(layer)  AND is Even(col) OR (isOdd(layer) AND isOdd(col)) then
                        BondAtoms(atom_id, atomid(layer-1, col))       // bond with atom in same
                column and previous row
        endfor
        BondAtoms(atom_id, atomid(layer, 1)    // close the layer
        atom_id++
endfor
Endproc
```

The algorithm had an average time complexity order of O(x^*l), with x being the number of layer atoms and l is the length of the tube.

The real length of the nanotube depended on the number of layers. For H layers, the approximate length (in Å) of the nanotube was expressed as Length = 1.5 + (2.25)*($H-1$). The constant values indicated in the previous expression are described in Fig. 3.

2.3. Defect incorporation

To create a defective CNT, the atom matrix for the armchair nanotube was modified by adding carbon dimers according to the patterns in Fig. 4. Depending on the distribution of the dimer insertions, a different type of defective nanotube (bumpy, zipper, multi-zipper) was obtained. The generation of haeckelite nanostructures could be achieved by the transversally insertion of carbon dimers. In our approach, the carbon dimers were all coaxially inserted along the nanotube axis. Their position in the tube was the factor that determined the type of defective nanotube.

To create a bumpy nanotube, carbon dimers were added in positions transversally located around the diameter of the nanotube. For a zipper nanotube, carbon dimers were inserted along the nanotube. For a multi-zipper nanotube, carbon dimers were inserted in alternating patterns of zippers along the nanotube.

The carbon dimer addition algorithms operated over contiguous layers of the nanotubes and were based on the location of the starting atom, where the insertion was going to take place. From

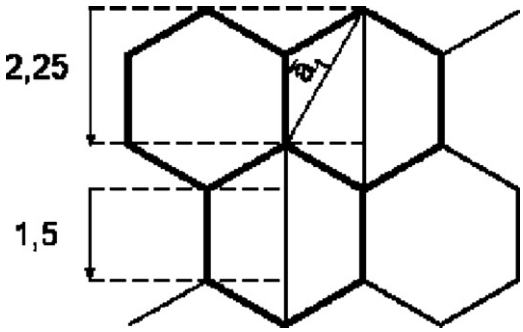

Fig. 3. Layer parameters used for estimating the length in Å.

this atom, labeled a (see Fig. 5), the next atom in the layer was selected (the b atom). The pair of atoms with the same position as a—b in the next layer (c and d) were then selected.

The next step was to break the a—b and c—d bonds. Subsequently, one carbon atom of the carbon dimer (labeled D_1) was inserted and bonded to atoms a and b. Similarly, the second atom of the carbon dimer, D_2, was inserted between the c and d atom pair. Finally, D_1 and D_2 were bonded to each other, as shown in Fig. 6.

The algorithm for building the Stone–Wales defect reorganized the bonding of the selected pair of contiguous atoms and the two adjacent atoms. This reorganized neighborhood was later geometrically optimized, and the selected atomic pair was rotated 90° to obtain the 5-7-7-5 defect, as shown in Fig. 7. This action was repeated, as needed, along the tube as long as the topological conditions existed. The conditions being that the atom pair must be surrounded by only hexagonal cycles and should not be at the border of the tube. When the transformation was repeated on an already transformed pair, the action was reversed.

2.4. Algorithm implementation

For algorithm implementation and testing, HyperChem, a widely used software package for molecular modeling and calculation [30], was used. This software package had several databases for the representation of complex structures, but it lacked one for general nanotube generation. However, it provided the capability to expand functionality through scripts written in Hcl (HyperChem command language) or Tcl/Tk (Tool command language/Toolkit). We were then able to completely integrate our algorithm into the HyperChem software and create a new tool to model various nanotube configurations and defects. The addition and implementation of our algorithm in HyperChem we named HyperTube. Of course, other calculation and modeling program suites have script execution capabilities and could have been used [31].

