

## APPENDIX – TINKER users guide for VEM tests of CNTs

### A.1 Virtual Experiment Method

The virtual experiment method (VEM) is a descriptive name for the research methodology used to develop continuum results from atomistic simulations. The base concept of this method is to perform atomic simulations which mimic basic macro-scale, engineering material tests on nanoscale objects. Currently, these simple tests are difficult to perform physically because of issues of scale. Common material tests, such as tension, torsion and cantilever bending can be simulated with atomistic simulations.

The VEM is in its most basic form a three step method. The first step is relaxation, the second step is the deformation and the third step is a minimization. The steps are listed below for clarity with the preprocessing (build) and postprocessing (analysis) steps also included.

#### A. Build

the CNT is created by estimating atomic positions

##### 1 Relaxation

minimize the potential energy of the structure to find the relaxed structure

##### 2 Deformation

deform the CNT by estimating new atomic positions corresponding to the deformed state

- repeat for as many deformation steps as necessary

apply appropriate boundary conditions

##### 3 Minimization

minimize the energy of the deformed structures to find the ‘true’ positions of atoms

- perform for each deformed state

#### B Analysis

strain energy and true deformation are available by comparing to the original, relaxed energy and position.

Initially, the atomic positions for the CNT (or more generally any molecule(s) to be studied) are input as educated guesses. For most MM simulations this also means defining the atom types and bonds between atoms. The potential energy between each bond is then minimized to find the ‘true’ relaxed molecular structure according to the type of MM potential set used. This relaxed structure is then deformed by estimating

new atomic positions corresponding to the type of experiment being performed. For example, to simulate tension in a nanotube each atom is moved by 1% of its original z-coordinate. The most appropriate boundary conditions are set on the atoms to insure the molecule will not relax back to its initial structure. The deformed structure is again energy minimized by allowing the other atom positions vary to find the atomic position with the minimum energy for the deformed molecule. By comparing the deformed structure (step 3) against the relaxed structure (step 1), the strain energy and tube deformations can be calculated. This is analogous to obtaining load and deflection data from a material test machine.

## A.2 TINKER

The Tinker molecular modeling package was developed at Washington University in St. Louis. It can be downloaded freely at the following website, <http://dasher.wustl.edu/tinker>. Executable, source code and an **extensive user's manual** are available.

Tinker was developed for general use in biochemistry molecular modeling. It has numerous potential sets including the mm2, mm3, Amber, Charm, OPLS and their variations (mm3pro, OPLSAA).

Tinker can be used either for molecular mechanics or dynamics simulations. The procedure outlined here are for molecular mechanics simulations. Because Tinker was developed primarily for biochemistry research, certain boundary conditions can not be met precisely and therefore the engineering analyst must be careful (see boundary condition section).

Tinker is a conglomeration of DOS executable programs run in series. The executables should all be run from the same directory along with the parameter sets (\*.prm files), molecule files (\*.xyz) and keyfiles (\*.key).

The VEM relevant Tinker programs, commands and characteristics are briefly discussed in the following sections. For a full discussion of the Tinker package see the user's manual.

### File Types.

Two main file types are used in the application of the VEM with Tinker, the \*.xyz and \*.key files. The \*.xyz file types define the molecular structure. They contain the information on atomic number, type, xyz cartesian coordinates and neighbor bonding (see later examples). If an energy minimization is performed on an \*.xyz file, Tinker outputs the results in another xyz file with a suffix number (for example, \*.xyz\_2). The code will use the highest numbered for solving or analyzing a new problem (for example minimizing nanotube.xyz\_2 to a more precise energy level will output as nanotube.xyz\_3).

The \*.key files contain the internal Tinker commands used for the simulation. The boundary condition commands such as *restrain-position* or *inactive* are applied here. When a solution routine is executed for an \*.xyz system, the routine immediately looks for a similarly named \*.key file for solution command instructions. If the keyfile is named differently than the \*.xyz file, then -k newname.key should be input into the command line. The default values are hard coded into the Tinker solving routines and are applied whenever commands are not directly specified in the \*.key file. Likewise, if the \*.key file is not given default values are used.

