Latex Films

Dow Chemical Project

Jason Crowley, David Lehtihet, Tod Pascal

Andres Jaramillo-Botero and William A Goddard III

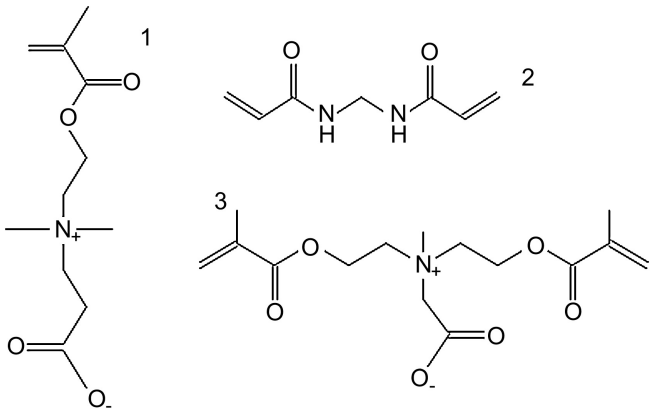
Outline

- Free-energy/entropies per water content
- Mechanical response

PREDICTING THE EQUILIBRIUM WATER CONTENT IN CBMA HYDROGELS FROM FIRST PRINCIPLE SIMULATIONS

DOW Chemical 6-27-3011

Carboxybetain methacrylate Hydrogels



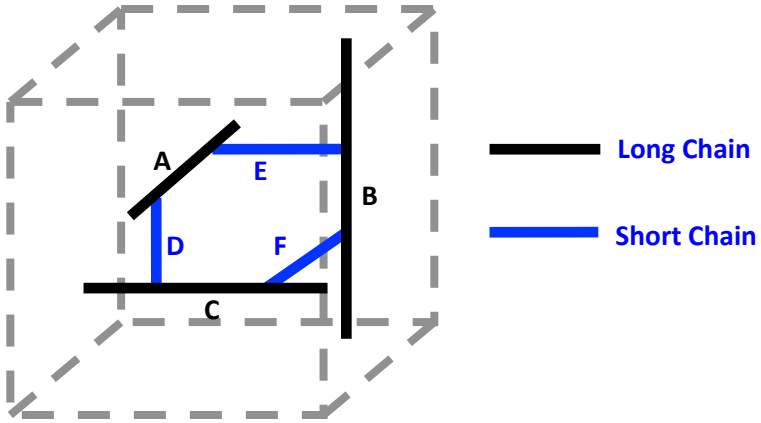
1. carboxybetain methacrylate (CBMA), **2**. *N,N'*-methylenebis (acrylamide) crosslinker **3.** carboxybetain dimethacrylate crosslinker

- superior suitability for biomedical applications
  - high hydration and ultra-low fouling
- Used as scaffolds in tissue engineering and joint replacment

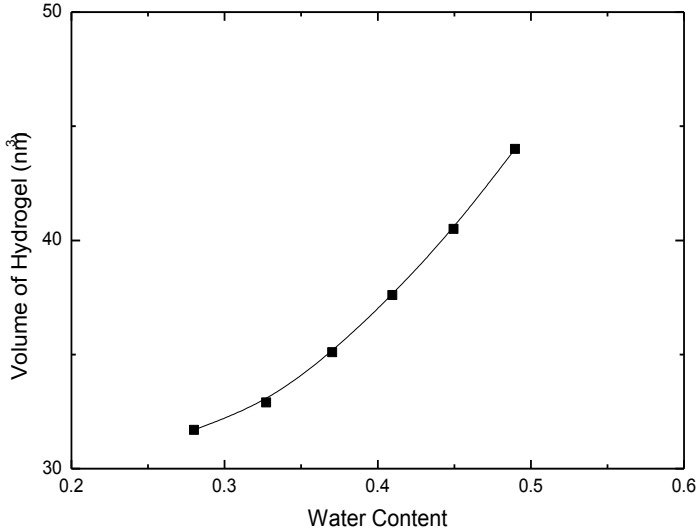
Physical crosslinking of zwitterionic polymer chains. (a) Inter-chain crosslinking; (b) Intra-chain crosslinking

Molecular Dynamics simulations

Water Content of Hydrogel	Number of Water Molecules
28%	335
33%	415
37%	502
41%	592
45%	697
49%	819
62%	1396
71%	2120
81%	3630
86%	5250
90%	8200

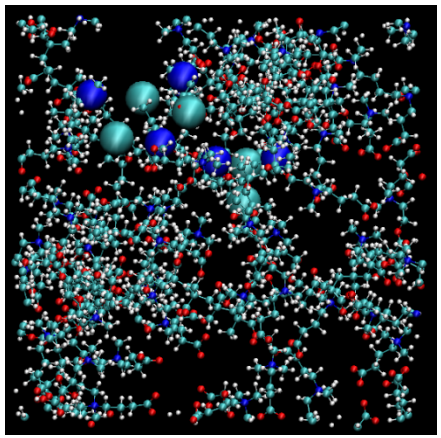


- Fully atomistic simulations
- Investigating the structural properties of water molecules in matrix

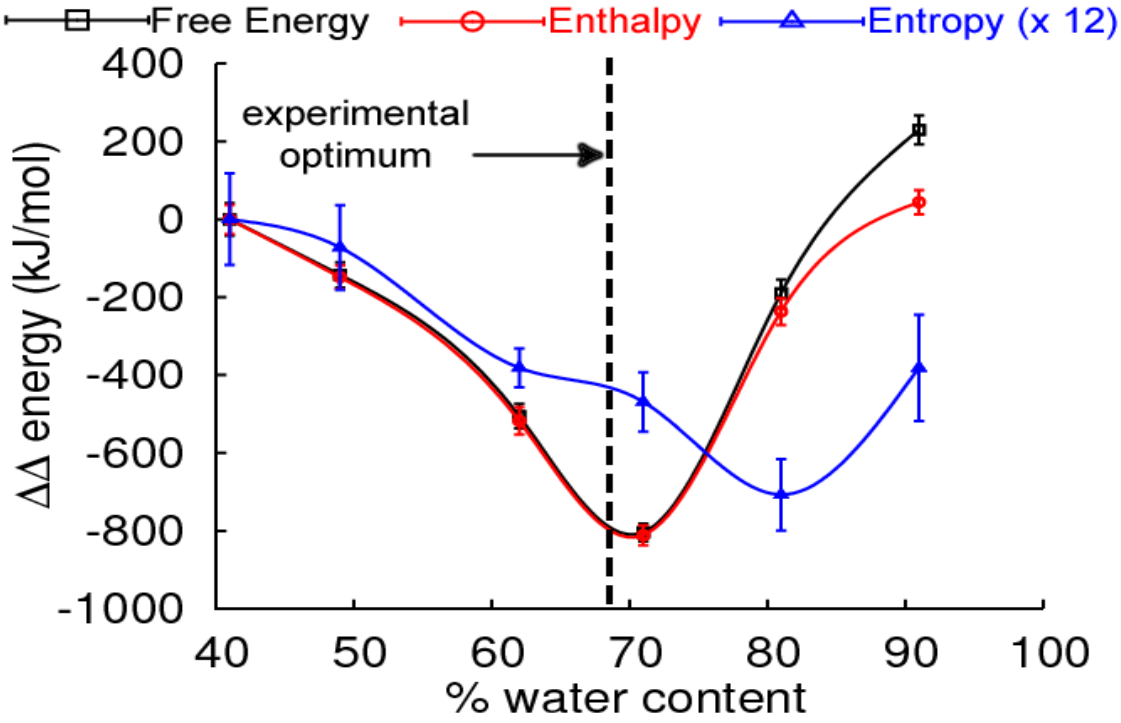


Volumes of hydrogels with various water contents.

Free Energy MD Simulations

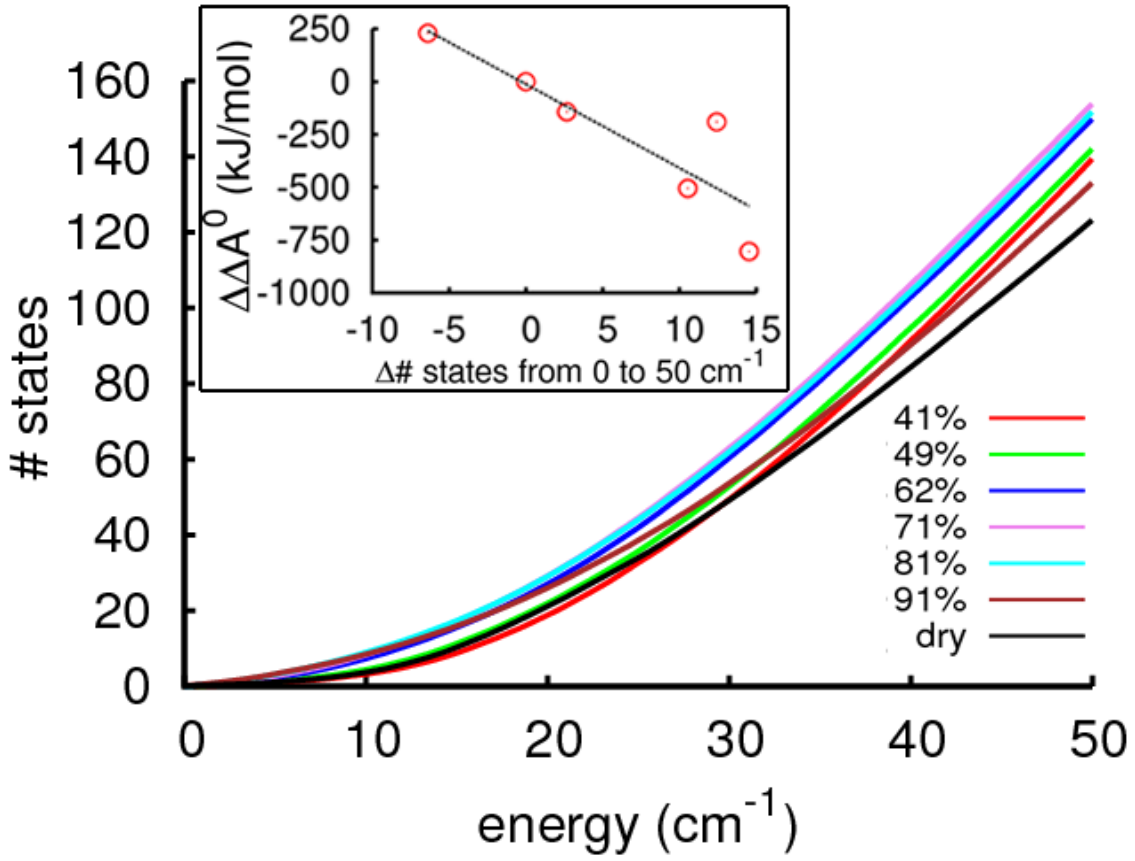


Snapshot of simulation cell



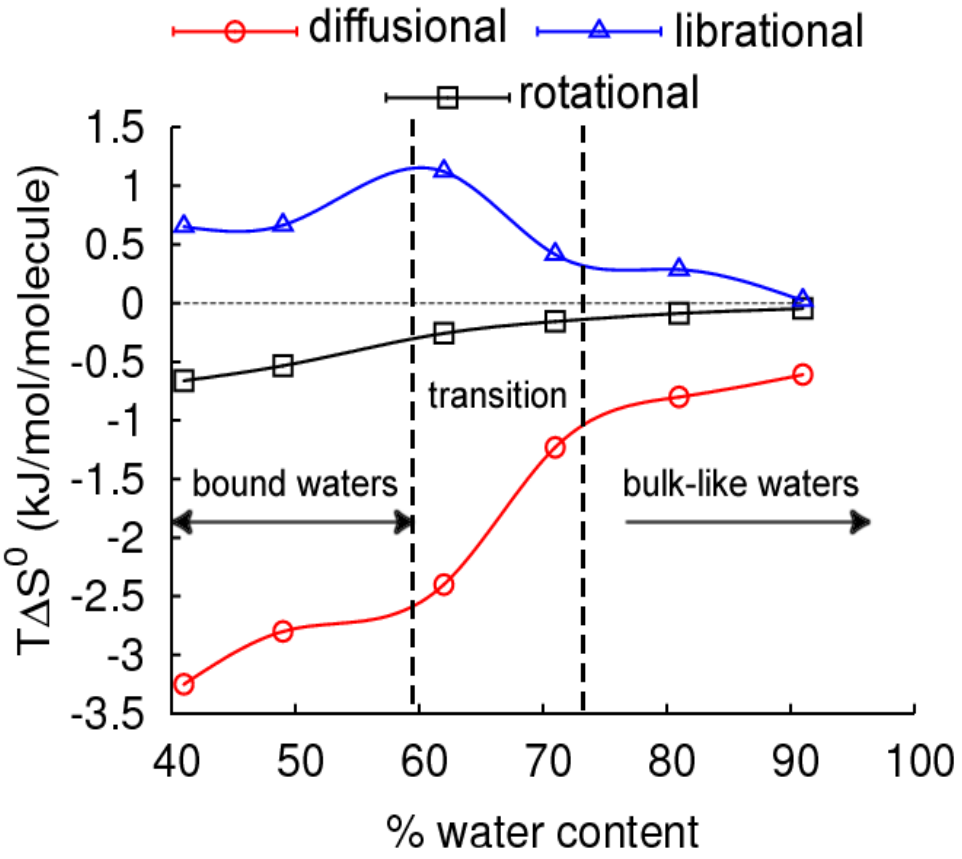
Able to predict the experimental optimal water content by considering the entropy of hydrogel