Scripting languages. Hcl allowed one to automate all HyperChem features, including modeling, calculation and even menu

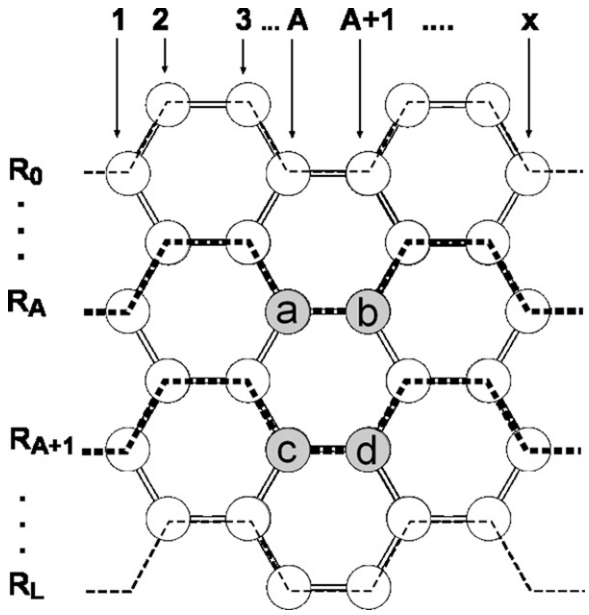

Fig. 5. Selection of the atoms a, b, c, and d among the layers.

modification. Tcl/Tk allowed for the creation of procedural scripts with rich user interfaces via the Tk extension.

The topology of the molecular structures was described in Hcl scripts. To do so, the only necessary information was the correct atom identifiers and the corresponding bonds between them. The geometry of the molecule was generated by HyperChem. The scripting software development process followed the classic waterfall model [32]: the main requirements were defined at the beginning of the development process, followed by the general design, and finally, the construction or writing of the script code.

The final application consisted of a set of Tcl/Tk/Hcl script files that were executed via a main Hcl script. An extra menu was added to HyperChem that contained two options, each with a different GUI (Graphical User Interface), "Regular Nanotube Generation" and "Defect-Containing Nanotube Generation." An overview of the modified main menu of HyperTube is shown in Fig. 8.

3. Results and discussion

The algorithms here developed implemented as script programs, called HyperTube, have capabilities to build saturated and unsaturated carbon nanotubes, and their corresponding defective nanotubes. Scripts are written in Hcl and Tcl/Tk and allow for working with commercial systems such as the software HyperChem [30]. The aim of HyperTube was to simplify nanotube topology generation by constructing the layers of the nanotube one atom at a time and, at the same time, interconnecting them, thereby rendering the roll-up process and overlapping of atoms unnecessary. In this

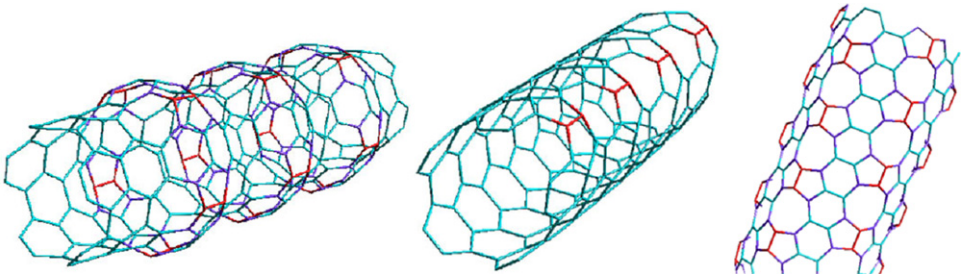

Fig. 4. Bumpy, zipper and multi-zipper nanotubes generated by HyperTube (from left to right, respectively; the added carbon dimers are highlighted in red).

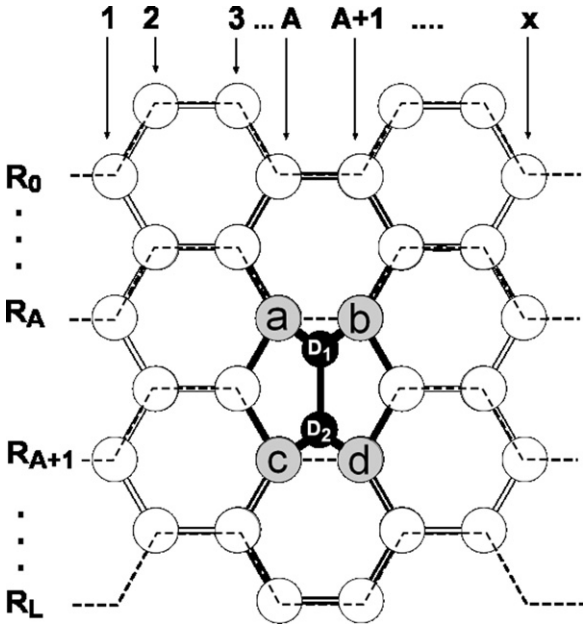

Fig. 6. Carbon dimer addition between the a–b and c–d atom pairs.

