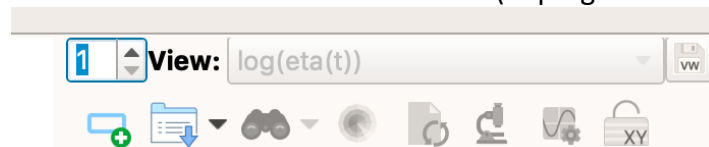# Crystal Application Tutorial: Comparing with steady state nucleation data
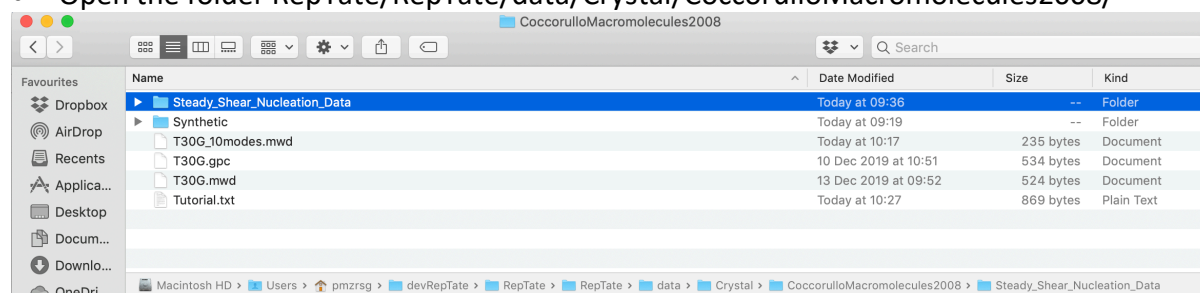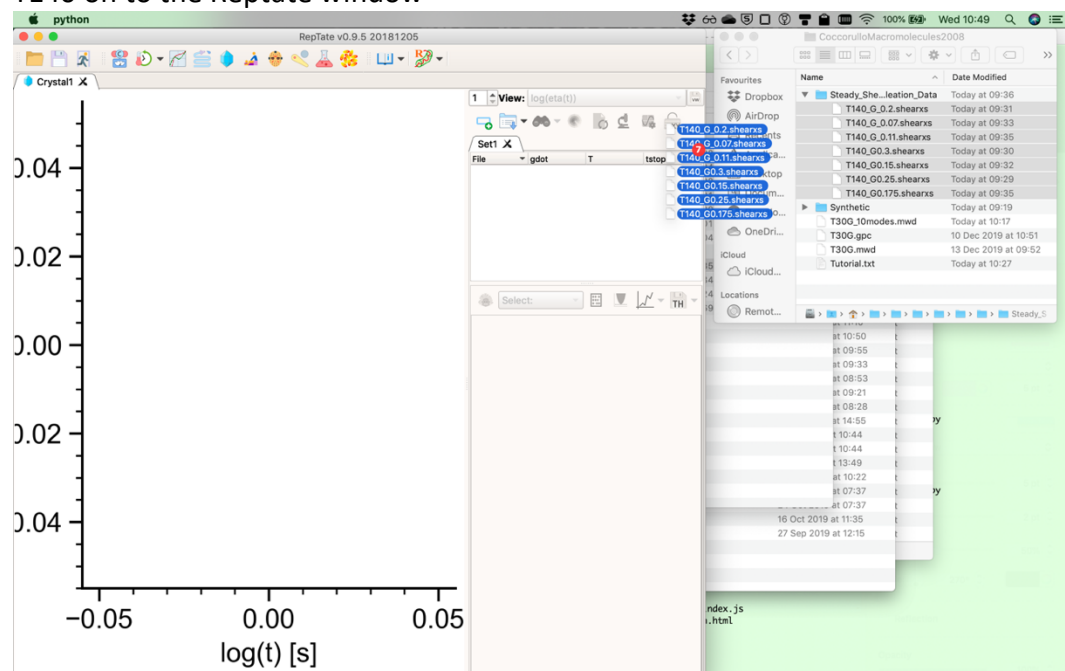
Load data and set the view

- Load the Crystal application (Click on the crystal application on the top toolbar)

