Documentation for calculating relaxation time from NIST Polymerization Stress Tensometer (SRI 6005)

If you are using this software please cite:

Sarkar, S., Baker, P. J., Chan, E., Lin-Gibson, S., & Chiang, M. (2017). Quantifying the sensitivity of network structure and properties from simultaneous measurements during photopolymerization. *Soft Matter*.

Directory Organization:

We recommend that the code directory **get_tau** and experimental data folder be organized in the following way.

get_tau	(contains python code for calculating relaxation time)
GlobalDataFolder	(contains all experimental data)
ExperimentFolder	(contains all trials of specific experiment)
<TrialName>.txt	(text file containing the information about the trial setup)
<TrialName>.csv	(Results of experiment in CSV format)

Example <TrialName>.txt file

Experimental Conditions

Measurements: Stress, Temperature, Degree of conversion

Beam type: Rigid steel

Sample Description: 70_30_50%
Diamater of sample (cm): 0.2500
Sample height (cm): 0.2000
C-Factor: 0.6250
Position of sample along the beam (cm): 20.0000
Compliance of the beam (cm/N): 1.2322E-3

Integration time (ms): 25.0000
Scans to average: 3.0000
Sample rate (s): 0.2000

Irradiation Mode: Standard
Start time of irradiation (s): 20.0000

Light Intensity (mW/cm2): 500.0000
Duration of irradiation (s): 40.0000
Duration of experiment: 10.00 minutes and 0.00 seconds

Additional comments on the experiment:

The NIST tensometer records the experimental condition in the above format. If the user's instrument records the information in a different way, it must be converted into the above one.

Example <TrialName>.csv

Time (s)	Voltage (V)	Disp. (cm)	Stress (MPa)	DC (%)	deltaT
0.142216	-0.00008416	-0.00000107	-0.00010018	2.926763	-0.12565
0.342656	-0.00009116	-0.00000107	-0.00010918	1.078467	0.016231
0.543096	-0.00026116	-0.00000207	-0.00031118	0.381026	0.300331
0.743536	-0.00071016	-0.00000707	-0.00084418	2.357989	0.959891
0.943976	-0.00145116	-0.00001407	-0.00172418	1.337635	2.112882

Lastly, we need a provide some additional information regarding for the material, which are provided using <inputfile>.txt.

# Inputs for folder location
Superfolder = GlobalDataFolder
Subfolder = ExperimentFolder
Testname = TrialName

Information about the composite
Initial viscosity (in Pa.s) = 1.0
High-frequency Youngs modulus (GPa) = 4.5
Maximum shrinkage strain = 0.10
Coefficient of thermal expansion (in 1/T) = 1E-4,0.5E-4
Molecular density (in moles/m^3) = 2500