work, we produced a simple algorithm structure and source code. By reducing the constitutive unit of the nanotube from a hexagonal cycle (used by the other systems) to the atom itself, the topological modifications and defects were more easily generated and later modified.

This application is able to automatically generate defective nanotubes containing either sp^2 or sp^3 C atoms. Other software for nanotube generation, such as CoNTub [29] or MCAD [28], does not generate nanotubes with defects neither saturated nanotubes. An earlier attempt at the topological generation of zigzag nanotubes was presented as a Tcl/Tk sample program [33] included on the website of HyperCube Inc. (the developers of HyperChem); however, it does not generate defective nanotubes.

HyperTube has several implications on modeling for nanotubes with different defects, such as:

1. *Hydrogen adsorption*. Hydrogen storage through adsorption mechanisms (chemisorption and physisorption) is an actual problem that merits analysis and research on the basis of hydrogen importance as an energy source. As was mentioned HyperTube has the ability of generating both particular carbon nanotube structures that can be unsaturated (sp^2 hybridized) and also the same carbon nanotube pattern but totally saturated (sp^3 hybridized) where hydrogen is chemisorbed in an exocyclic way. This unique feature of HyperTube facilitates hydrogen chemisorption-energy calculations for potential new nanotube derivative-material useful for storing hydrogen. Using density functional theory and the HyperTube tool we have reported exothermic values of chemisorption-energy per atom of hydrogen chemisorbed from −29.2 kcal/mol to −35.2 kcal/mol for the hydrogen chemisorption on nitrogen-containing carbon nanotubes with small diameters (∼0.3 nm) and high nitrogen contents (∼32%) [20].
2. *Vacancies*. An example of these defects is provided in supplementary information part of this paper. For obtaining a nanotube with vacancies using HyperTube, it is necessary only to remove one or more atoms in a perfect nanotube to get mono- or multiple-vacancy defects at different positions and also with a required variable vacancy density.

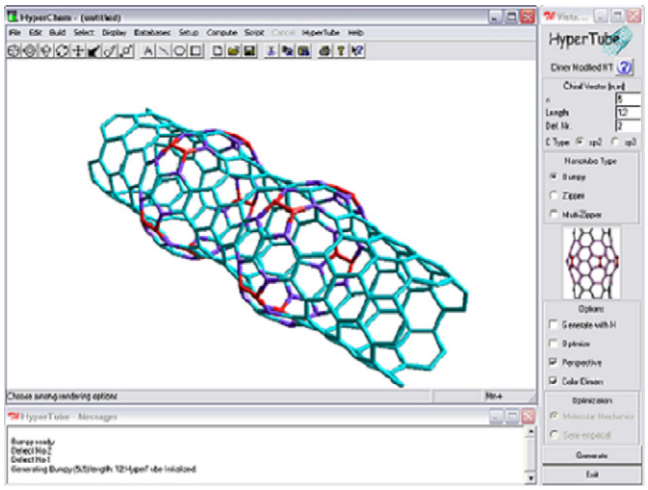

Fig. 8. Main view of HyperTube and one generated defective nanotube.