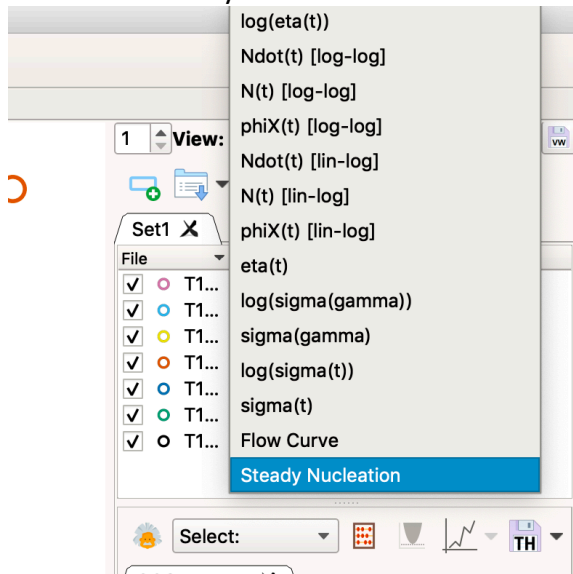- Reduce the number of views to 1 (Top right corner)

- Open the folder RepTate/RepTate/data/Crystal/CoccorulloMacromolecules2008/

- From the folder 'Steady_Shear_Nucleation_Data' drag and drop all files that begin with T140 on to the Reptate window
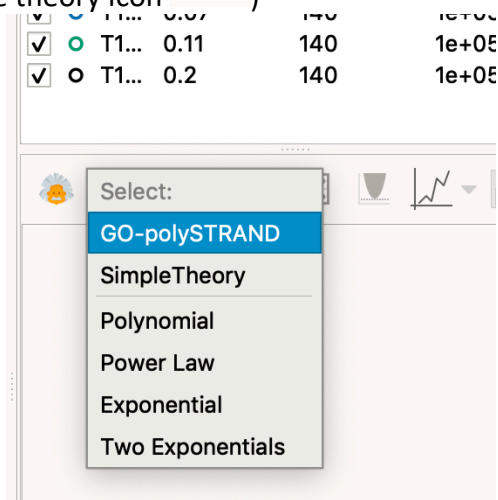
- Select 'Steady Nucleation' View
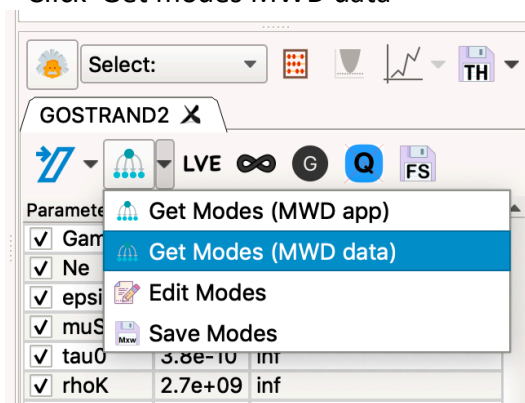

Set-up a fast-running calculation

- Load GO-polyStrand model (choose the model from the drop down list and then click
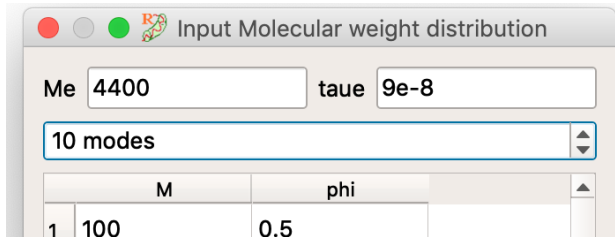
  the theory icon   )
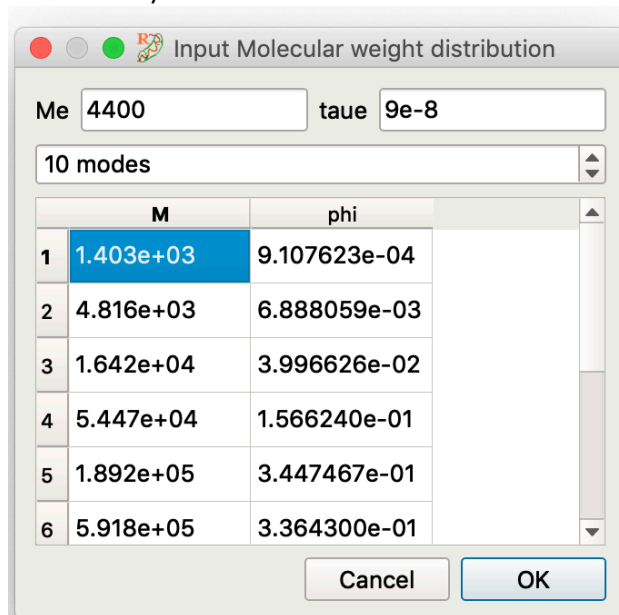