Insights into the role of water



Water enhances the low frequency breathing modes of the hydrogel at low water content

The entropy of water inside hydrogels



- Diffusional entropy increases continously
- Librational entropy decreases as water molecules leave surface of hydrogel and enters quasi-liquid state in hydrogel pore

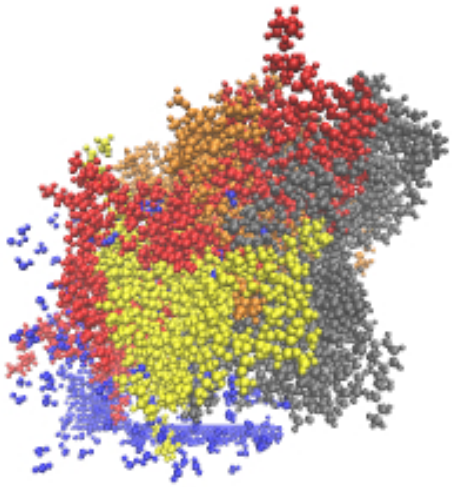
Conclusions

- Using computational tools developed at Goddard lab, we are able to predict the experimental optimal water content of CBMA hydrogel
- The enthalpy dominates the interactions in the systems
- Water acts to enhance the low energy vibrational state of the hydrogel before equilibrium by binding to surface
- Water transitions into a quasi-liquid phase at higher content, destabilizing hydrogel matrix

HYDROPOHOBIC

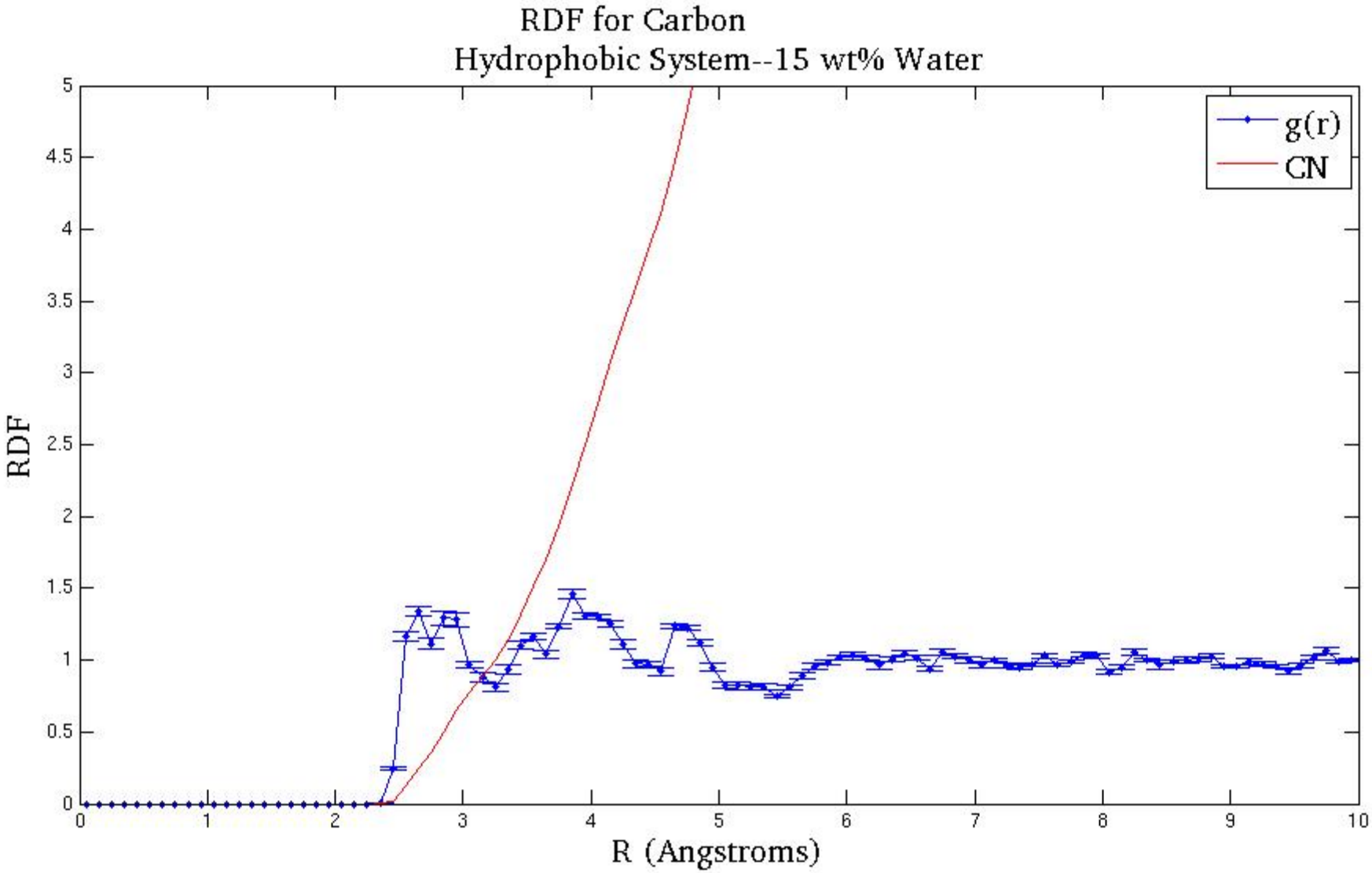
Preparation of Solvated Structures

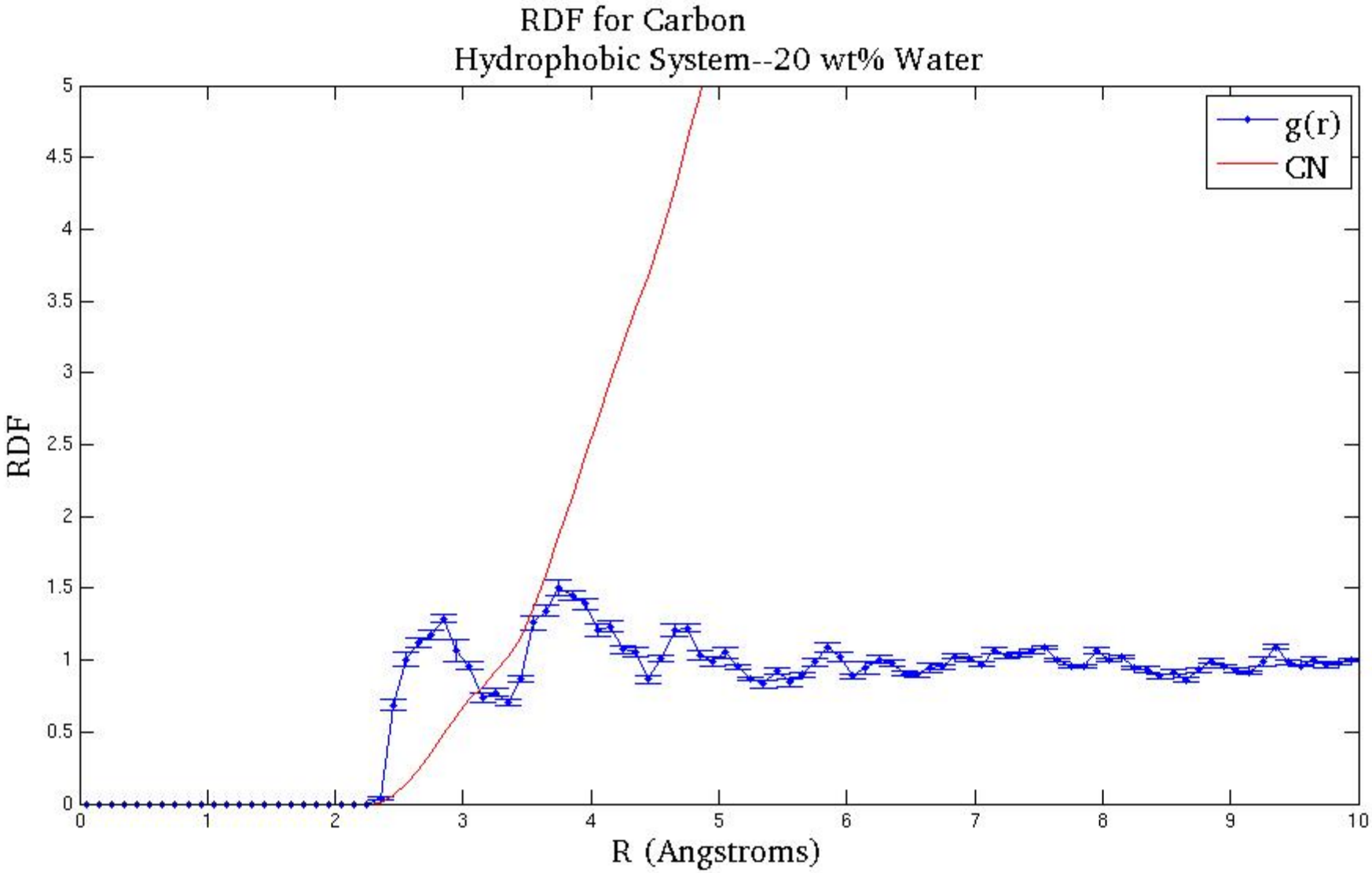
- Start from equilibrated (density ~1) structure
- Add water (05-40 wt%), remove bad contacts
- Expand to density 1
- One CED cycle
- NVT equilibration at density ~1
- Further NVT for 2PT