This kind of defects has recently been studied looking for the energy band gap modulation of a (10,5) chiral carbon nanotube with a mono-vacancy defect using ab initio calculations [34] to analyze the variation in the local energy gap according to the direction and strength of an external applied electric field. When the external electric field is applied along the axis of the mono-vacancy defective nanotube, the local energy gap increases first with the strength of the field (from 0 to 0.4 V/Å) and then decreases (when the field strength increases from 0.4 to 0.7 V/Å). This effect is not observed when the external electric field is applied in the perpendicular direction. The described orientation effect of an external electric field gives some flexibility

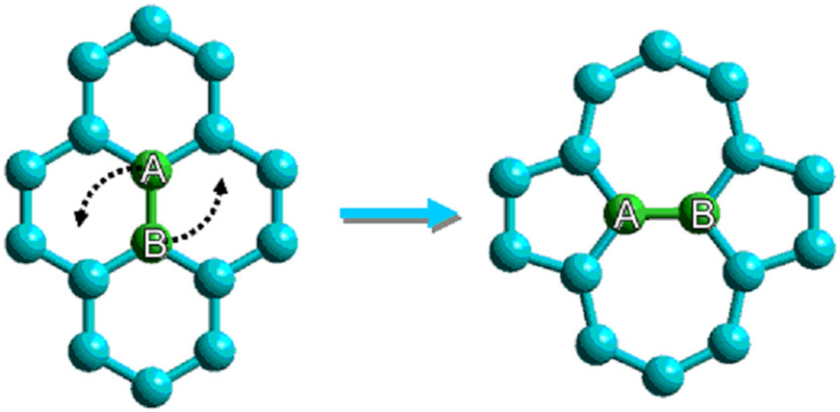

Fig. 7. Representation of the Stone–Wales transformation.

to select a suitable local energy gap range for specific applications in the electronic area. Using HyperTube, carbon nanotubes can be doped with different atoms, and this particular research could be enriched.

The same research group studying the variation in the band structure of three different single walled carbon nanotubes (5,5), (10,0), and (10,5), using the first-principle density functional theory (DFT) calculations [35], found that the properties of the nanotubes can be tuned by controlling the mono-vacancy defect density. They explain that on the base of a strain increase due to dangling bonds, the twofold coordinated carbon protrude outward of the nanotube reducing the local energy gap.

Another study on vacancy defects refers to induced magnetism in graphene and graphene ribbons [36], which can be extended to carbon nanotubes. The electronic properties of the defects resulting from the removal of atoms from a graphene depend on the sublattice imbalance, where spin interactions between two magnetic defects of the same imbalance can be ferromagnetic, antiferromagnetic or annihilating depending on the density of monoatomic vacancies in such a way that a very dilute monoatomic vacancy is related to a paramagnetic effect; on the contrary, a high density monoatomic vacancy produces an annihilating effect. On the other hand it is known that nanoporous graphene is magnetic but when it is completely saturated with hydrogen, magnetism disappears [37]. Again for a wider knowledge on the effect of different defective nanotubes, HyperTube could be of some help also for this type of research.

3. *Stone–Wales defects*. The algorithm for the Stone–Wales defects created here allows the user to select the place of the defect formation, and the density of such defects. Liu et al. have studied the impact these defects have on nonlinear optical behavior of carbon nanotubes [38], where it is shown that Stone–Wales defects produce an increase on the static first hyperpolarizability (β_0) 10^3 times respect of carbon nanotubes with no defect. According to that research in order to enhance nonlinear optical effects is appropriate to consider a strategy of controlling the defects introduced in the nanotubes.

   Also mechanical studies on nanotubes show that Stone–Wales defects decrease critical buckling force, pressure, and strain of single walled CNTs, under axial compression leading to more reliable design of nanostructures [39].
4. *Bumps*. For CNTs with bumps it was demonstrated [40] that CNT bumps can achieve high gain and high thermal conductivity in high-frequency high-power amplifiers of mobile communication systems. Semiconductor products are continuously improving their performance. With the aim of controlling heat transfer that affect semiconductor chips, modeling of CNTs with bumps would be facilitated through the use of HyperTube by allowing for the study on the effect of some physical parameters such as the diameter, the length or the number of bumps on nanotube conductivity parameters (i.e., valence band maximum state, conduction band minimum state).