- Click 'Get modes MWD data'

-In the pop-up window set Me=4400, tau_e=9.0E-8 and the number of modes to 10
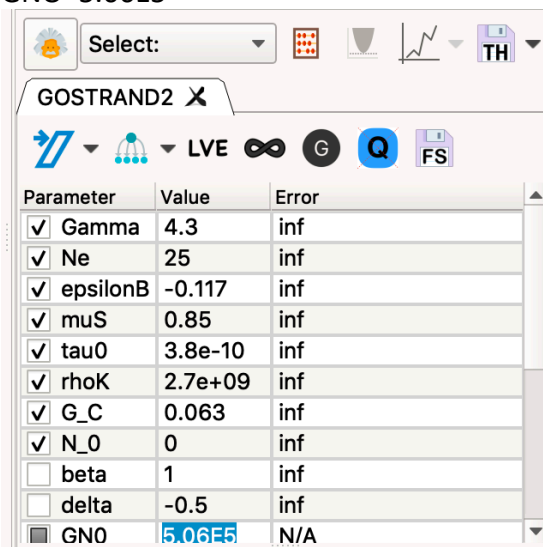

In a text editor, open 'T30G_10modes.mwd' and copy whole file contents to the clipboard.

- Click on the first element of the table and paste the copied file (use ctrl-v or a similar keyboard shortcut)


Close the mode window by clicking 'Ok'

- Back in the theory window, turn on the modulus correction button and set Gamma=4.3 and GNO=5.06E5
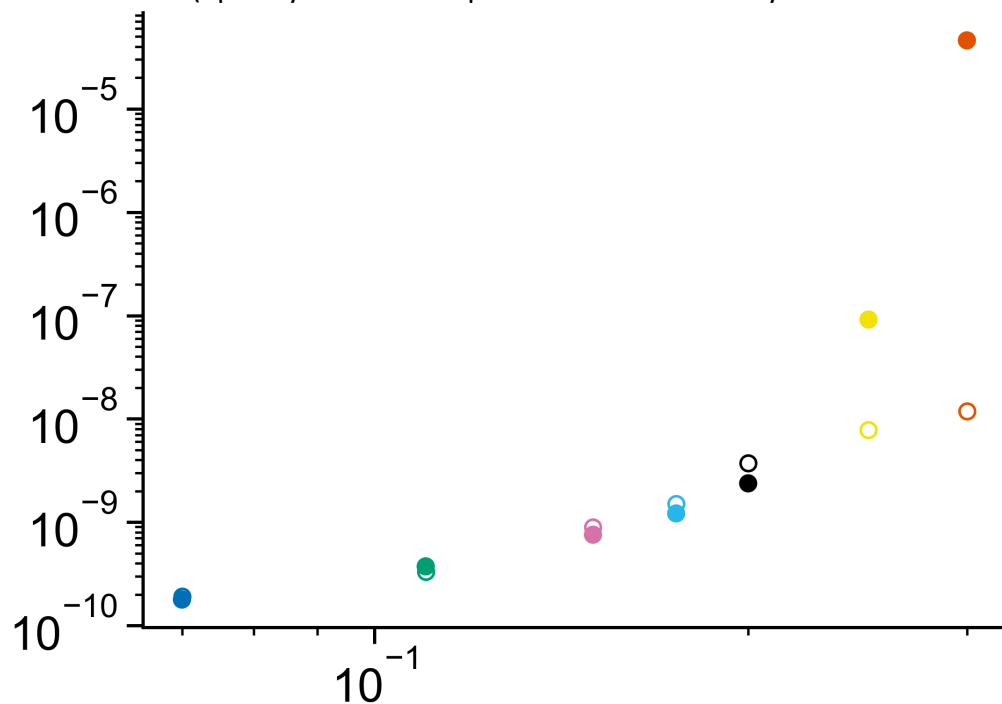
- Other parameters default to the correct values, here's a full list.
  - Gamma   4.3
  - Ne   25
  - epsilonB   -0.117
  - muS   0.85
  - tau0   3.8e-10
  - rhoK   2.7e+09
  - G_C   0.063
  - N_0   0
  - beta   1
  - GN0   506000