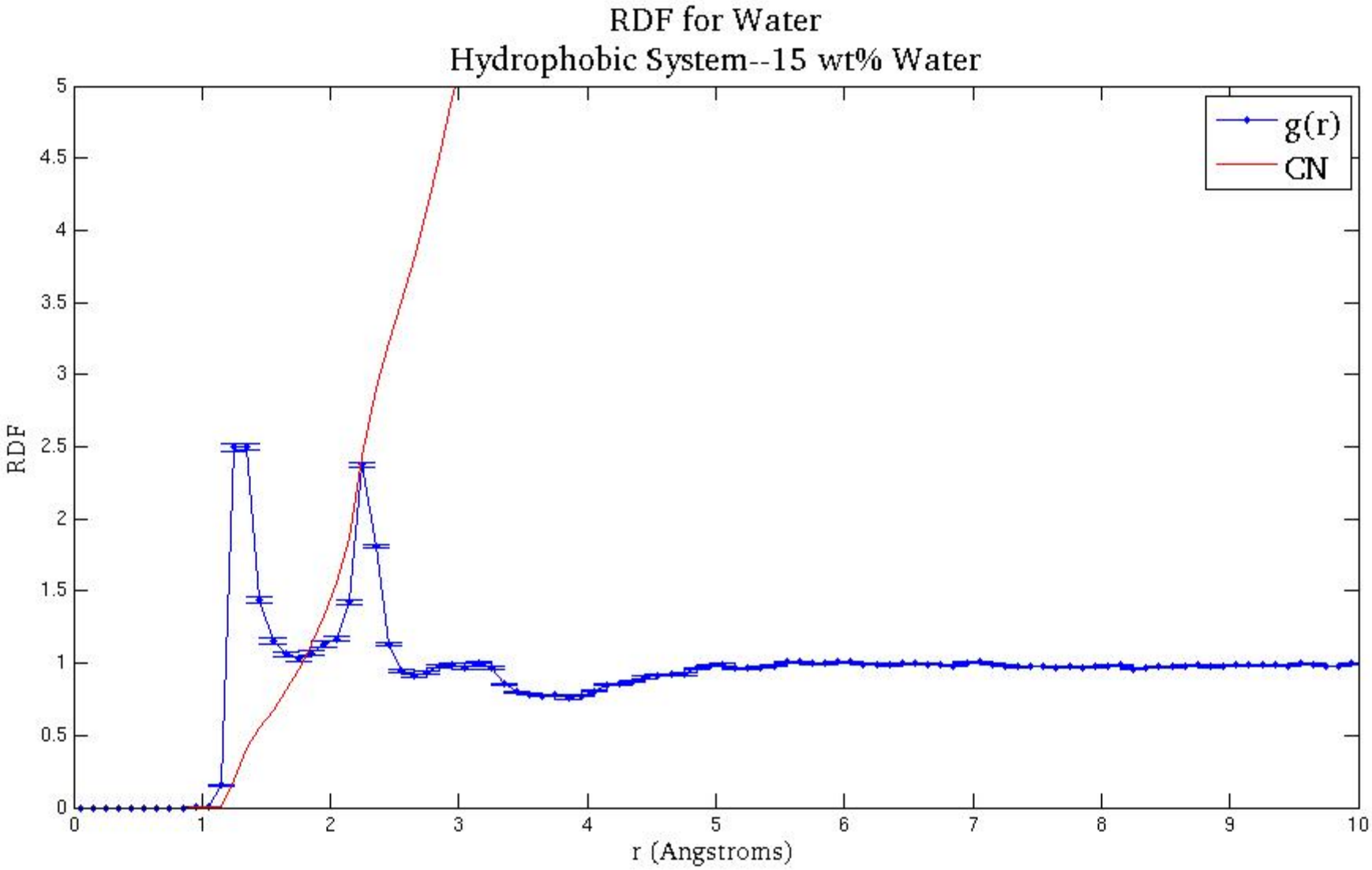


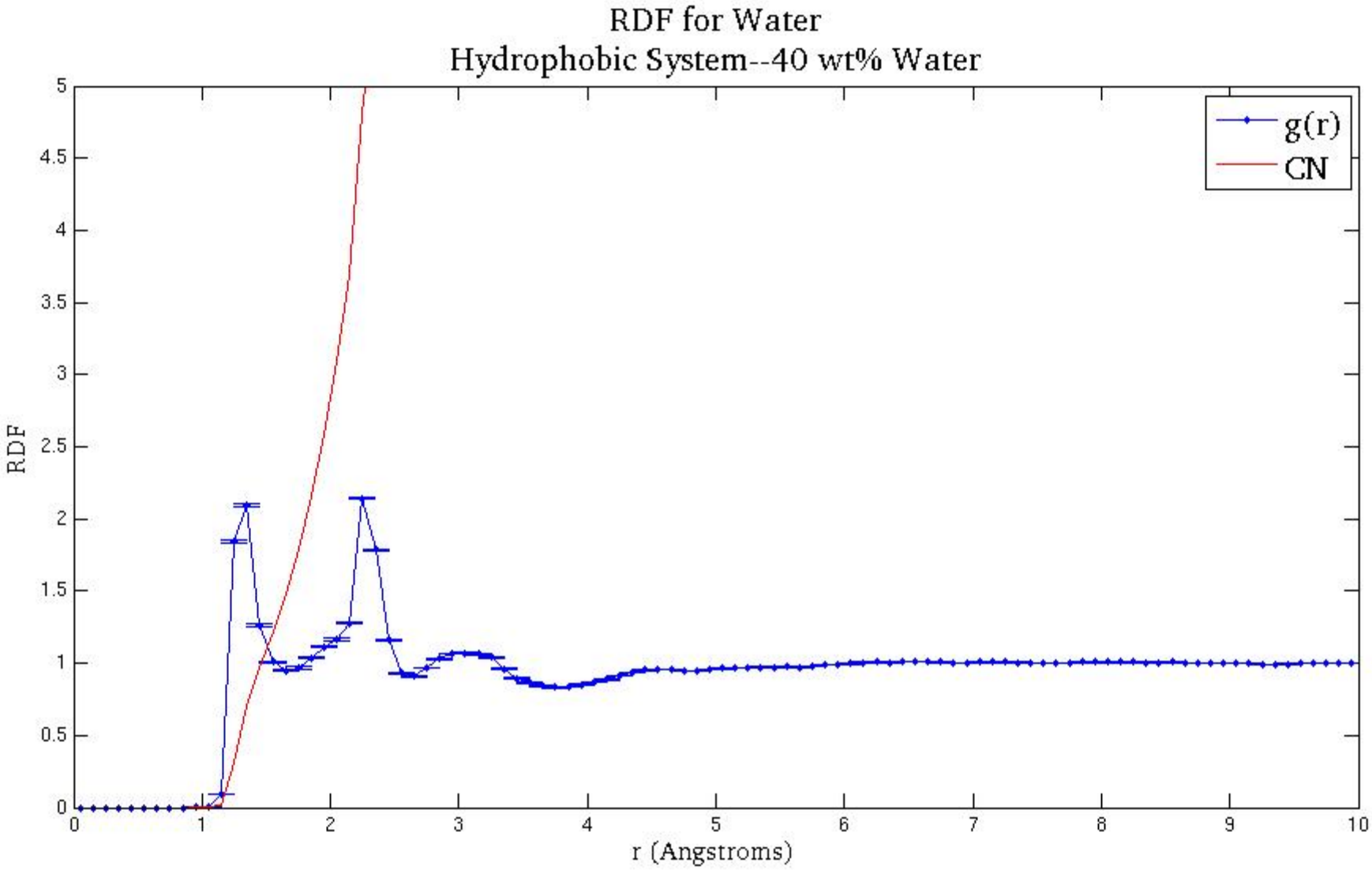
Equilibration

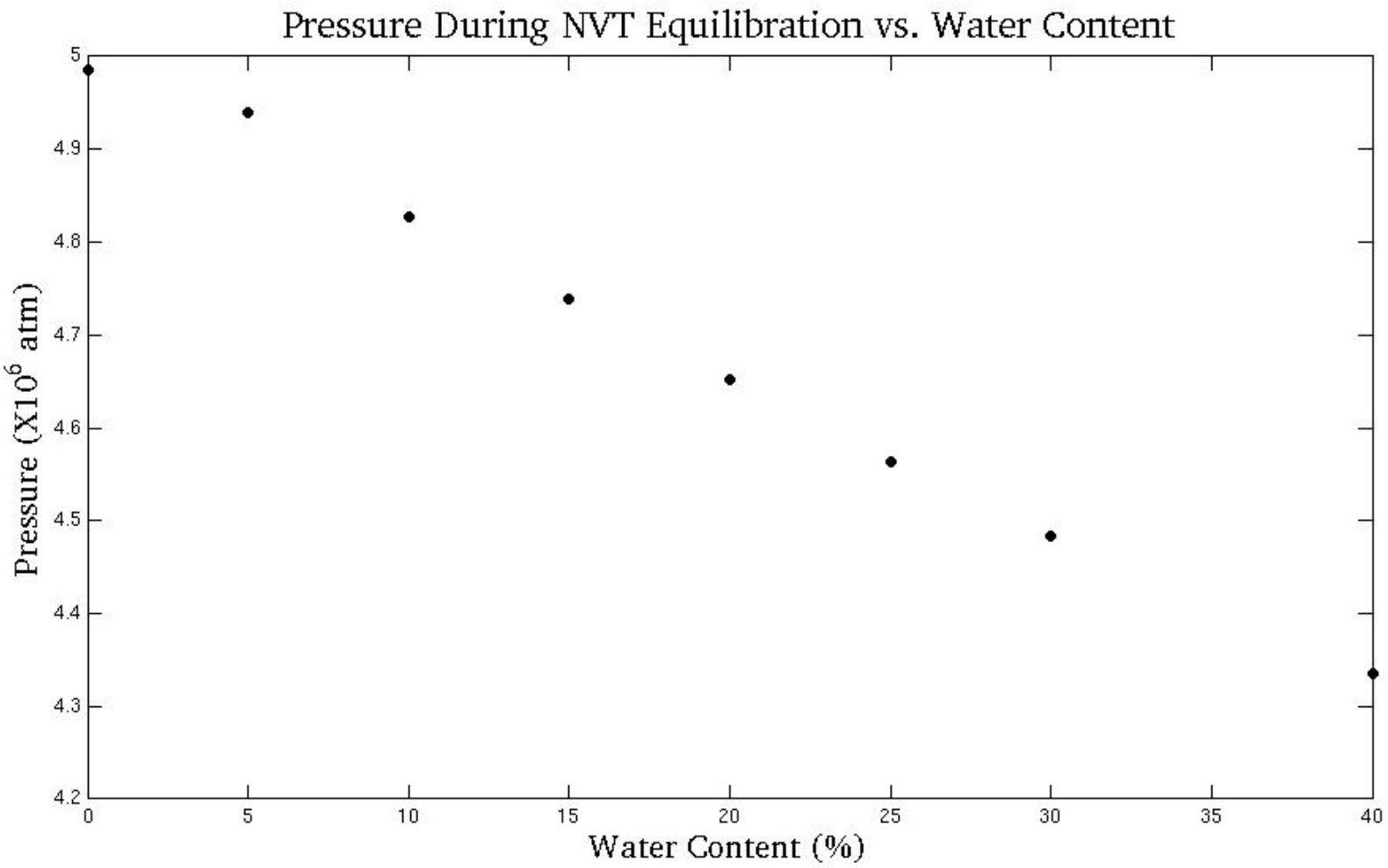
- Minimize at 0K
- Heat 10-298K, 50ps NVE
- Expand to density ~1 at 298K
- CED: Double volume while heating 298-600K over 50ps
- CED: Compress while cooling 600-298K over 200ps
- 100ps NVT at 298K, density ~1 (compute RDF,MSD)
- 10ps NVT at 298K for 2PT

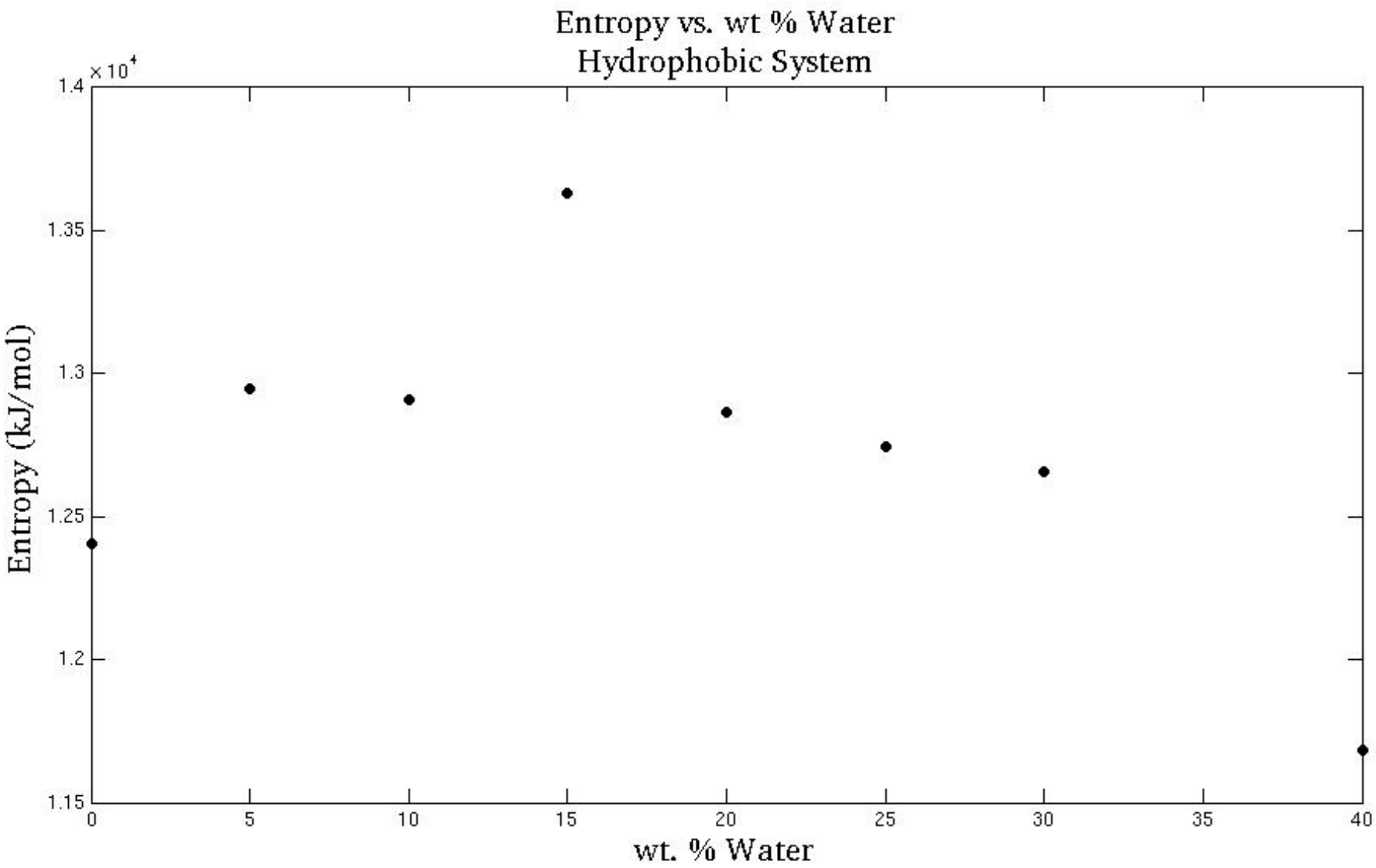

RDF for Carbon
Hydrophobic System--15 wt% Water
g(r)
CN
RDF
R (Angstroms)
0
0.5
1
1.5
2
2.5
3
3.5
4
4.5
5
0
1
2
3
4
5
6
7
8
9
10


RDF for Carbon
Hydrophobic System--20 wt% Water
g(r)
CN
RDF
R (Angstroms)
0
0.5
1
1.5
2
2.5
3
3.5
4
4.5
5
0
1
2
3
4
5
6
7
8
9
10


RDF for Water
Hydrophobic System--15 wt% Water
g(r)
CN
RDF
r (Angstroms)
0
0.5
1
1.5
2
2.5
3
3.5
4
4.5
5
0
1
2
3
4
5
6
7
8
9
10