5. *Nanobuds and non-covalent CNT surface modifiers*. Generation of nanobuds can be done by constructing a nanotube and then importing a fullerene and manually bonding them. Also, if we have available the geometry data for a fullerene, it will be possible to generate nanobuds by joining the fullerene to the nanotube moiety (an example of a relaxed nanobud structure built with the aid of HyperTube is presented in Supplementary Information). As it is known, nanotubes without any defect tend to aggregate into bundles and ropes, due to the van der Waals interactions between each other, having solubility problems, and difficulties to be functionalized. However, fullerenes can easily react, for instance with amines. Having both structures together provides a means for functionalizing the nanotube [41]. Different nanobuds structures can be envisaged and modeled with the help of HyperTube. Also, this tool should contribute to the search of novel non-covalent CNT-surface modifiers that can interact with a relatively strong attraction with the nanotube which can provide different sites of interaction with the tube sidewalls with the aim to guarantee mechanical stability. As a result nanotubes could be homogeneously managed in various media.
6. *Zipper*. Dimer addition into carbon nanotubes makes zipper nanotubes which have octagons surrounded by pentagons. This feature offers just the geometric dimensions that have been considered as very useful to be bonded to Ultrananocrystalline™ diamond (novel form of nanocarbon developed at Argonne Laboratories that can be deposited on many different surfaces) with the aim of optimizing the combined properties of both, with applications in the field of thermoelectric materials with implications in a more efficiently electricity production from solar or thermal power generation [5]. Further studies on these structures can optimize their properties upon desired applications. HyperTube could help to model zipper nanotubes having different physical properties.

Other software as the Homology Modeling Professional [42], created to model biological molecules like proteins, was also developed using Tcl/Tk scripts. The utilization of an internal Tcl interpreter is the main architectural difference between it, which uses an external interpreter, and HyperTube. The idea behind this was to simplify the installation process for HyperTube, requiring only the set of HyperTube scripts and the licensed HyperChem software. HyperTube algorithms are available as supporting information and scripts are available on request.

4. Conclusions

The development of ad hoc algorithms that allowed for the atomic coordinates of a large variety of nanotubes, with or without defects, having either sp^2 or sp^3 carbon atoms and with varying diameters along the nanotube was presented. These algorithms are based on atomic units that form interconnected layers in a specific way to obtain a desired nanotube topology. Therefore, nanotubes with defects, such as bumpy, zipper, and multi-zipper, can be automatically created in a portable format. Regular zigzag, chiral, and armchair nanotubes (with hexagonal cycles only) can be later altered with vacancies or SW defects.

As it was discussed above, the potential implications of the algorithms here developed for generating defects related to Stone–Wales, bumps, zipper, nanobuds, vacancies, doped, and saturated/unsaturated nanotubes are quite wide and could be of help for modeling nanotubes with desired properties in the field of hydrogen adsorption, electronic area, magnetism, nonlinear optical properties, buckling behavior, thermal conductivity, electricity more efficiently produced, etc., where an appropriate defect design is needed.

Layer “stacking-up” algorithms developed allowed for the generation of defective nanotubes in one simple step. Tcl/Tk script implementation of algorithms, developed here, could be of general use. We have shown an application where an extra menu, containing independent easy-to-use GUIs, was added to the geometry generation tools of HyperChem.

All of the nanotubes generated here can be exported to other molecular design applications where they can be functionalized, doped in different ways, with or without vacancies, and modified at will to evaluate their theoretical properties. Therefore, HyperTube could be a useful and easy-to-use tool in a field of research that undergoes continuous development.

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Appendix A. Supplementary data

Supplementary data associated with this article can be found, in the online version, at http://dx.doi.org/10.1016/j.jmgm.2012.05.001.

References

[1] J.M. Marulanda, Carbon Nanotubes, In-Tech, India, 2010.
[2] D.L. Shenkenberg, Can the miracles promised by carbon nanotubes be realized? Biophotonics International (2008) 34–36.
[3] M.D. Ganji, Behavior of a single nitrogen molecule on the pentagon at a carbon nanotube tip: a first-principles study, Nanotechnology 19 (2008) 025709.1–025709.5.
[4] D. Tománek, Preface and introduction to carbon nanotubes: advanced topics in the synthesis, structure, properties and applications, in: A. Jorio, M.S. Dresselhaus, G. Dresselhaus (Eds.), Topics in Applied Physics, vol. 111, Springer, Berlin, 2008.
[5] E. Brown, Carbon Nanotube Building Blocks Open up Possibilities for Advanced Electronics, Argonne National Laboratory. http://www.physorg.com/news71333426.html (accessed February 2012).