### Potentials & Parameter Sets.

Various potentials used in common commercial and academic molecular dynamics packages are available in Tinker. These potentials have been refit to conform to the Tinker potential equation. The potentials are available as Tinker parameter sets (\*.prm files). The parameter sets have been tested and validated versus the original potential results. Each parameter set defines the atom types slightly differently, therefore, each \*.xyz file is specific to one set. Any parameter set may be used with any Tinker routine and is generally part of the input parameters. (Note: the Tersoff-Brenner potential is a very specific C-C bonding potential and is not included with the Tinker package).

### Solution Routines.

Two main solution routines are used in the VEM procedure, the minimize and newton programs. Both minimize the potential energy of a molecular structure or system by repositioning of the atoms until a specified gradient is found. A root mean square (rms)

gradient value of 0.001 was found to be the best choice for the convergence of both energy and position in this study (the default value is 0.01).

#### MINIMIZE.EXE

The minimize.exe routine uses a steepest descent type algorithm to find the minimum energy of a structure. The minimize routine is a slower routine, especially around the minimum energy, but is more accepting of initially poor molecular structures. For most nanotube cases, the initial molecular positions are adequate and minimize.exe is not the best choice.

#### NEWTON.EXE

The newton.exe routine is a solution algorithm that can adaptively incorporate several different minimization methods (Newton-Rhapson, negative curvature, etc.). The newton.exe routine requires the Hessian matrix (second derivatives) to run which may become a problem for very large systems. For many simulations it is a faster routine because it does not oscillate around the minimum energy well. In the current study, a single run of newton.exe, to an rms gradient of 0.001, was used and solution times were acceptable.

#### Processing Routines.

Only a few processing routines are needed for the VEM. They are described individually below.

#### XYZEDIT.EXE

This program allows the user to directly manipulate a molecular structure. It was primarily used to move atom #1 from its relaxed position to the coordinates of [0,0,0] to help post- and intermediate-processing.

#### ANALYZE.EXE

This program was used to calculate the energy of a molecular structure. Several post-processing analyses are available with analyze.exe. The primary function of analyze.exe was to obtain the total energy of a molecular structure. This option outputs the total potential energy of the molecule and the contributions of different terms to the total. For example, with the mm3 parameter set the total contribution of all six terms are output (bond stretching, angle bending, stretch-bend, angle-angle, out of plane bend,

torsional angle, and Van der Waals). Another option is also available which outputs these same values for each individual atom.

#### XYZPDB.EXE

This routine is useful to create \*.pdb files (protein data base) from \*.xyz files. The \*.pdb format is a commercial molecular structure format that many molecular modeling and visualization programs accept. In particular the visualization package, Visual Molecular Dynamics (VMD), accepts the \*.pdb format but not the \*.xyz format.

#### Keyfile Commands.

##### Boundary Conditions.

inactive [integer list]

The inactive command removes the listed atoms (the integer list) from those that can be moved during the minimization process. The FEM analogy to these boundary conditions is to fix the displacement degrees of freedom to zero for each node. In Tinker, this is the only method for insuring displacements to be zero (Tinker will not fix atomic positions for only 1 or 2 axes). This can cause problems for various experiments, (i.e. necking in tension).

restrain-position [1 integer & 4 real numbers]

The restrain-position command constrains an atom to a position by means of an external force (defined by a harmonic potential). The integer is the atom number, the first 3 real numbers are the constraint position and the final number is the constraint force in kcal/A<sup>2</sup> (default is 100.0). Note that the constraining force is radial and cannot be specified for different cartesian directions. This command can substitute as a loose boundary condition when some relaxation is required and absolute position not required.

A-axis [1 real number]

This command sets the periodic box size in the *x*-direction. B-axis and C-axis are used to set the box sizes in the *y* and *z* axes respectively. The periodic box is positioned around the center of the molecule. For work with nanotubes the open ended atoms must be bonded across the box boundaries to obtain a periodic tube (approximating an infinite tube). By changing the C-axis value, the nanotube may be axially deformed (*z*-direction) without applying any boundary conditions.