- Hit compute, and the calculation should take about 15 secs (depending on how good your laptop is!)
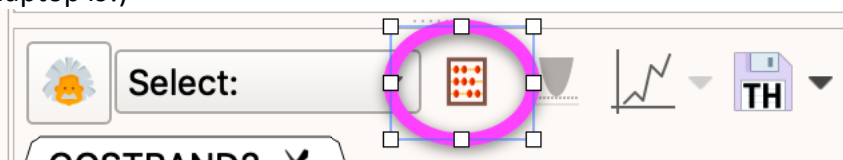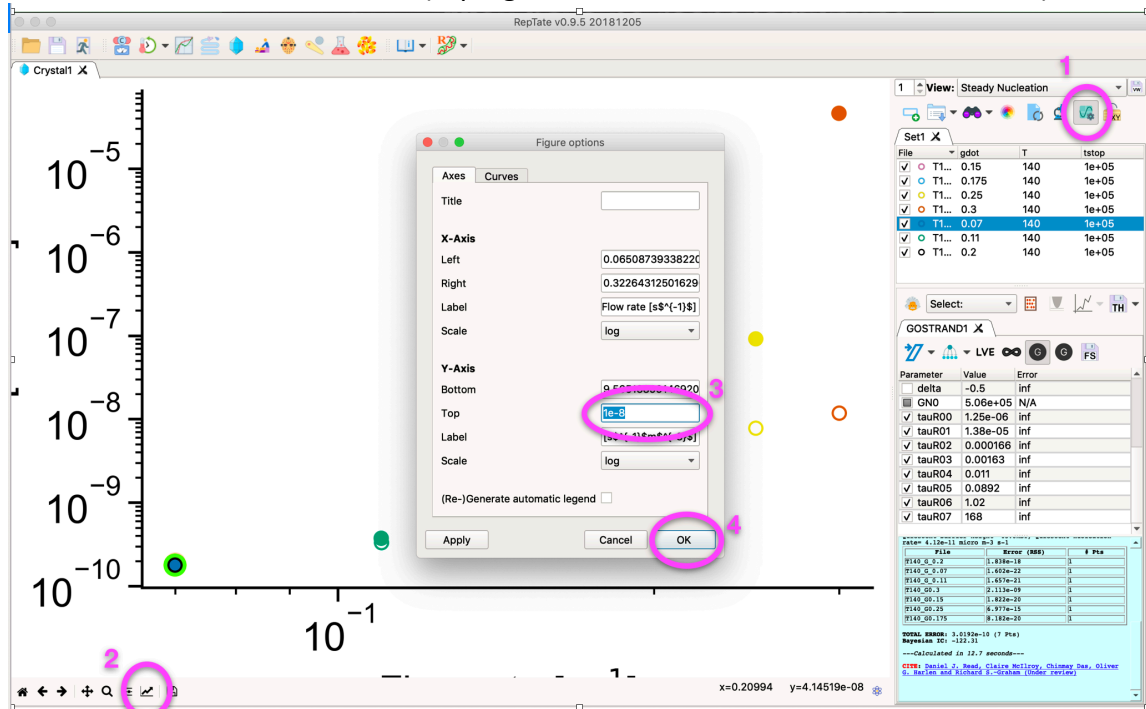

- You should see (open symbols are experiments and closed symbols are the model)
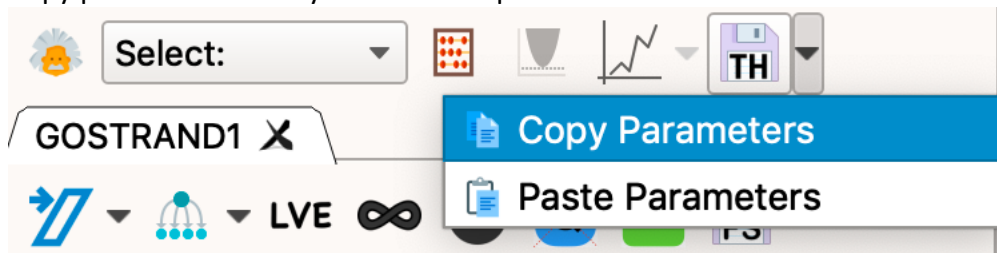
Adjusting the view

- Click 'show/hide' toolbar' (top right corner underneath the views selector)