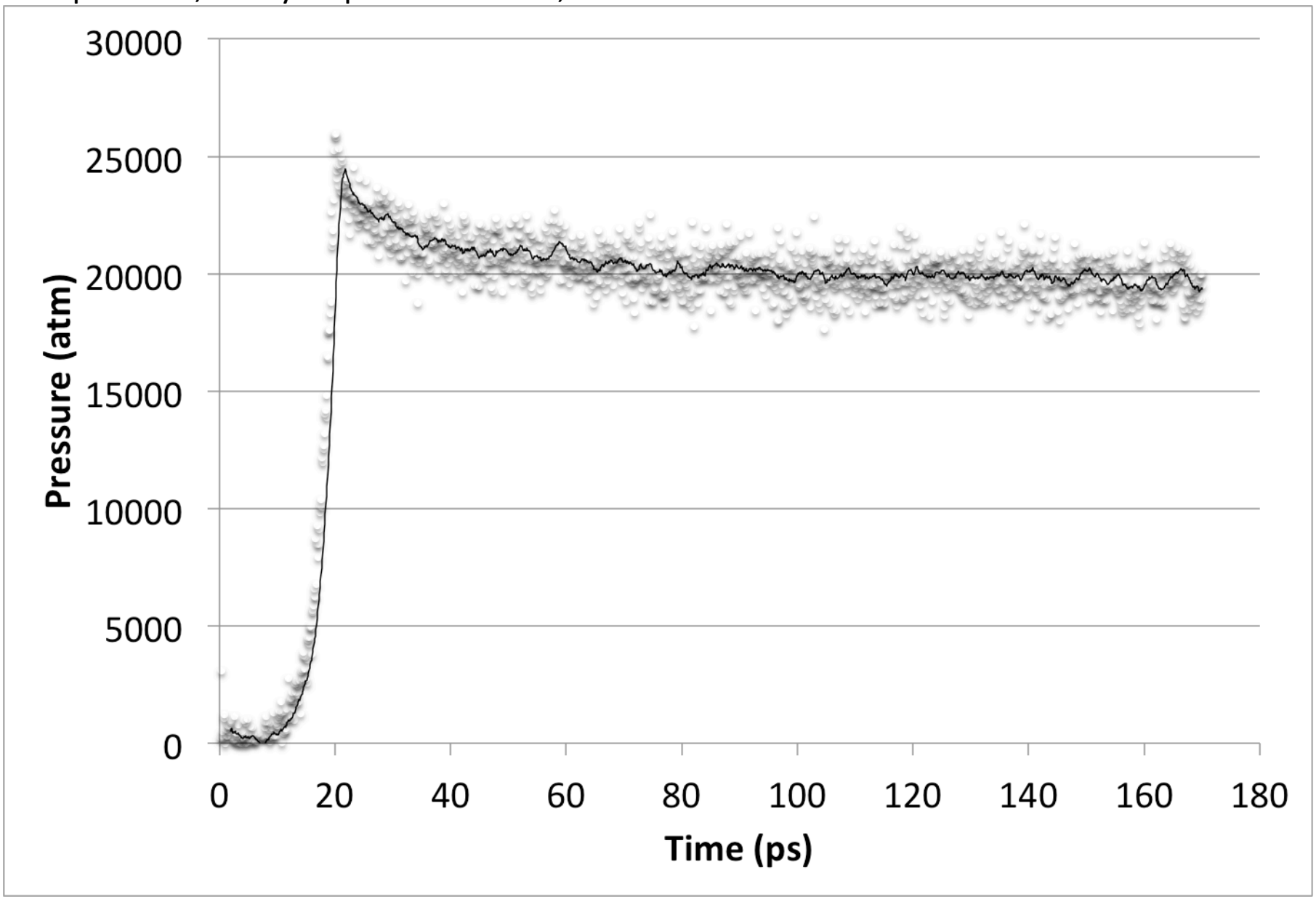

RDF for Water
Hydrophobic System--40 wt% Water
g(r)
CN
RDF
r (Angstroms)
0
0.5
1
1.5
2
2.5
3
3.5
4
4.5
5
0
1
2
3
4
5
6
7
8
9
10


Pressure During NVT Equilibration vs. Water Content
Pressure (X10^6 atm)
Water Content (%)
5
4.9
4.8
4.7
4.6
4.5
4.4
4.3
4.2
0
5
10
15
20
25
30
35
40

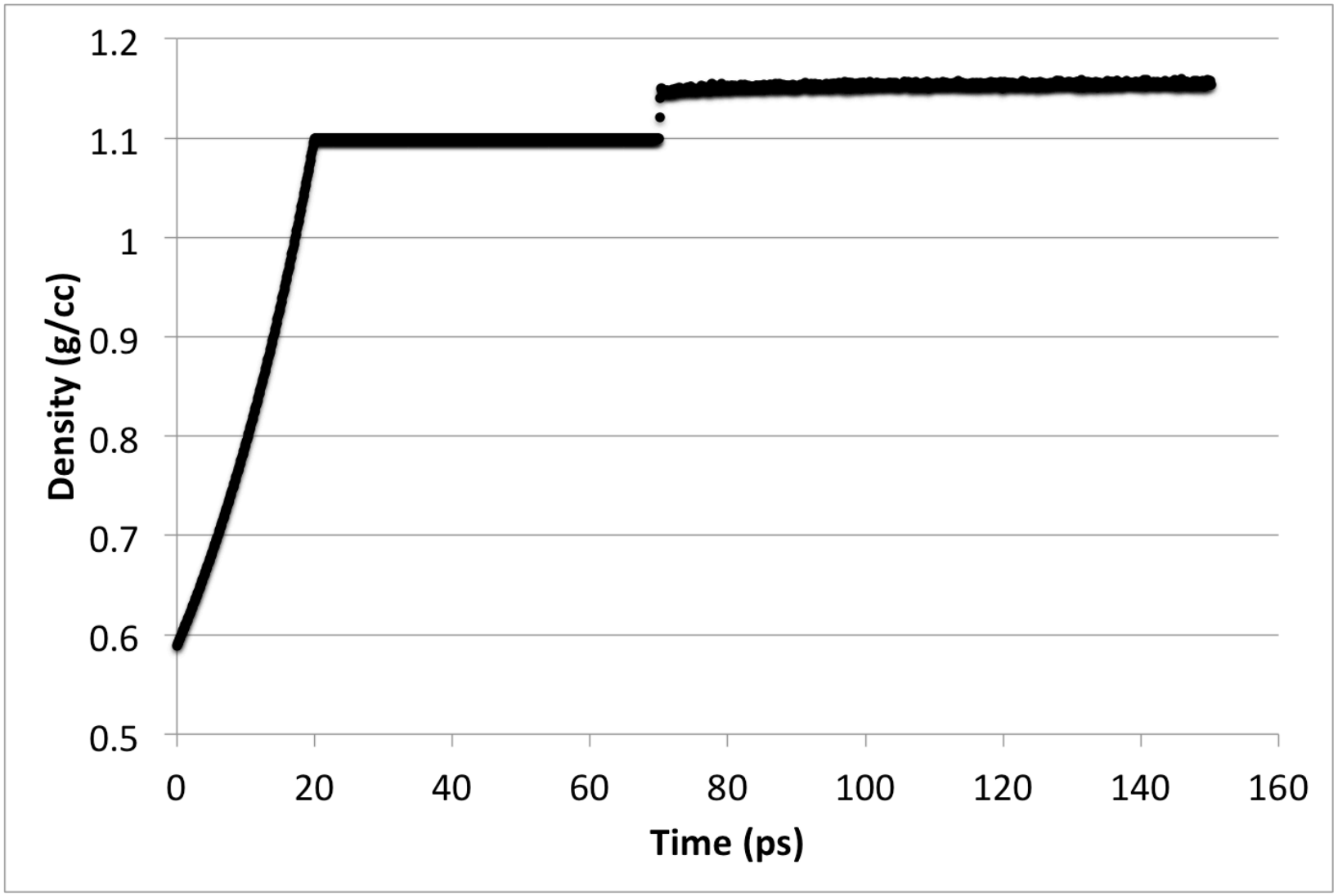

Entropy vs. wt % Water
Hydrophobic System
x 10^4
1.4
1.35
1.3
1.25
1.2
1.15
Entropy (kJ/mol)
0
5
10
15
20
25
30
35
40
wt. % Water

HYDROPHILIC

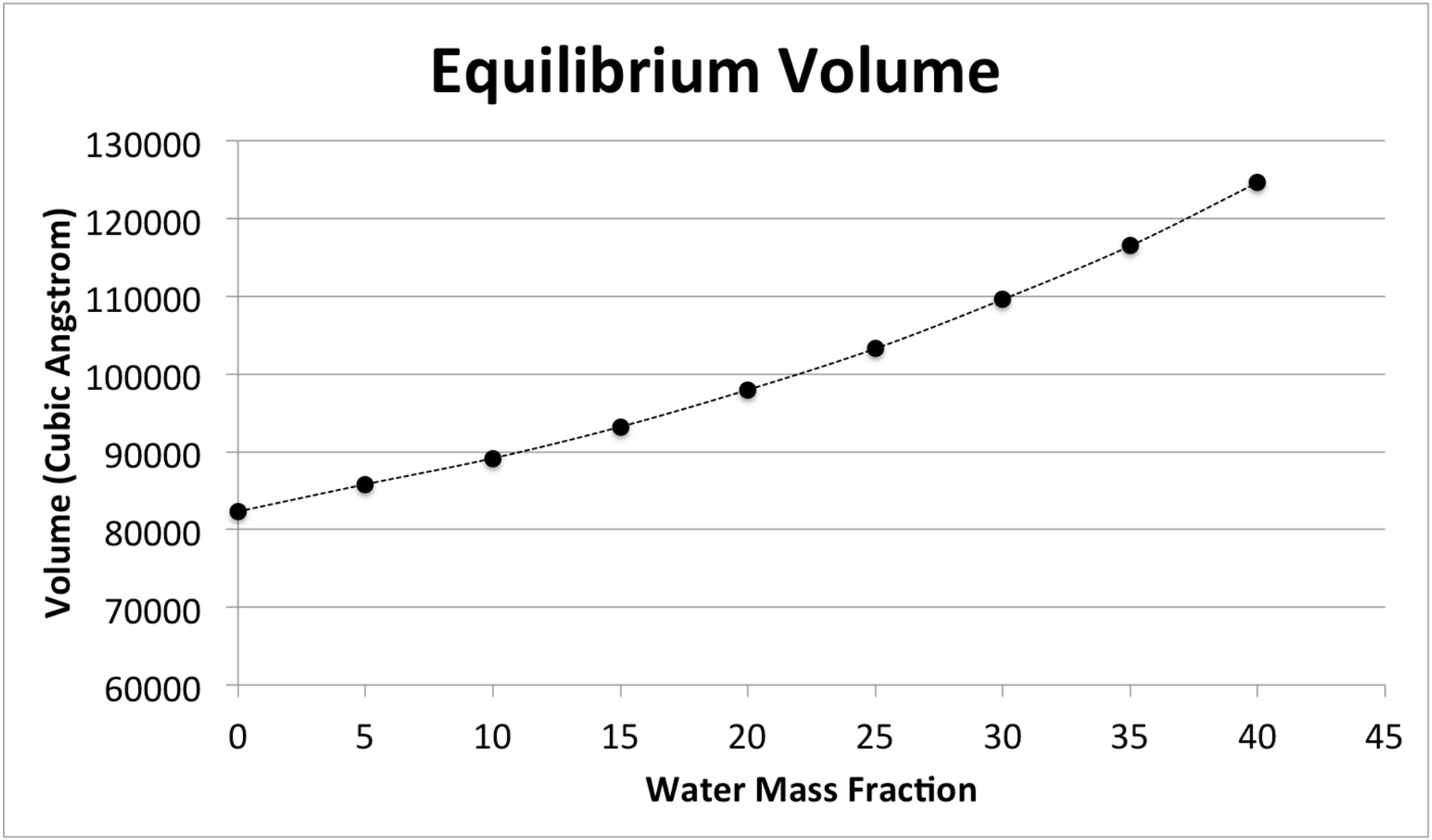
Preparation:
Vacuum System was compressed to experimental density to measure equilibrium pressure, for hydrophilic case: 20,000 atm