## External Programs & Packages.

### User Programs.

All user developed programs for use with the Tinker Package have the superfix 'aa\_' before their executable name. These programs were developed to create and manipulate nanotubes in the Tinker \*.xyz format. The programs were written in FORTRAN and are DOS executable applications. The most current versions are described below.

#### *aa\_zz-swnt.exe*

This program creates zig-zag type [n,0] single wall nanotubes. Input parameters are the filename, base vector 'n' (number of circumferential carbon rings), lengthwise, double carbon ring rows (2 adjacent hoops or carbon-bond rings), and parameter type (mm2 or mm3). The nanotubes are open ended or periodic as defined by the user.

#### *aa\_xmol.xyz.exe*

This program changes \*.xmol type molecule files into \*.xyz files that Tinker can use. This allows for the use of make\_tube\_ncsu.exe which can make any open ended [a,b] type of carbon nanotube.

#### *aa\_deform-man.exe*

This program deforms a nanotube \*.xyz file in one of several deformation modes. The input parameters are the deformation type, deformation magnitude (described for each), and the number of substeps. The program outputs an \*.xyz file for each substep of deformation as well as a \*.key file defining the boundary conditions. A suffix is added to the original filename defining the deformation type and substep for each file.

axial deformation (tension/compression). The axial deformation option asks for the desired axial percent strain of deformation (negative values for compression). The deformations are performed by simply moving each atom as a percent of its z coordinate. Atoms near the end faces are fixed (inactive command in the keyfile), which will cause the relaxed to structure to neck in the middle as would a macro-scale test specimen.

torsion. The torsion option asks for the total twist deformation in degrees. The deformation is simply a trigonometric function in x & y (the tube axes must coincide with

the  $z$ -axis). The boundary conditions (same atoms held inactive for the same nanotube) are the same as for the tension case.

bending. The cantilever bending option asks for the number of diameters of out of plane displacement. Each atom is then moved in the  $x$ -direction as a third order polynomial function of its  $z$  coordinate. Each atom is also moved inwards in the  $z$ -direction, as input by the user, to account for the axial deflection of the tube. The boundary condition is fixed (inactive) at the base end using the inactive command. The out of plane displacement is held by fixing (inactive) a three coincident atoms near the loaded end to its deformed position. This method lessens the local indentation of the nanotube due to point loading compared to holding a single atom and the end. Unfortunately, by fixing the atom locations, the user must perform a convergence test for each out of plane deflection to find the proper amount of axial relaxation of the tube. This is an artifact of the use of the inactive command as a boundary condition. The restrain-position command was attempted for this deformation mode, but found to be an unreliable method.

buckling. It was found that small geometric perturbations lower the critical buckling strain of MM simulations. Without perturbations the simulations did not yield consistent results. With small sinusoidal perturbations the MM models, consistent results were found for both columnar and shell buckling modes. The buckling routine moves the atoms axially in the same manner as the tension routine. The atoms are moved laterally in the  $x$ -direction in a clamped-clamped sinusoidal wave. The amplitude of the wave is input as a function of the tube length.

radial expansion. This option moves any atom radially ( $x,y$  positions) as a percent of its current radius. This option is generally used on DWNTs to apply an external or internal pseudo-pressure on an adjacent wall via the van der Waals forces.

#### *aa\_mwntcombine*

This program places any number of \*.xyz SWNT files together to create a multi-walled nanotube (MWNT). It is left up to the user to input proper SWNT sizes to create viable MWNTs. It should also be noted that this MWNT must also be relaxed even if the SWNT components were relaxed structures.

### *aa-compobox*

This program creates a nanotube polyethylene composite box. The box is periodic in all three directions. The nanotube, already previously created and relaxed, is placed first. The polyethylene matrix is then positioned around the nanotube using a random walk technique. The user inputs restrictions and constants on the polyethylene chain size and cross-linking.