Numerical calculation details
Calculation time (s) = 250.0

Regularization parameter = 1E-2
Denoising window = 5

# Analysis outname
Casename = TrialAnalysis

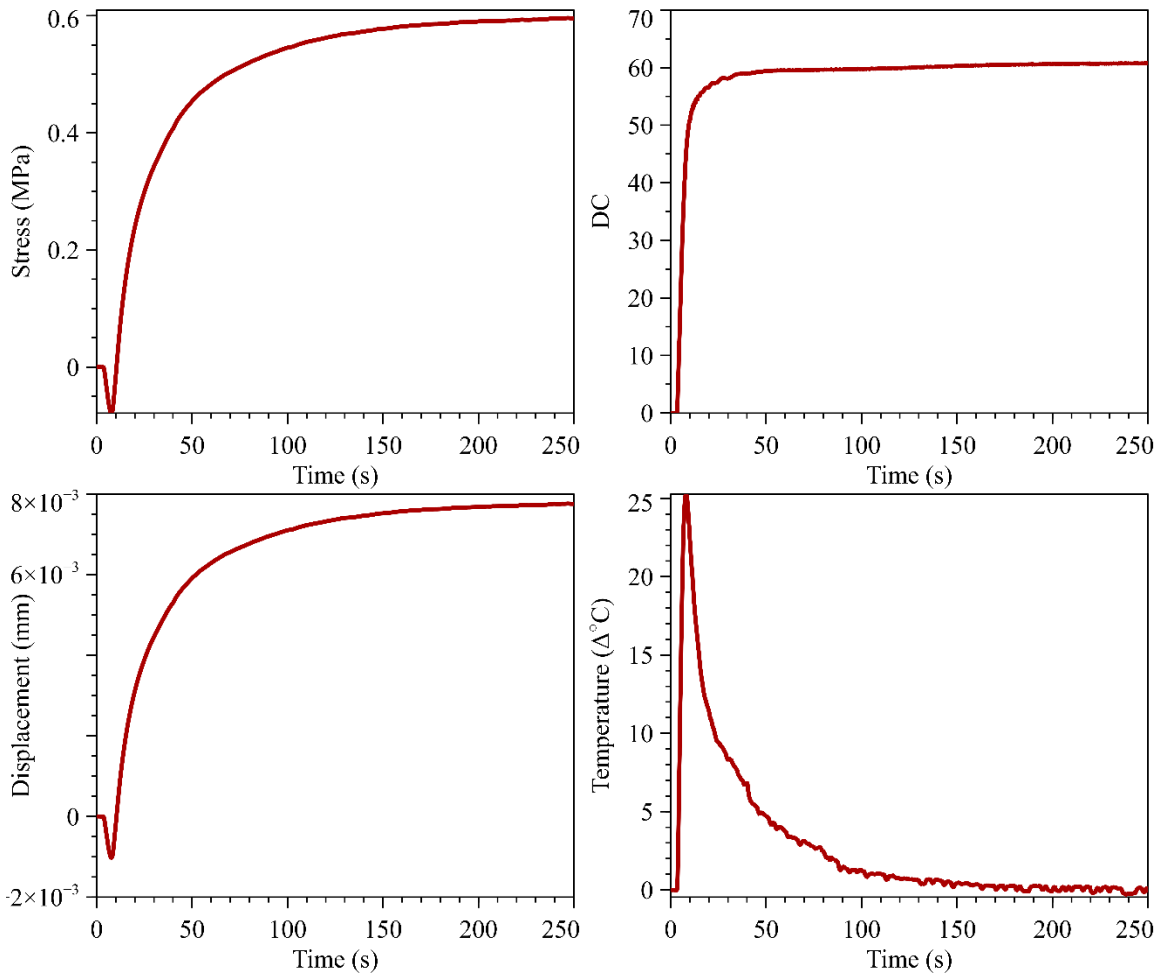
The coefficient of thermal expansion asked for are the limiting values for the resin and the cured polymer at a high DC.

Once, the input file and rest of the information has been organized. The code can be executed as,

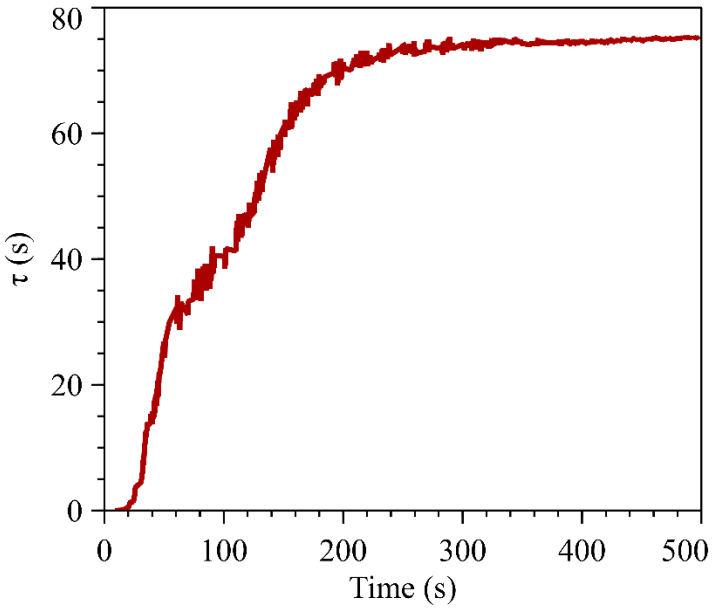
python get_tau/get_tau.py -i <inputfile>.txt

The outputs of the calculation will be stored in a folder <Casename> under the directory ExperimentFolder.

Sample Inputs:



Sample Output:



Evaluating the effect of interaction energy and clustering using effective conductivity theory

The code for calculating the scaling law for diffusion coefficient with Degree of Conversion is available in the folder **scaling_law** under **photocureRT.**

Usage:

$ python scaling_law.py -h
Usage: scaling_law.py [option1] arg1 [option2] arg2 [option3] arg3

Options:
-h, --help show this help message and exit
-z COORD Coordination number of the lattice
-e ENERGY Energy of interaction as a factor f to kT (i.e. e = f kT).
-c BIAS Bias for clustering (no bias: c = 1, strictly biased: c = 0).

Example:

$python scaling_law.py -z 6 -e 10 -c 0.1