[6] X. Xiong, J. Ouyang, W.R.G. Baeyens, J.R. Delanghe, X. Shen, Y. Yang, Enhanced separation of purine and pyrimidine bases using carboxylic multiwalled carbon nanotubes as additive in capillary zone electrophoresis, Electrophoresis 27 (2006) 3243–3253.
[7] S.H. Yang, W.H. Shin, J.K. Kang, The nature of graphite- and pyridine like nitrogen configurations in carbon nitride nanotubes: dependence on diameter and helicity, Small 4 (2008) 437–441.
[8] K.M. Alam, A.K. Ray, A hybrid density functional study of zigzag SiC nanotubes, Nanotechnology 18 (2007) 495706.1–495706.10.
[9] R. Saito, M. Fujita, G. Dresselhaus, M.S. Dresselhaus, Electronic structure of chiral graphene tubules, Applied Physics Letters 60 (1992) 2204–2206.
[10] N. Hamada, S. Sawada, A. Oshiyama, New one-dimensional conductors: grafite microtubules, Physical Review Letters 68 (1992) 1579–1581.
[11] J.C. Charlier, Defects in carbon nanotubes, Accounts of Chemical Research 35 (2002) 1063–1069.
[12] J.C. Charlier, T.W. Ebessen, Ph. Lambin, Structural and electronic properties of pentagon–heptagon pair defects in carbon nanotubes, Physical Review B 53 (1996) 11108–11113.
[13] M. Stenberg, L.A. Curtiss, D.M. Gruen, G. Kedziora, D.A. Horner, P.C. Redfern, et al., Carbon ad-dimer defects in carbon nanotubes, Physical Review Letters 96 (2006) 075506.1–075506.4.
[14] D.A. Horner, P.C. Redfern, M. Stenberg, P. Zapol, L.A. Curtiss, Increased reactivity of single wall carbon nanotubes at carbon ad-dimer defect sites, Chemical Physics Letters 450 (2007) 71–75.
[15] D. Orlikowski, M. Buongiorno Nardelli, J. Bernholc, C. Roland, Ad-dimers on strained carbon nanotubes: a new route for quantum dot formation? Physical Review Letters 83 (1999) 4132–4135.
[16] L. Chico, V.H. Crespi, L.X. Benedict, S.G. Louie, M.L. Cohen, Pure carbon nanoscale devices: nanotube heterojunctions, Physical Review Letters 76 (1996) 971–974.
[17] Ph. Lambin, V. Meunier, Connecting carbon nanotubes with pentagon–heptagon pair defects. http://perso.fundp.ac.be/~(phlambin/Nanotube/knee.html (accessed February 2012).
[18] Y.Y. Xia, J.Z.H. Zhu, M.W. Zhao, F. Li, B.D. Huang, Y.J. Ji, et al., Enhancement of hydrogen physisorption on single-walled carbon nanotubes resulting from defects created by carbon bombardment, Physical Review B 71 (2005) 075412.1–075412.8.
[19] V. Ruangpornvisuti, Molecular modelling of dissociative and non-dissociative chemisorption of nitrosamine on closed-ended and open-ended pristine and Stone–Wales defective (5,5) armchair single-walled carbon nanotubes, Journal of Molecular Modeling 16 (2010) 1127–1138.
[20] M.L. Contreras, R. Rozas, Nitrogen-containing carbon nanotubes. A theoretical approach, in: S. Bianco (Ed.), Carbon Nanotubes – From Research to Applications, InTech, Croatia, 2011, pp. 3–26 (Chapter 1) http://www.intechopen.com/articles/show/title/nitrogen-containing-carbon-nanotubes-a-theoretical-approach
[21] X. Hu, Z. Zhou, Q. Lin, Y. Wu, Z. Zhang, High reactivity of metal-free nitrogen-doped carbon nanotube for the C—H activation, Chemical Physics Letters 503 (2011) 287–291.
[22] H. Li, I. Kim, Fabrication and application of carbon nanotube-based hybrid nanomaterials by means of non-covalently functionalized carbon nanotubes, in: S. Bianco (Ed.), Carbon Nanotubes. From Research to Applications, InTech, Croatia, 2011, pp. 211–228 (Chapter 13).