### External Packages

#### make tube ncsu.exe

This program creates [a,b] SWNTs in an \*.xmol format. It was created at North Carolina State Univ. for distribution to the scientific community.

#### Visual Molecular Dynamics (VMD).

VMD is a public domain package for molecular visualization created and distributed to the scientific community by the University of Illinois. It recognizes the \*.pdb and \*.xmol file formats. VMD is a powerful tool with numerous viewing options.

### A.3 Tinker VEM Procedure

The details of implementing the VEM procedure with Tinker are outlined with an example tension test on a very short (10,0) nanotube. Four nanotube SWNT structures are shown in Tinker \*.xyz format on the following pages. The first tube is the initially generated atomic structure shorttube.xyz. The second tube is the relaxed version of the tube as minimized by the mm3 parameter set. The third tube is the estimated deformed structure, with a keyfile. The fourth tube is the minimized deformed structure ready for structural analysis along with the DOS command sequence to accomplish it.

The header comments in italics are not part of the \*.xyz file, but are notes written here for clarity. The first line of the \*.xyz file is the title line which begins with the number of atoms in the structure and ends as a comment line. The rest of the file is dedicated to the atomic positions and bonding (connectivity). The format is as follows:

atom number, atom type, x-location, y-loc., z-loc., bonded atoms 1,2,3 & 4 as needed

shorttube.xyz  
 [10,0] SWNT, open ended  
 mm3 parameter set  
 estimated atomic structure  
 estimated length = 7.00 Å  
 total energy = 766.02 Kcal/mole

40	hoop cells:	5	zig-zag SWNT	xyz file	d= 3.86	ang	ar= 2.18	mm3
1	C	1.929651	.000000	.000000	2	6	10	
2	C	.596295	1.835207	.000000	2	7	6	
3	C	-1.561121	1.134220	.000000	2	8	7	
4	C	-1.561120	-1.134221	.000000	2	9	8	
5	C	.596295	-1.835207	.000000	2	10	9	
6	C	1.561120	1.134220	.700000	2	2	11	1
7	C	-.596295	1.835207	.700000	2	3	12	2
8	C	-1.929651	.000000	.700000	2	4	13	3
9	C	-.596295	-1.835207	.700000	2	5	14	4
10	C	1.561121	-1.134220	.700000	2	1	15	5
11	C	1.561120	1.134220	2.100000	2	17	16	6
12	C	-.596295	1.835207	2.100000	2	18	17	7
13	C	-1.929651	.000000	2.100000	2	19	18	8
14	C	-.596295	-1.835207	2.100000	2	20	19	9
15	C	1.561121	-1.134220	2.100000	2	16	20	10
16	C	1.929651	.000000	2.800000	2	11	21	15
17	C	.596295	1.835207	2.800000	2	12	22	11
18	C	-1.561121	1.134220	2.800000	2	13	23	12
19	C	-1.561120	-1.134221	2.800000	2	14	24	13
20	C	.596295	-1.835207	2.800000	2	15	25	14
21	C	1.929651	.000000	4.200000	2	26	30	16
22	C	.596295	1.835207	4.200000	2	27	26	17
23	C	-1.561121	1.134220	4.200000	2	28	27	18
24	C	-1.561120	-1.134221	4.200000	2	29	28	19
25	C	.596295	-1.835207	4.200000	2	30	29	20
26	C	1.561120	1.134220	4.900000	2	22	31	21
27	C	-.596295	1.835207	4.900000	2	23	32	22
28	C	-1.929651	.000000	4.900000	2	24	33	23
29	C	-.596295	-1.835207	4.900000	2	25	34	24
30	C	1.561121	-1.134220	4.900000	2	21	35	25
31	C	1.561120	1.134220	6.300000	2	37	36	26
32	C	-.596295	1.835207	6.300000	2	38	37	27
33	C	-1.929651	.000000	6.300000	2	39	38	28
34	C	-.596295	-1.835207	6.300000	2	40	39	29
35	C	1.561121	-1.134220	6.300000	2	36	40	30
36	C	1.929651	.000000	7.000000	2	31	35	
37	C	.596295	1.835207	7.000000	2	32	31	
38	C	-1.561121	1.134220	7.000000	2	33	32	
39	C	-1.561120	-1.134221	7.000000	2	34	33	
40	C	.596295	-1.835207	7.000000	2	35	34	