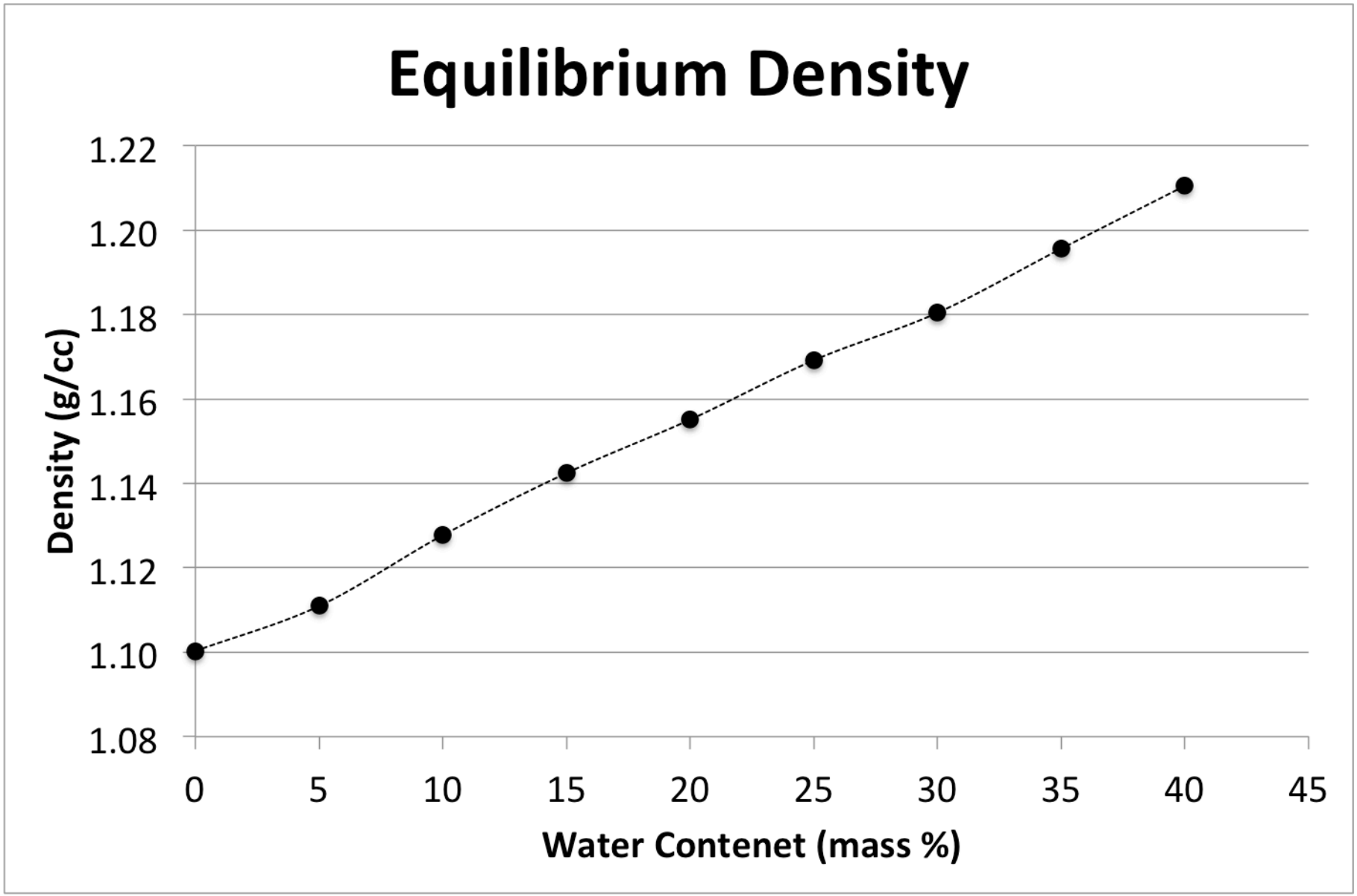


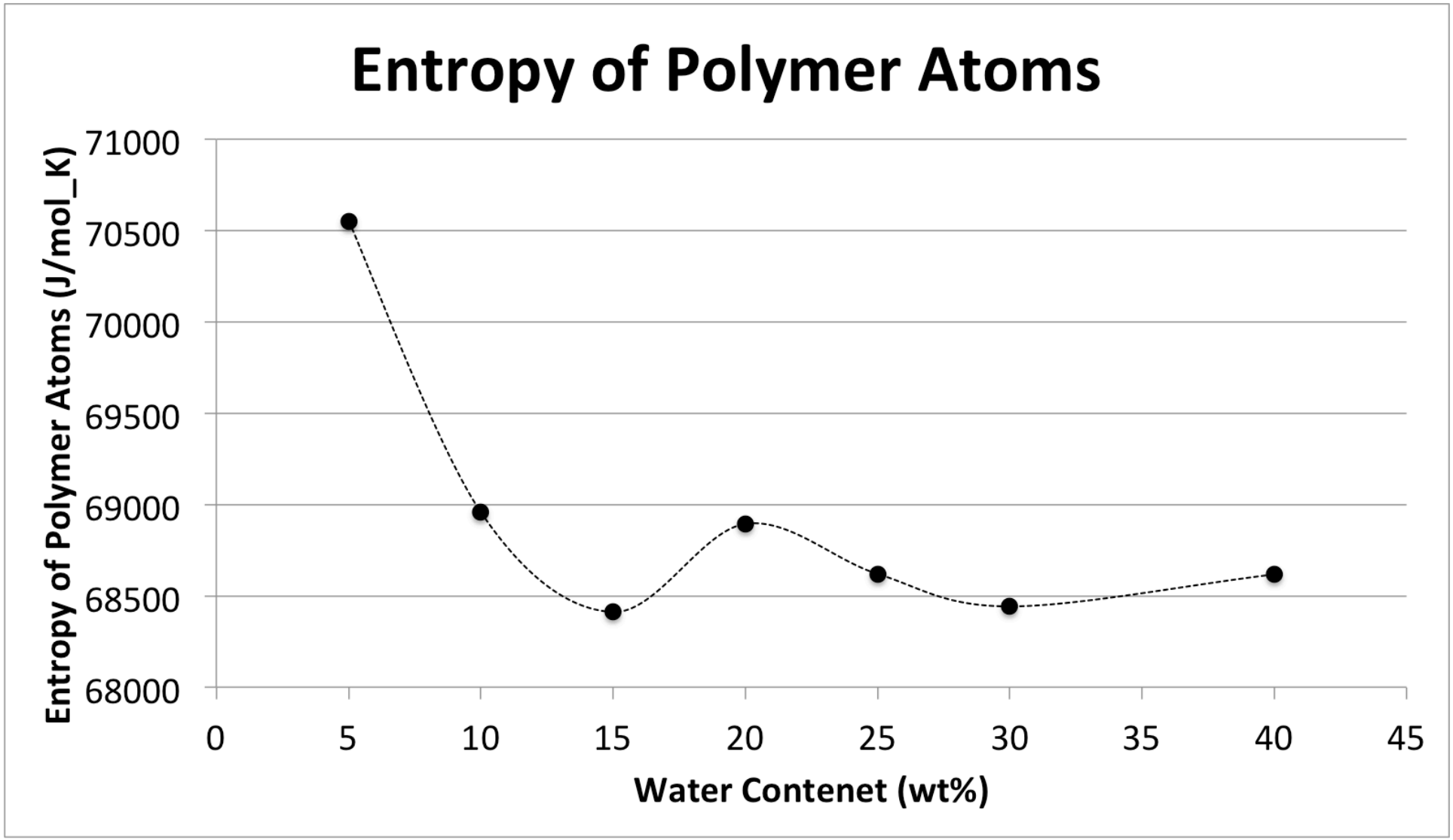
Preparation:
Polymer systems were prepared at low density (~0.5 g/cc) and appropriate number of water molecules were randomly added. System allowed to equilibrate NVT for 50 ps, compressed over 20 ps to a density of 1.1 g/cc, allowed to relax here for 50 ps NVT, then subjected to ~100 ps NPT to attain final density.

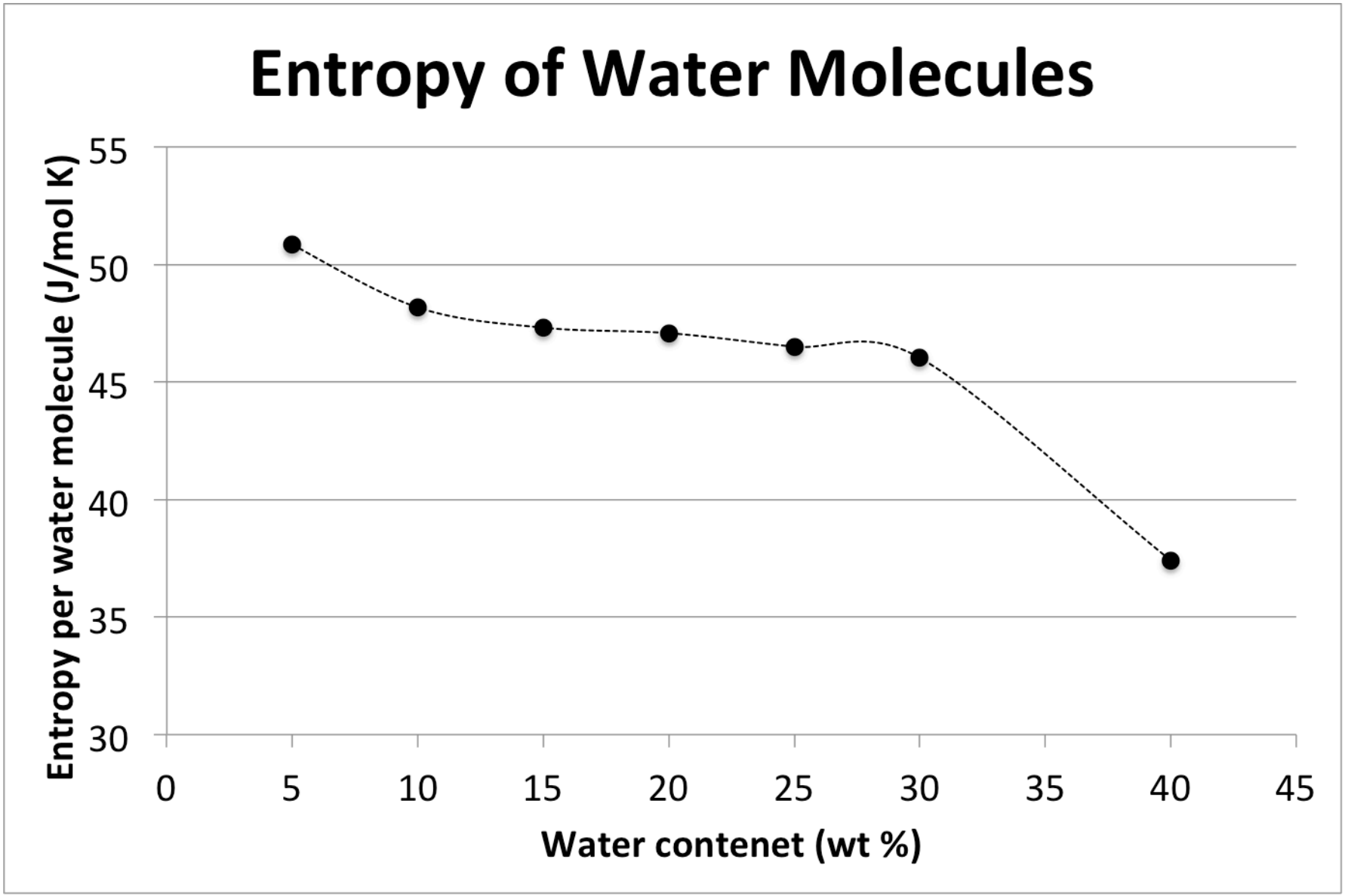


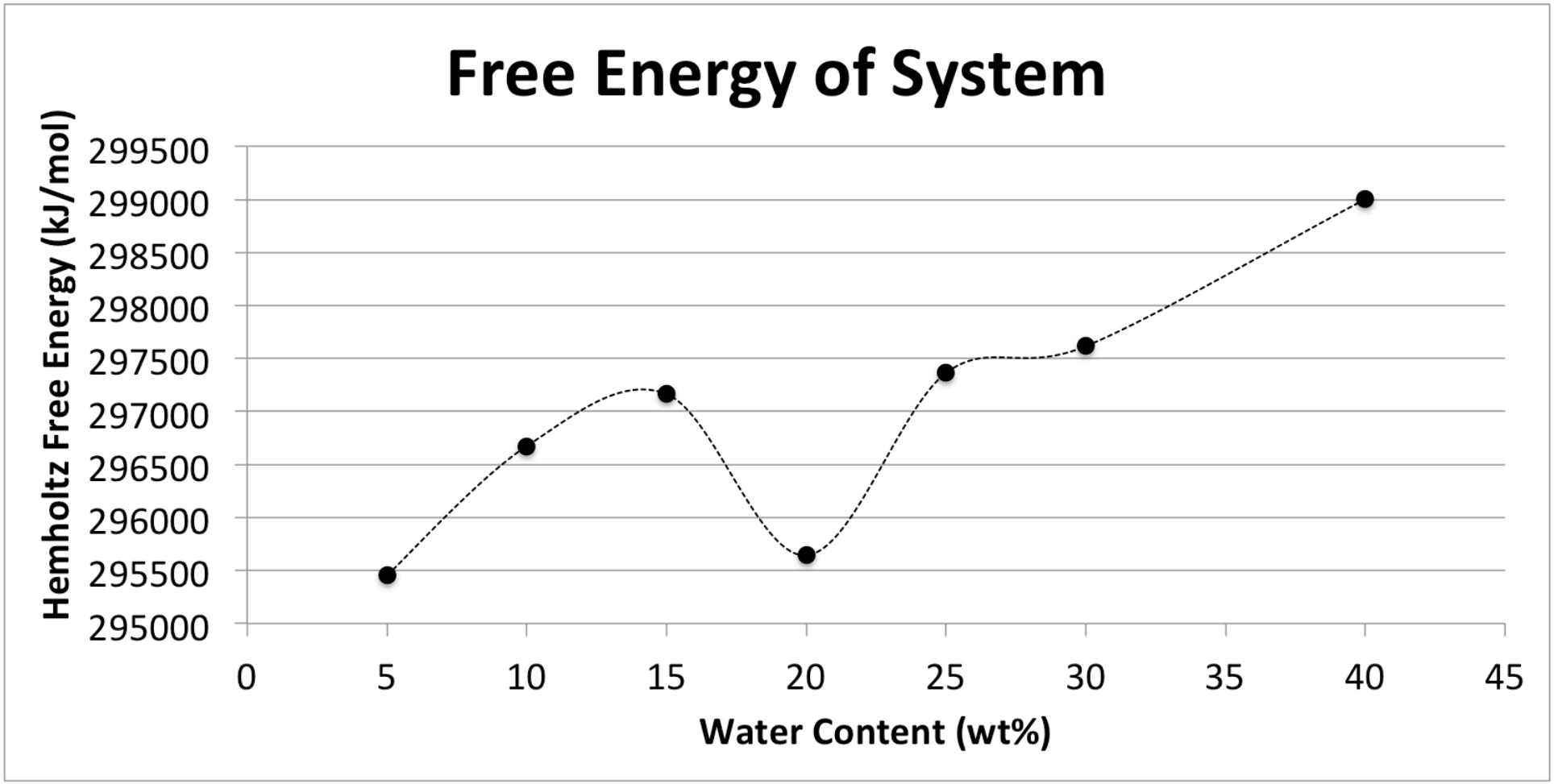
Results for Hydrophilic System:




Equilibrium Density
Density (g/cc)
1.22
1.20
1.18
1.16
1.14
1.12
1.10
1.08
0
5
10
15
20
25
30
35
40
45
Water Contenet (mass %)


Entropy of Polymer Atoms
Entropy of Polymer Atoms (J/mol_K)
71000
70500
70000
69500
69000
68500
68000
0
5
10
15
20
25
30
35
40
45
Water Contenet (wt%)


Entropy of Water Molecules
Entropy per water molecule (J/mol K)
55
50
45
40
35
30
0
5
10
15
20
25
30
35
40
45
Water contenet (wt %)


Free Energy of System
Hemholtz Free Energy (kJ/mol)
299500
299000
298500
298000
297500
297000
296500
296000
295500
295000
0
5
10
15
20
25
30
35
40
45
Water Content (wt%)

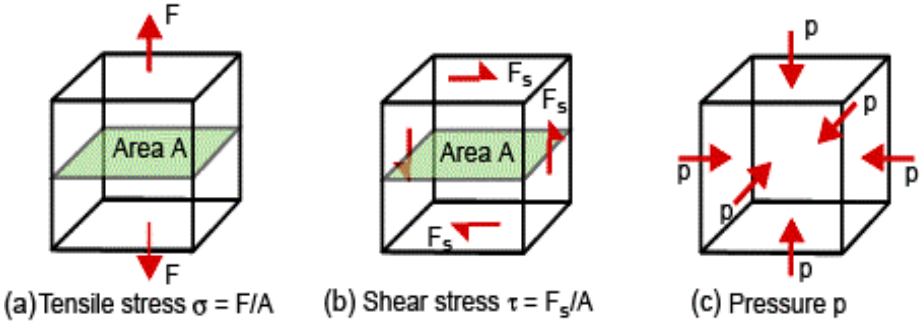
Stress-Strain, Poisson's Ratio, Elastic moduli and other mechanical properties

Hardness [nanoindentation]

MM/MD to calculate elastic constants, moduli and other mechanical properties

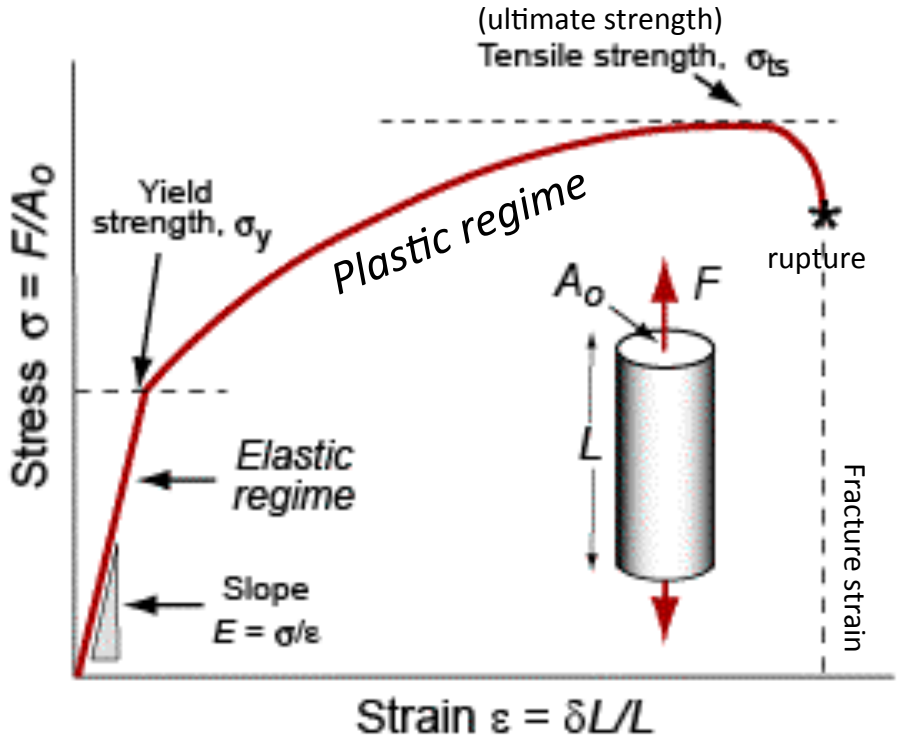
OUTLINE

Stress-Strain



$$\sigma = E\varepsilon \qquad \sigma_S = G\gamma \qquad p = K\Delta$$

Tensile Stress	Shear stress	Pressure
Young's modulus	Shear Modulus	Bulk modulus
Tensile strain	Shear strain	Dilation



- Young's modulus describes the material's response to linear strain
- Shear modulus describes the material's response to shearing strains
- Bulk modulus describes the material's response to uniform pressure

Poisson's Ratio
Transverse strain
Axial strain

$$\nu = -\frac{\varepsilon_t}{\varepsilon}$$

Stress

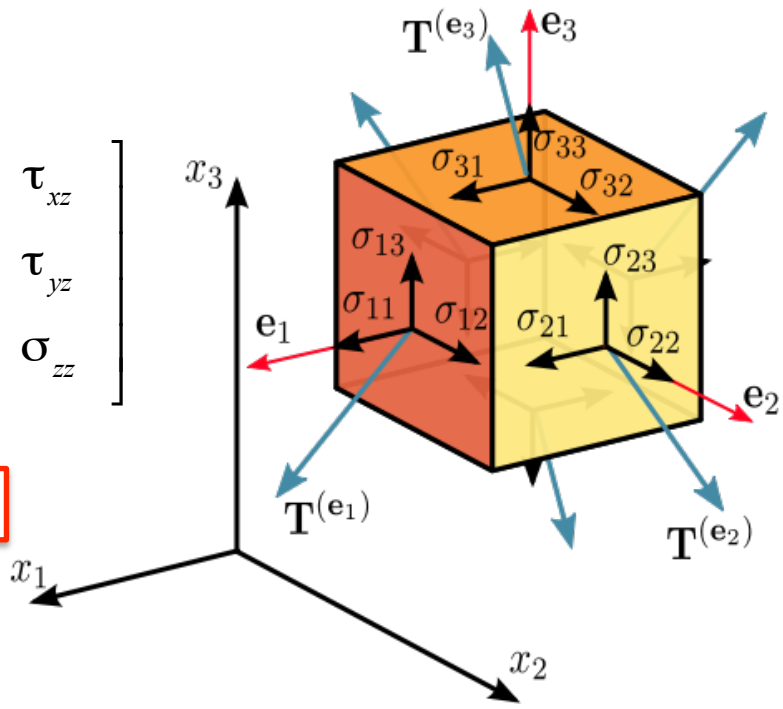
- The stress (Force/Area) at any point in a continuum object, is defined completely, for small deformations, by the symmetric Cauchy stress tensor,

1 normal and 2 shear components per plane

$$\sigma = \sigma_{ij} = \begin{bmatrix} T^{(e_1)} \\ T^{(e_2)} \\ T^{(e_3)} \end{bmatrix} = \begin{bmatrix} \sigma_{xx} & \sigma_{xy} & \sigma_{xz} \\ \sigma_{yx} & \sigma_{yy} & \sigma_{yz} \\ \sigma_{zx} & \sigma_{zy} & \sigma_{zz} \end{bmatrix} = \begin{bmatrix} \sigma_{xx} & \tau_{xy} & \tau_{xz} \\ \tau_{yx} & \sigma_{yy} & \tau_{yz} \\ \tau_{zx} & \tau_{zy} & \sigma_{zz} \end{bmatrix}$$

shear stresses

normal stresses

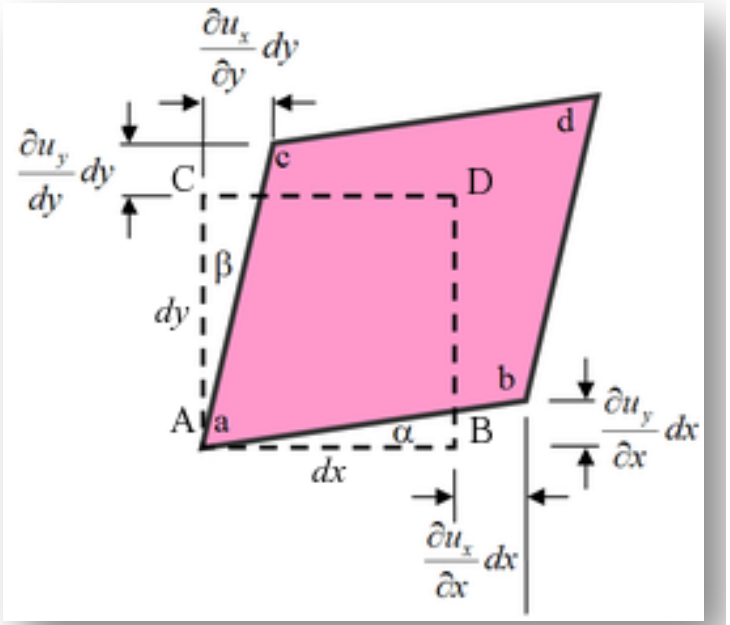


Strain

- A material with dimension $dx \times dy$ is deformed (by a force), and the infinitesimal vector that describes the difference between initial and final positions for each point in the object is,

$$u(x,y,z) = \left[u(x,y,z), v(x,y,z), w(x,y,z)\right]^T$$

- Its gradient (a tensor) describes the directional changes in every Cartesian direction



$$u\nabla = \begin{bmatrix} \partial u/\partial x & \partial u/\partial y & \partial u/\partial z \\ \partial v/\partial x & \partial v/\partial y & \partial v/\partial z \\ \partial w/\partial x & \partial w/\partial y & \partial w/\partial z \end{bmatrix}$$

$$\|\nabla u\| \ll 1 \rightarrow \frac{\nabla u + \nabla u^T}{2} = \varepsilon \rightarrow \varepsilon = \varepsilon_{kl} = \begin{bmatrix} \varepsilon_{xx} & \varepsilon_{xy} & \varepsilon_{xz} \\ \varepsilon_{yx} & \varepsilon_{yy} & \varepsilon_{yz} \\ \varepsilon_{zx} & \varepsilon_{zy} & \varepsilon_{zz} \end{bmatrix} = \begin{bmatrix} \varepsilon_{xx} & 0.5\gamma_{xy} & 0.5\gamma_{xz} \\ 0.5\gamma_{zx} & \varepsilon_{yy} & 0.5\gamma_{yz} \\ 0.5\gamma_{zx} & 0.5\gamma_{zy} & \varepsilon_{zz} \end{bmatrix}$$

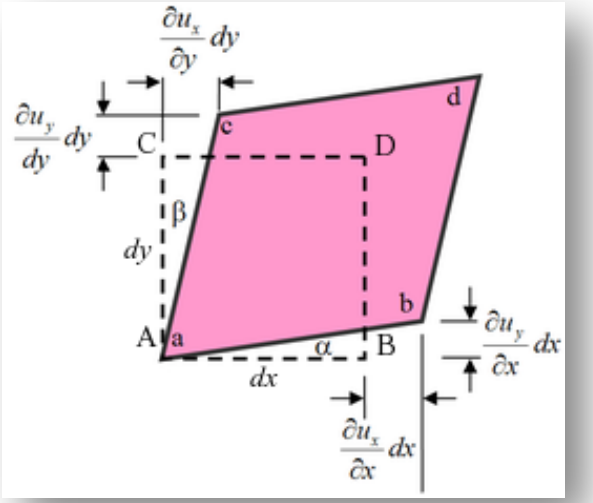
shear engineering strains

normal stresses

Strain

- Strains can be defined geometrically,

$$\overline{ab} = \sqrt{\left(\partial x + \frac{\partial u_x}{\partial x}dx\right)^2 + \left(\frac{\partial u_y}{\partial x}dx\right)^2} = \sqrt{1 + 2\frac{\partial u_x}{\partial x} + \left(\frac{\partial u_x}{\partial x}\right)^2 + \left(\frac{\partial u_y}{\partial x}\right)^2}\,dx$$