[23] T. Yumura, A density functional theory study of chemical functionalization of carbon nanotubes – toward site selective functionalization, in: J.M. Marulanda (Ed.), Electronic Properties of Carbon Nanotubes, InTech, India, 2011, pp. 309–328 (Chapter 14).
[24] M.L. Contreras, D. Avila, J. Alvarez, R. Rozas, Exploring the structural and electronic properties of nitrogen-containing exohydrogenated carbon nanotubes: a quantum chemistry study, Structural Chemistry 21 (2010) 573–581.
[25] G. Sánchez-Pomales, C. Pagán-Miranda, L. Santiago-Rodríguez, C.R. Cabrera, DNA-wrapped carbon nanotubes: from synthesis to applications, in: J.M. Marulanda (Ed.), Carbon Nanotubes, In-Tech, India, 2010, pp. 721–748 (Chapter 35).
[26] M.M.A. Rafique, J. Iqbal, Production of carbon nanotubes by different routes—a review, Journal of Encapsulation and Adsorption Science 1 (2011) 29–34.
[27] S. Maruyama, Nanotube coordinate generator with a Viewer for Windows. http://www.photon.t.u-tokyo.ac.jp/~(maruyama/wrapping3/wrapping.html (accessed December 2011).
[28] M.L. Contreras, E. Benítez, J. Alvarez, R. Rozas, Algorithm for nanotubes computer generation with different configurations, Algorithms 2 (2009) 108–120, http://www.mdpi.com/1999-4893/2/1/108
[29] S. Melchor, J. Dobado, CoNTub: an algorithm for connecting two arbitrary carbon nanotubes, Journal of Chemical Information and Computer Science 44 (2004) 1639–1646.
[30] HyperChem Release 7.5, Hypercube Inc., 1115 NW 4th Street, Gainesville, Florida 32601, USA, 2012.
[31] Schrodinger, Schrödinger, LLC, New York, NY, 2011.
[32] R.S. Pressman, Software Engineer. A Practitioner's Approach, 5th ed., MacGraw-Hill, Madrid, 2002.
[33] HyperCube, Inc. http://www.computationalchemistry.com/support/download/Scripts/index.htm (accessed February 2012).
[34] Y.P. Luo, L.G. Tien, C.H. Tsai, M.H. Lee, F.Y. Li, Effect of vacancy defect on electrical properties of chiral single-walled carbon nanotube under external electrical field, Chinese Physics B 20 (2011) 017302-1–017302-5.
[35] Y.P. Luo, L.G. Tien, C.H. Tsai, M.H. Lee, F.Y. Li, Dependence of the electrical properties of defective single-walled carbon nanotubes on the vacancy density, Chinese Physics B 20 (2011) 087303-1–087303-7.
[36] J.J. Palacios, J. Fernández-Rossier, Vacancy induced magnetism in graphene and graphene ribbons, Physical Review B 77 (2008) 195428-1–195428-14.
[37] S. Li, H.M. Zhao, P. Jena, Ti-doped nano-porous graphene: a material for hydrogen storage and sensor, Frontiers of Physics 6 (2011) 204–208.
[38] Z.B. Liu, Z.J. Zhou, Z.R. Li, Q.Z. Li, F.Y. Jia, J.B. Cheng, et al., What is the role of defects in single-walled carbon nanotubes for nonlinear optical property? Journal of Materials Chemistry 21 (2011) 8905–8910.
[39] A.R. Ranjbartoreh, G. Wang, Effect of topological defects on buckling behavior of single-walled carbon nanotube, Nanoscale Research Letters 6 (2011) 28-1–28-5.
[40] T. Iwai, Y. Awano, Carbon nanotube bumps for thermal electric conduction in transistor, Fujitsu Scientific and Technical Journal 43 (2007) 508–515.
[41] H. Li, I. Kim, Fabrication and applications of carbon nanotube-based hybrid nanomaterials by means of non-covalently functionalized carbon nanotubes, in: S. Bianco (Ed.), Carbon Nanotubes – From Research to Applications, InTech, Croatia, 2011, pp. 211–228 (Chapter 13).
[42] Institute of Molecular Function, Homology Modeling for HyperChem. http://www.molfunction.com/software1.htm (accessed February 2012).