shorttube.xyz\_2

relaxed [10,0] SWNT structure

relaxed length = 6.6 Å

total energy = 705.91 Kcal/mole (RMS gradient = 0.001)

```
40 hoop cells: 5 zig-zag SWNT xyz file d= 3.86 ang ar= 2.
 1 C 1.886495 0.000412 0.195271 2 6 10
 2 C 0.583272 1.793915 0.195311 2 6 7
 3 C -1.525168 1.108699 0.195182 2 7 8
 4 C -1.525033 -1.108290 0.195061 2 8 9
 5 C 0.583490 -1.793249 0.195116 2 9 10
 6 C 1.586583 1.152707 0.818608 2 1 2 11
 7 C -0.605354 1.864763 0.818551 2 2 3 12
 8 C -1.959906 0.000144 0.818390 2 3 4 13
 9 C -0.605127 -1.864310 0.818348 2 4 5 14
10 C 1.586724 -1.151987 0.818483 2 1 5 15
11 C 1.567172 1.138572 2.170243 2 6 16 17
12 C -0.598020 1.841940 2.170187 2 7 17 18
13 C -1.936043 0.000072 2.170029 2 8 18 19
14 C -0.597795 -1.841632 2.169987 2 9 19 20
15 C 1.567311 -1.138001 2.170120 2 10 16 20
16 C 1.918776 0.000271 2.824413 2 11 15 21
17 C 0.593166 1.824583 2.824454 2 11 12 22
18 C -1.551493 1.127596 2.824323 2 12 13 23
19 C -1.551355 -1.127476 2.824200 2 13 14 24
20 C 0.593388 -1.824201 2.824256 2 14 15 25
21 C 1.918717 0.000198 4.174861 2 16 26 30
22 C 0.593107 1.824509 4.174902 2 17 26 27
23 C -1.551552 1.127523 4.174770 2 18 27 28
24 C -1.551414 -1.127549 4.174648 2 19 28 29
25 C 0.593329 -1.824275 4.174704 2 20 29 30
26 C 1.567056 1.138428 4.829124 2 21 22 31
27 C -0.598136 1.841795 4.829067 2 22 23 32
28 C -1.936160 -0.000072 4.828909 2 23 24 33
29 C -0.597912 -1.841777 4.828867 2 24 25 34
30 C 1.567195 -1.138145 4.829000 2 21 25 35
31 C 1.586349 1.152416 6.180763 2 26 36 37
32 C -0.605588 1.864472 6.180706 2 27 37 38
33 C -1.960140 -0.000147 6.180545 2 28 38 39
34 C -0.605361 -1.864601 6.180503 2 29 39 40
35 C 1.586489 -1.152278 6.180637 2 30 36 40
36 C 1.886206 0.000053 6.804001 2 31 35
37 C 0.582983 1.793556 6.804041 2 31 32
38 C -1.525457 1.108340 6.803912 2 32 33
39 C -1.525322 -1.108649 6.803791 2 33 34
40 C 0.583202 -1.793608 6.803846 2 34 35
```