- Click the 'Edit axis' button ( ) to bring up the axis properties
- Change the Y-Axis: Top value to '1e-8'
- Click 'Apply' or 'Ok'

## Comparing with the 'average stress model'

- Copy parameters from your data comparison above

- Create a new GO-polyStrand model
- Paste the model parameters. (This create an identical copy of the model above)
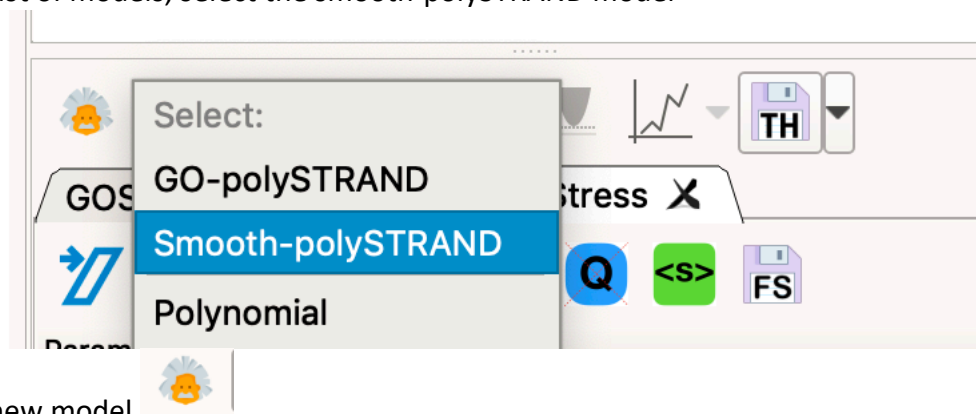- Double click on the name of theory and rename it to 'Average Stress'
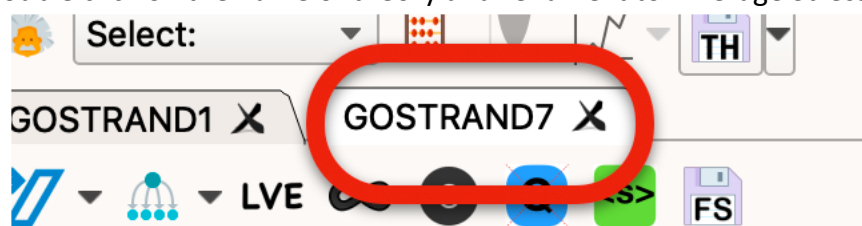
- Click the 'average stress' button and run the model
- Towards the top of the window click 'View All Theories' to show both theories on the same plot.
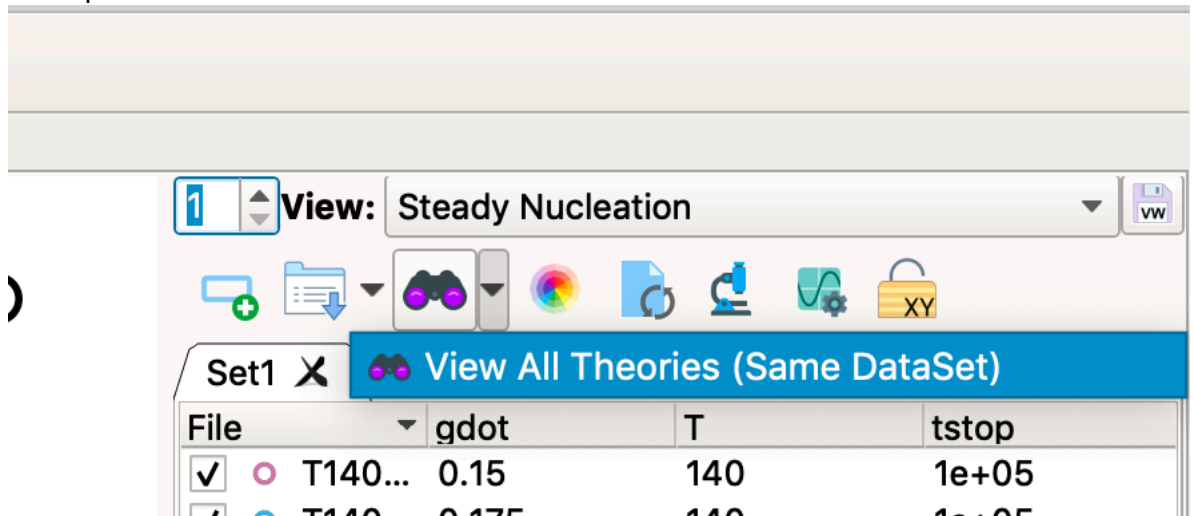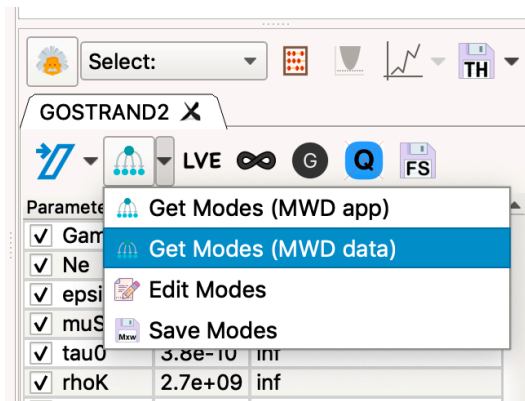