- For small displacement gradient, $\|\nabla u\| \ll 1$

$$\overline{ab} \approx dx + \frac{du_x}{dx}dx$$

- **Normal strain**

$$\varepsilon_x = \frac{\overline{ab} - \overline{AB}}{\overline{AB}} = \frac{\partial u_x}{\partial x}$$

$$\varepsilon_y = \frac{\partial u_y}{\partial y}$$

$$\varepsilon_z = \frac{\partial u_z}{\partial z}$$

Shear Strain

$$\gamma_{xy} = \alpha + \beta \qquad tan(\alpha) = \frac{\frac{\partial u_y}{\partial x}dx}{dx + \frac{\partial u_x}{\partial x}dx} = \frac{\frac{\partial u_y}{\partial x}}{1 + \frac{\partial u_x}{\partial x}};\; tan(\beta) = \frac{\frac{\partial u_x}{\partial y}dy}{dy + \frac{\partial u_y}{\partial y}dy} = \frac{\frac{\partial u_x}{\partial y}}{1 + \frac{\partial u_y}{\partial y}}$$

For small rotations (i.e. $\tan(\alpha)\approx\alpha$ and $\tan(\beta)\approx\beta$), and small displacement gradients (i.e. $\alpha\approx du_y/dx$ and $\beta=du_x/dy$),

$$\gamma_{xy} = \frac{\partial u_y}{\partial x} + \frac{\partial u_x}{\partial y} \Rightarrow \gamma_{xz} = \frac{\partial u_x}{\partial z} + \frac{\partial u_z}{\partial x} \Rightarrow \gamma_{yz} = \frac{\partial u_y}{\partial z} + \frac{\partial u_z}{\partial y}$$

Atomic virial stresses and continuum stress

- The average virial stress, Π, in a representative volume, Θ, containing a number of atoms is given by,

$$\boldsymbol{\Pi} = \frac{1}{\Theta} \sum_{\mathbf{x}_i \in \Theta} (\Theta_i \boldsymbol{\Pi}_i) = \frac{1}{\Theta} \sum_{\mathbf{x}_i \in \Theta} \left(-m_i \dot{\mathbf{u}}_i \otimes \dot{\mathbf{u}}_i + \frac{1}{2} \sum_{j \neq i} \mathbf{x}_{ij} \otimes \mathbf{f}_{ij} \right)$$

- Zhou [8] and Zhou and McDowell [9] have suggested that the first, dynamical, term in the average virial formula above should not participate since the desired continuum Cauchy stress is supposed to represent mechanical forces only. Based on the conservation principles they suggested that the Cauchy stress be equal to the mechanical term in the

$$\boldsymbol{\sigma} = \frac{1}{2\Theta} \sum_{\mathbf{x}_i \in \Theta} \sum_{j \neq i} \mathbf{x}_{ij} \otimes \mathbf{f}_{ij} \longrightarrow \sigma_{xx} = E_x \varepsilon_{xx} + \alpha \varepsilon_{xx}^2$$

Virial stress method

Egami et al (1980), Cheung and Yip (1991), Horstemeyer and Baskes (1999) and Zhou (2003)

Stress-Strain Relationship

- The stress and strain tensors are linearly related by the **elastic constants** (which characterize the stiffness of a material) in the limit of infinitesimal deformation as $\sigma_{ij}=C_{ijkl}\varepsilon_{kl}$, i.e. every member of ε_{kl} will cause a stress in σ_{ij}
- For example, for the first term

$$C_{ijkl} = \frac{\partial \sigma_{ij}}{\partial \varepsilon_{kl}}$$

$$\sigma_{xx}=C_{xxxx}\varepsilon_{xx}+C_{xxxy}\varepsilon_{xy}+C_{xxxz}\varepsilon_{xz}+C_{xxyx}\varepsilon_{yx}+C_{xxyy}\varepsilon_{yy}+C_{xxyz}\varepsilon_{yz}+C_{xxzx}\varepsilon_{zx}+C_{xxzy}\varepsilon_{zy}+C_{xxzz}\varepsilon_{zz}$$

- **81 C_{ijkl} in total ! but only 21 are unique (symmetry)**
- Rewriting the stress and strain tensors as vectors, and using engineering strain, the stress-strain relationship in terms of the **stiffness matrix Q(C)** is

Voigt notation

$$\begin{bmatrix} \sigma_1 \\ \sigma_2 \\ \sigma_3 \\ \sigma_4 \\ \sigma_5 \\ \sigma_6 \end{bmatrix} = \begin{bmatrix} Q_{11} & Q_{12} & Q_{13} & Q_{14} & Q_{15} & Q_{16} \\ Q_{12} & Q_{22} & Q_{23} & Q_{24} & Q_{25} & Q_{26} \\ Q_{13} & Q_{23} & Q_{33} & Q_{34} & Q_{35} & Q_{36} \\ Q_{14} & Q_{24} & Q_{34} & Q_{44} & Q_{45} & Q_{46} \\ Q_{15} & Q_{25} & Q_{35} & Q_{45} & Q_{55} & Q_{56} \\ Q_{16} & Q_{26} & Q_{36} & Q_{46} & Q_{56} & Q_{66} \end{bmatrix} \begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \varepsilon_3 \\ \varepsilon_4 \\ \varepsilon_5 \\ \varepsilon_6 \end{bmatrix}$$

1:xx,2:yy,3:zz,4:yz-zy,5:xz-zx,6:xy-yz

$$\varepsilon = Q^{-1}\sigma = S\sigma$$

Compliance Matrix

Stiffness Matrix

General anisotropic linear elastic stress-strain with thermal strain

General stress-strain relationship: $\sigma_{ij} = C_{ijkl}\left(\varepsilon_{kl} - \alpha_{kl}\Delta T\right)$

And its inverse: $\varepsilon_{ij} = S_{ijkl}\sigma_{kl} + \alpha_{ij}\Delta T$

Temperature reduces strength !!

By definition: $C_{ijkl} = \dfrac{\partial \sigma_{ij}}{\partial \varepsilon_{kl}}$ and $\sigma_{ij} = \dfrac{\partial U}{\partial \varepsilon_{ij}}$ $\longrightarrow$ $\dfrac{\partial^2 U}{\partial \varepsilon_{ij}\partial \varepsilon_{kl}} = \dfrac{\partial^2 U}{\partial \varepsilon_{kl}\partial \varepsilon_{ij}}$

- Where strain E density: $U = \frac{1}{2}C_{ijkl}\left(\varepsilon_{ij} - \alpha_{ij}\Delta T\right)\left(\varepsilon_{kl} - \alpha_{kl}\Delta T\right) = \frac{1}{2}S_{ijkl}\sigma_{ij}\sigma_{kl}$
- Tensor symmetries follow: $C_{ijkl} = C_{klij} = C_{jikl} = C_{ijlk}$

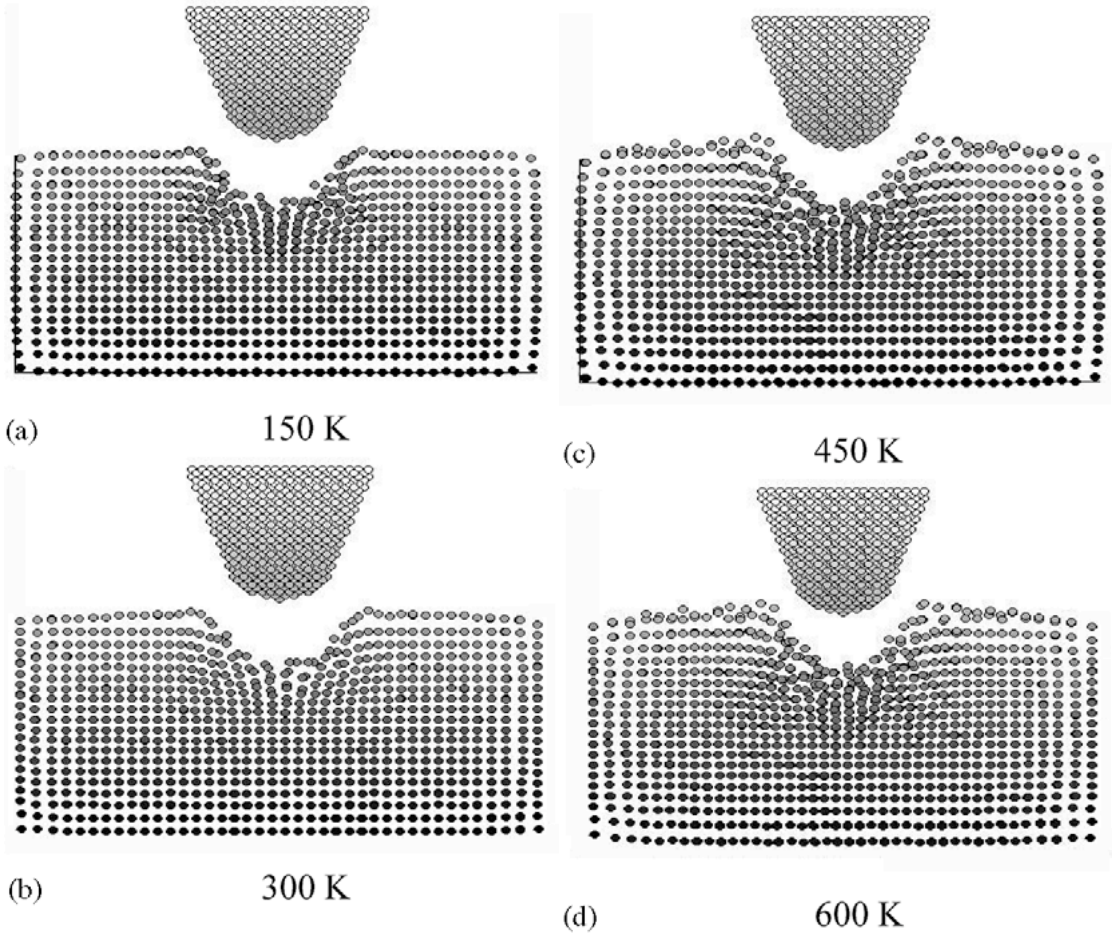
EC relationships in materials with cubic symmetry:

$$E = \left(c_{11}^2 + c_{12}c_{11} - 2c_{12}^2\right)/\left(c_{11} + c_{12}\right) \qquad \nu = c_{12}/(c_{11} + c_{12}) \qquad \mu = c_{44}$$

$$c_{11} = E(1-\nu)/(1-\nu-2\nu^2) \qquad c_{12} = E\nu/(1-\nu-2\nu^2) \qquad A = \frac{2\mu(1+\nu)}{E} = \frac{2c_{44}}{c_{11}-c_{12}}$$

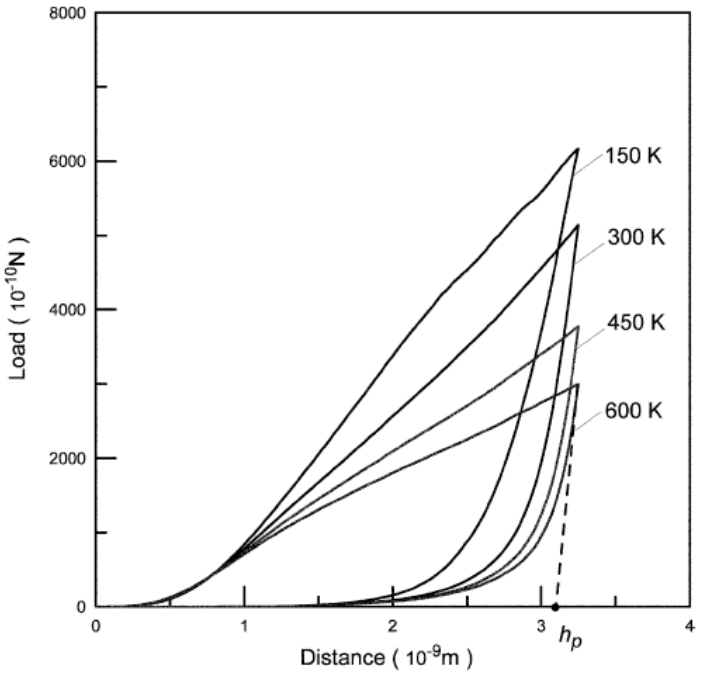
Hardness (nanoindentation)

- Resistance to local plastic deformation.