*shorttube2\_t01.xyz*

*shorttube.xyz\_2 strained to  $\epsilon_z = 0.10$  using *aa\_deformman.exe**

```
40  substrain: .10000      original file: shorttube2.xyz
  1  C      1.886495      .000412      .000000      2      6      10
  2  C      .583272      1.793915      .000044      2      6      7
  3  C     -1.525168      1.108699     -.000098      2      7      8
  4  C     -1.525033     -1.108290     -.000231      2      8      9
  5  C      .583490     -1.793249     -.000171      2      9      10
  6  C      1.586583      1.152707      .685671      2      1      2      11
  7  C     -.605354      1.864763      .685608      2      2      3      12
  8  C     -1.959906      .000144      .685431      2      3      4      13
  9  C     -.605127     -1.864310      .685385      2      4      5      14
10  C      1.586724     -1.151987      .685533      2      1      5      15
11  C      1.567172      1.138572      2.172469      2      6      16      17
12  C     -.598020      1.841940      2.172408      2      7      17      18
13  C     -1.936043      .000072      2.172234      2      8      18      19
14  C     -.597795     -1.841632      2.172188      2      9      19      20
15  C      1.567311     -1.138001      2.172334      2     10      16      20
16  C      1.918776      .000271      2.892056      2     11      15      21
17  C      .593166      1.824583      2.892101      2     11      12      22
18  C     -1.551493      1.127596      2.891957      2     12      13      23
19  C     -1.551355     -1.127476      2.891822      2     13      14      24
20  C      .593388     -1.824201      2.891883      2     14      15      25
21  C      1.918717      .000198      4.377549      2     16      26      30
22  C      .593107      1.824509      4.377594      2     17      26      27
23  C     -1.551552      1.127523      4.377449      2     18      27      28
24  C     -1.551414     -1.127549      4.377315      2     19      28      29
25  C      .593329     -1.824275      4.377377      2     20      29      30
26  C      1.567056      1.138428      5.097238      2     21      22      31
27  C     -.598136      1.841795      5.097176      2     22      23      32
28  C     -1.936160     -.000072      5.097002      2     23      24      33
29  C     -.597912     -1.841777      5.096955      2     24      25      34
30  C      1.567195     -1.138145      5.097102      2     21      25      35
31  C      1.586349      1.152416      6.584041      2     26      36      37
32  C     -.605588      1.864472      6.583979      2     27      37      38
33  C     -1.960140     -.000147      6.583801      2     28      38      39
34  C     -.605361     -1.864601      6.583755      2     29      39      40
35  C      1.586489     -1.152278      6.583902      2     30      36      40
36  C      1.886206      .000053      7.269603      2     31      35
37  C      .582983      1.793556      7.269647      2     31      32
38  C     -1.525457      1.108340      7.269505      2     32      33
39  C     -1.525322     -1.108649      7.269372      2     33      34
40  C      .583202     -1.793608      7.269433      2     34      35
```

*shorttube2\_t.key*

*keyfile containing fixed boundary conditions at open ends of tube (not recommended, but easy to show)*

```
inactive -1 5
inactive 36
inactive 37
inactive 38
inactive 39
inactive 40
cutoff 10.0
```

shorttube2\_t01n.xyz

shorttube2 strained and minimized to deformed structure using Newton to rms value of 0.01 and keyfile

newton shorttube2\_t01 -k shorttube\_t2 mm3 a a 0.001

total energy = 844.3025 Kcal/mole (RMS gradient = 0.01)