Comparing with the smooth-polySTRAND model

- From the list of models, select the smooth-polySTRAND model

- And click new model
- Add modes as before: Click 'Get modes MWD data'

- In the pop-up window set Me=4400, tau_e=9.0E-8 and the number of modes to 10

In a text editor, open 'T30G_10modes.mwd' and copy whole file contents to the clipboard.

- Click on the first element of the table and paste the copied file (use ctrl-v or a similar keyboard shortcut)

- Scroll down to the last mode and increase it from 1.9e8 to 3e8

Close the mode window by clicking 'Ok'

- Back in the theory window, turn on the modulus correction button and set Gamma=4.3 and GNO=5.06E5.
- Other parameters default to the correct values, here's a full list.
    - Gamma   4.3
    - Kappa0   0.1
    - Qs0   30
   - Ne   25
    - epsilonB   0.044
    - muS   0.94

- tau0   7.4e-10
- rhoK   2.7e+09
- G_C   0.063
- N_0   0

The values of epsilonB and muS are different to the GO-polyStrand model comparison because the roughness penalty changes the quiescent barrier. These parameters produce the same quiescent barrier for the two models.

- Click 'View All Theories' as above.

## Comparing with experiments at 144°C

- Double click on the Crystal application tab and rename this to '140oC'
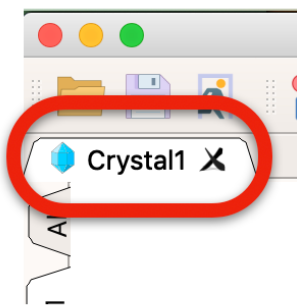
- Open a new Crystal Application and rename this to '144oC'
- In the '144oC' application reduce the number of views to 1
- Go back to the folder with the experimental data in ('CoccorulloMacromolcules2008') and drag all files that begin T144 onto the Reptate window
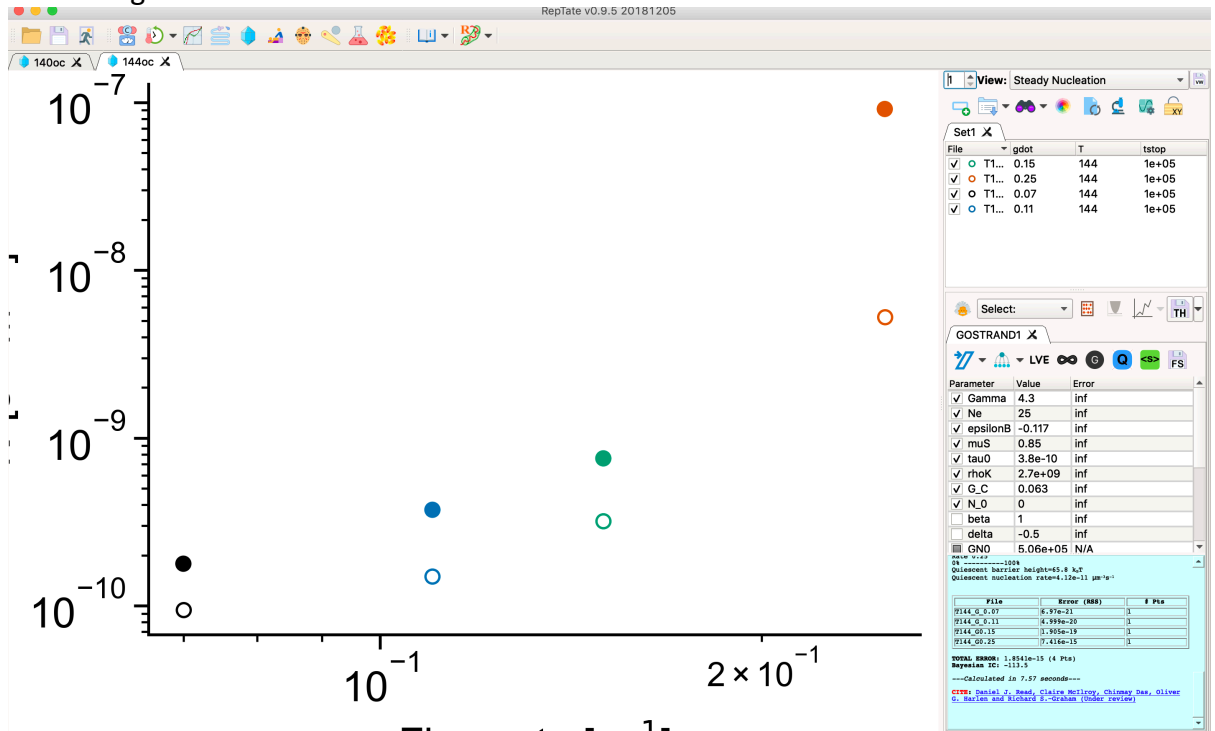- Make this view 'Steady Nucleation'