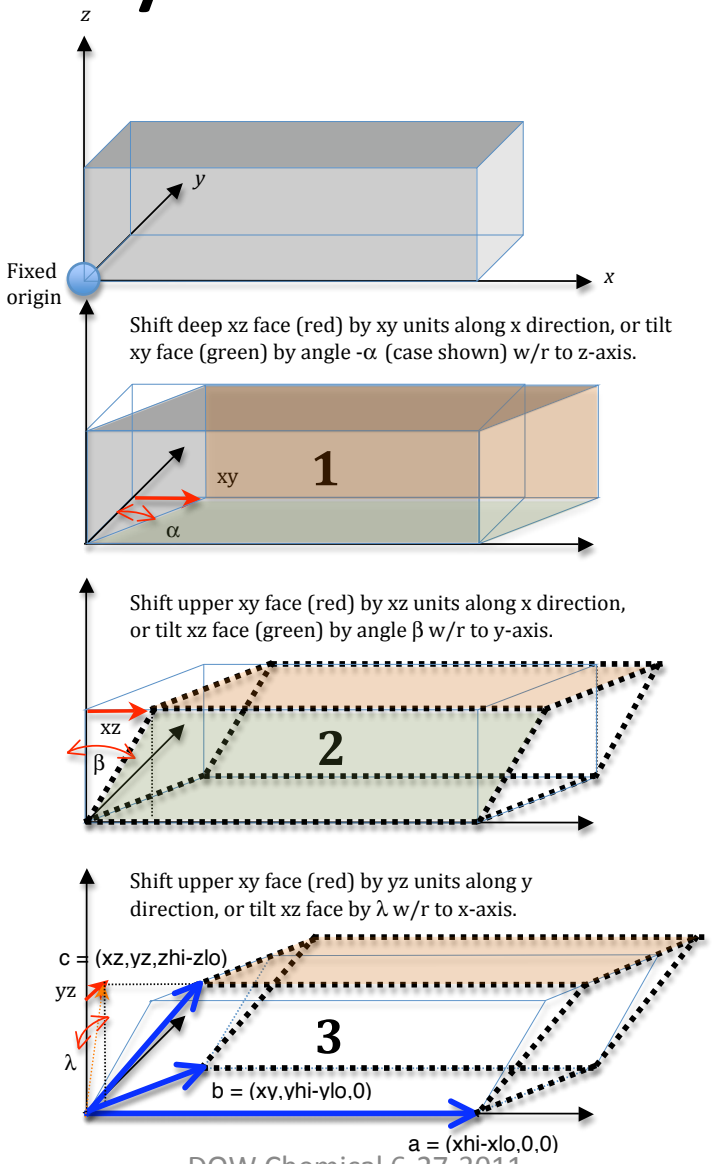


$$H = \frac{W_{max}}{A}$$

Max indentation load / Contact area



Triclinic Systems in LAMMPS



Using MM to compute 0K elastic constants (e.g. LAMMPS)

1

```
# 1. Simulation settings
boundary        p p p
newton          on
units           electron
atom_style      hybrid charge electron
read_data       data.diamond

# 2. Global variables
# conversions
variable        gpa equal 1e-9
# displacement
variable        up equal 1.0e-6
# minimization parameters
variable        etol equal 0.0
variable        ftol equal 1.0e-10
variable        maxiter equal 1000
variable        maxeval equal 5000
variable        dmax equal 1.0e-2
```

2

```
variable        temp equal lx
variable        lx0 equal ${tmp} …

# 3. Setup potential, min and out params
pair_style      eff/cut 40.340355
pair_coeff      * *
neigh_modify    once no every 1 delay 0 check yes
                one 40000 page 400000

# Setup minimization style
min_style       cg
min_modify      dmax ${dmax} line quadratic

# Setup output
thermo          1
thermo_style    custom step pe press pxx
                pyy pzz pxy pxz pyz lx ly lz vol
```

$$P = \frac{Nk_BT}{V} + \frac{\sum_i^N r_i \bullet f_i}{dV}$$

Using MM to compute 0K elastic constants (e.g. LAMMPS)

3

```
# 4. Initial system state
fix             1 all box/relax aniso 0.0
minimize        ${etol} ${ftol} ${maxiter} ${maxeval}
# Define constants from pressure tensor components
variable        tmp equal pxx
variable        pxx0 equal ${tmp}
                … (pyy0,pzz0,pyz0,pxz0,pxy0)
# 5. Derivatives w.r.t. strain components
variable        d1 equal -(v_pxx1-${pxx0})/(v_delta/
                v_len0)*${gpa}
variable        d2 equal -(v_pyy1-${pyy0})/(v_delta/
                v_len0)*${gpa}
variable        d3 equal -(v_pzz1-${pzz0})/(v_delta/
                v_len0)*${gpa}
variable        d4 equal -(v_pyz1-${pyz0})/(v_delta/
                v_len0)*${gpa}
variable        d5 equal -(v_pxz1-${pxz0})/(v_delta/
                v_len0)*${gpa}
variable        d6 equal -(v_pxy1-${pxy0})/(v_delta/
                v_len0)*${gpa}
```

4

```
# 6. Write initial system state restart
write_restart   restart.initial
# 7. uxx Perturbation
variable        len0 equal ${lx0}
# Reset box / simulation parameters
clear
read_restart    restart.initial
include         steps 3 (i.e. repeat code here)
# Negative deformation
variable        delta equal -${up}*${len0}”
displace_box    all x delta 0 ${delta} units box”
# Relax atoms positions
minimize        ${etol} ${ftol} ${maxiter} ${maxeval}
# New stress tensor, and variables
variable        tmp equal pxx
variable        pxx1 equal ${tmp}
                …  (pyy1,pzz1,pyz1,pxz1,pxy1)
# Compute elastic constant from Pressure tensor
variable        C1neg equal ${d1}
                … C2neg,C3neg,C4neg,C5neg,C6neg
```

Using MM to compute 0K elastic constants (e.g. LAMMPS)

5

```
# Reset box / simulation parameters
clear
read_restart        restart.initial
include             steps 2,5,6 (i.e. repeat code here)

# Positive deformation
variable            delta equal ${up}*{len0}
displace_box        all x delta 0 ${delta} units box
# Relax atoms positions
minimize      ${etol} ${ftol} ${maxiter} ${maxeval}

# New stress tensor, and vars
variable            tmp equal pxx
variable            pxx1 equal ${tmp}
                    …  (pyy1,pzz1,pyz1,pxz1,pxy1)

# Compute positive elastic cons from P
variable      C1pos equal ${d1}
              … C2pos,C3pos,C4pos,C5pos,C6pos
```

6

```
# 8. Average + and - constants
variable      C11 equal 0.5*(${C1neg}+${C1pos})
variable      C21 equal 0.5*(${C2neg}+${C2pos})
variable      C31 equal 0.5*(${C3neg}+${C3pos})
variable      C41 equal 0.5*(${C4neg}+${C4pos})
variable      C51 equal 0.5*(${C5neg}+${C5pos})
variable      C61 equal 0.5*(${C6neg}+${C6pos})
```

9. Repeat 7-8 for Uyy, Uzz, Uyz, Uxz, Uxy perturbations

10. Average symmetric components

11. Use elastic constants to compute elastic properties (B,K,E,..,etc.)

Finite Temperature Elastic Moduli with NVT-MD [Elastic Modulus (100)]

```
# Initialize
variable        sname index diamond
variable        dt equal 0.001
timestep        ${dt}
# Minimize and equilibrate
…
# Strain
….
fix             1 all nvt/sllod/eff 300.0 300.0 0.1
fix             2 all deform 1 x erate 1e-3 remap v units box

restart         100 ${sname}.nvt_strain.restart1 ${sname}.nvt_strain.restart2
thermo          100
compute         strain all ${step}*${dt}/lx
thermo_style    custom step strain etotal pe ke temp pxx pyy pzz pxy pxz pyz
compute         astress all stress/atom
compute         peatom all pe/atom
compute         keatom all ke/atom/eff
dump            1 all custom 100 ${sname}.nvt_strain.lammpstrj id type x y z spin radius vx vy vz vr fx fy fz rf
dump            2 all custom 100 ${sname}.nvt_stress id c_astress[1] c_astress[2] c_astress[3] c_astress[4] c_astress[5] c_astress[6]

run             1000000
```

NVT-SLLOD: position-dependent streaming velocity, associated with box deformation, is subtracted from each atom's actual velocity to yield a thermal velocity which is used for temperature computation and thermostatting

Can use regular NVT, but, remap x (solids)

use engineering strain and NOT true strain

Finite Temperature Elastic Moduli with NVT-MD [Shear Modulus – manual deformation [100]]

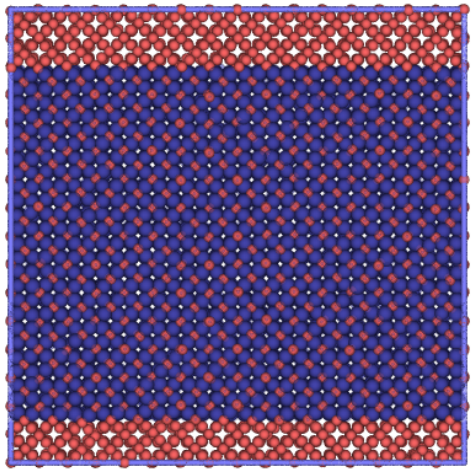
```
region        lower block INF INF INF INF INF 8.07856425 units box
region        upper block INF INF INF INF 72.707078331 INF units box
group         lower region lower;          group        upper region upper
group         boundary union lower upper;
group         mobile subtract all boundary
# Just move nuclei (eFF)
set           group lower type 1;          set          group upper type 1

# temp controllers
compute       new2d mobile temp/partial/eff 1 1 0
# Move
fix           1 all nve/eff
fix           2 boundary setforce 0.0 0.0 0.0 [rf=0]

# Shear
velocity      upper set 1.0 0 0 sum yes units box;
velocity      mobile ramp vx 0.0 1.0 z -0.0524425 80.7332 sum yes units b
# Make sure temperature in boundary remains at setpoint
fix           3 mobile temp/rescale 10 300.0 300.0 10.0 1.0
fix_modify    3 temp new2d

compute       peatom all pe/atom;
compute       keatom all ke/atom/eff; compute       astress all stress/atom
dump          1 all custom 500 ${sname}.shear id type x y z spin radius vx vy vz vr c_peatom c_keatom c_astress[1] c_astress[2] c_astress[3] …
thermo_modify temp new2d
run           20000
```

- Unit cell can be orthorhombic [finite xy]
- Use non-periodic x and y (s)
- Very cumbersome, but you're in control of every variable
- Strain = displacement of upper region



Finite Temperature Elastic Moduli with NVT-MD [Shear Modulus – using deformation (100)]

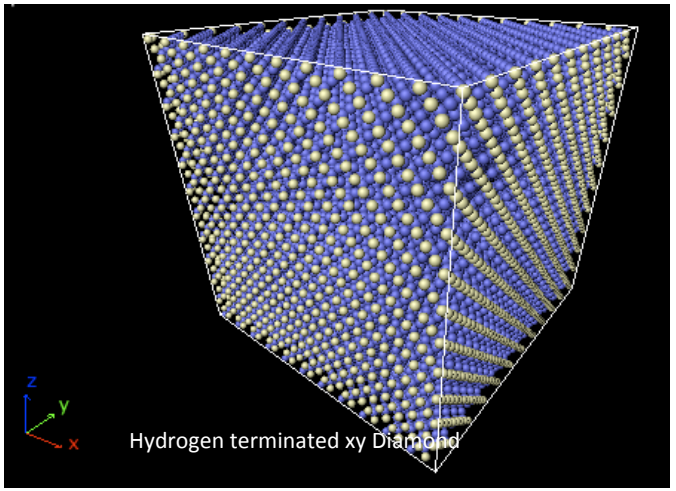
Finite versus infinite cell boundaries and triclinic symmetry

Much simpler !!

```
# Initialize
variable        sname index diamond
variable        dt equal 0.001
timestep        ${dt}
# Minimize and equilibrate
…
# Strain
….
fix             1 all nvt/sllod/eff 300.0 300.0 0.1
fix             2 all deform 1 xy erate 1e-3 remap v units box

restart         100 ${sname}.nvt_strain.restart1 ${sname}.nvt_strain.restart2
thermo          100
compute         strain all ${step}*${dt}/lx
thermo_style    custom step strain etotal pe ke temp pxx pyy pzz pxy pxz pyz
compute         astress all stress/atom
compute         peatom all pe/atom
compute         keatom all ke/atom/eff
dump            1 all custom 100 ${sname}.nvt_strain.lammpstrj id type x y z spin radius vx vy vz vr fx fy fz rf
dump            2 all custom 100 ${sname}.nvt_stress id c_astress[1] c_astress[2] c_astress[3] c_astress[4] c_astress[5] c_astress[6]

run             1000000
```



- Elastic Constant C11all = 2219.675 GPa
- Elastic Constant C22all = 1914.59 GPa
- Elastic Constant C33all = 2356.21 GPa
- Elastic Constant C12all = 985.08 GPa
- Elastic Constant C13all = 1764.0175 GPa
- Elastic Constant C23all = 548.37 GPa
- Elastic Constant C44all = 460.118515 GPa
- Elastic Constant C55all = 954.10055 GPa
- Elastic Constant C66all = 796.4444 GPa
- Elastic Constant C14all = -277.836825 GPa
- Elastic Constant C15all = -458.8013 GPa
- Elastic Constant C16all = -988.6811 GPa
- Elastic Constant C24all = 189.045385 GPa
- Elastic Constant C25all = 380.313975 GPa
- Elastic Constant C26all = -234.76535 GPa
- Elastic Constant C34all = -524.984345 GPa
- Elastic Constant C35all = -943.305825 GPa
- Elastic Constant C36all = -644.928075 GPa
- Elastic Constant C45all = 434.09374 GPa
- Elastic Constant C46all = 212.9396225 GPa
- Elastic Constant C56all = 173.12035 GPa