strain energy = 844.30 - 705.91 = 138.39 Kcal/mol

40								
1	C	1.886495	0.000412	0.000000	2	6	10	
2	C	0.583272	1.793915	0.000044	2	6	7	
3	C	-1.525168	1.108699	-0.000098	2	7	8	
4	C	-1.525033	-1.108290	-0.000231	2	8	9	
5	C	0.583490	-1.793249	-0.000171	2	9	10	
6	C	1.551830	1.127452	0.715146	2	1	2	11
7	C	-0.592081	1.823906	0.715088	2	2	3	12
8	C	-1.916949	0.000142	0.714923	2	3	4	13
9	C	-0.591858	-1.823455	0.714880	2	4	5	14
10	C	1.551965	-1.126744	0.715018	2	1	5	15
11	C	1.541796	1.120131	2.180056	2	6	16	17
12	C	-0.588325	1.812106	2.180001	2	7	17	18
13	C	-1.904674	0.000073	2.179846	2	8	18	19
14	C	-0.588105	-1.811798	2.179805	2	9	19	20
15	C	1.541931	-1.119567	2.179935	2	10	16	20
16	C	1.898741	0.000267	2.902963	2	11	15	21
17	C	0.586977	1.805528	2.903003	2	11	12	22
18	C	-1.535285	1.115821	2.902875	2	12	13	23
19	C	-1.535149	-1.115700	2.902756	2	13	14	24
20	C	0.587195	-1.805152	2.902810	2	14	15	25
21	C	1.898685	0.000199	4.366622	2	16	26	30
22	C	0.586921	1.805458	4.366662	2	17	26	27
23	C	-1.535340	1.115752	4.366533	2	18	27	28
24	C	-1.535205	-1.115771	4.366414	2	19	28	29
25	C	0.587140	-1.805222	4.366469	2	20	29	30
26	C	1.541683	1.119990	5.089620	2	21	22	31
27	C	-0.588437	1.811964	5.089565	2	22	23	32
28	C	-1.904787	-0.000068	5.089409	2	23	24	33
29	C	-0.588218	-1.811943	5.089368	2	24	25	34
30	C	1.541818	-1.119707	5.089499	2	21	25	35
31	C	1.551601	1.127168	6.554546	2	26	36	37
32	C	-0.592307	1.823621	6.554487	2	27	37	38
33	C	-1.917178	-0.000139	6.554321	2	28	38	39
34	C	-0.592086	-1.823744	6.554279	2	29	39	40
35	C	1.551739	-1.127026	6.554417	2	30	36	40
36	C	1.886206	0.000053	7.269603	2	31	35	
37	C	0.582983	1.793556	7.269647	2	31	32	
38	C	-1.525457	1.108340	7.269505	2	32	33	
39	C	-1.525322	-1.108649	7.269372	2	33	34	
40	C	0.583202	-1.793608	7.269433	2	34	35	

# Aaron Sears

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1150 Bozeman Trail  
Bozeman MT, 59715  
(406) 570-9600  
*asears@vt.edu*  
*aaron.sears@coe.montana.edu*

## EDUCATION

**Doctoral candidate, Engineering Science and Mechanics**  
Virginia Polytechnic Institute and State University (def. 11/7/06)  
*Mechanics of carbon nanotubes; development of continuum models from molecular simulations*

**Master of Science, Mechanical Engineering**  
Montana State University-Bozeman ('99)  
*Experimental Validation of Finite Element Techniques for Buckling & Postbuckling of Composite Sandwich Shells*

**Bachelor of Science, Mechanical Engineering**  
Washington University in St. Louis ('95)

## AWARDS

Virginia Space Grant Consortium Graduate Fellow ('03-'05)

## PUBLICATIONS

Published Papers(2): *Macroscopic properties of carbon nanotubes from molecular mechanics simulations*, Phys. Rev. B (69) 2004,  
*Buckling of multi-walled carbon nanotubes in axial compression*, Physical Review B (73) 2006

## PRESENTATIONS

Conference Presentations (3): *Design considerations for buckling in composite wind turbine blades*, AIAA Conference (2000),  
*Carbon nanotube mechanics*, Virginia Space Grant Consortium Conference (2004, 2005)

## EXPERIENCE

Research Associate, Montana State University ('06-present)  
damage initiation in composite joints under multi-axial load  
Instructor, Montana State University ('06-present)  
ME 102, Engineering Computer Applications  
Graduate Research Assistant, Virginia Tech ('01-'05)  
Project Manager, SHARP@MSU ('00-01)  
(SHARP = Slender High Altitude Research Projectile)  
design & construct the 'S1' re-entry vehicle structure  
manage 1 full-time engineer and 8 undergraduate students  
integrate with collaborative groups at Stanford & Wyoming  
Graduate Teaching & Research Assistant, MSU ('96-99)  
Lab Assistant, Composites Group MSU ('92, 93)  
Youth Soccer Coach ('95-present)  
Bozeman High School, FC Bozeman, New River United