- Create new GO-polySTRAND theory
- Go back to the '140oC' tab, return to the GO-polySTRAND model and copy the GO-model parameters
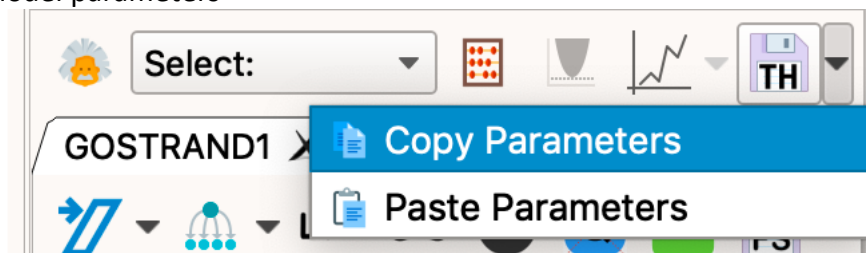

- Return to 144 and paste these parameters onto the theory
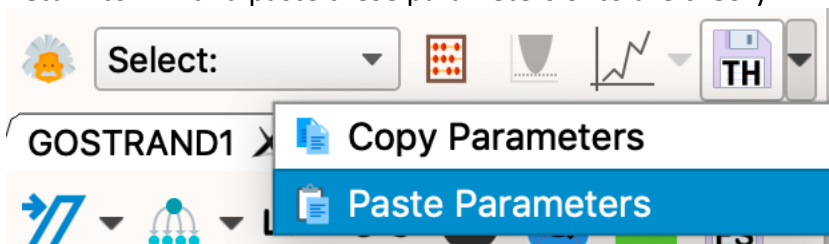
- Run the model to confirm that this gives the predictions for 140. You should see something like

- Change epsilonB to -0.118

- Rerun the model to get improved agreement.
- Repeat the steps above to make an 'Average Stress' model
- Create a new smooth-PolySTRAND model, copy the parameters for this model from 140°C into this new model and change epsilonB to 0.0429 to give reasonable agreement for all rates.
- Repeat all of the above steps to create new tab for the data at 138°C. For the GO-polySTRAND model use epsilon=-0.01146 and for 0.0463 for the smooth-polyStrand model.

Things to try

- Change Gamma to adjust the sensitivity to shear
- Make *small* changes to epsilonB to adjust the quiescent barrier (equivalent to changing temperature)
- Adjust tau0 to scale all nucleation rates
- Change the molecular weight distribution by clicking 'Get modes (MWD data)' and changing the Molar Mass values (M) by hand. You can also change phi but this needs to add up to 1.
- For the smooth polystrand model try changing Qs0.
- For the GO-polyStrand model, increase the resolution of the molecular weight distribution by copy/pasting the modes from the file 'T30G.mwd' (this has 23 modes, should give similar results and will take a 4 mins to calculate)