Determining the validity of Guinier analysis in slit-smeared small angle scattering data

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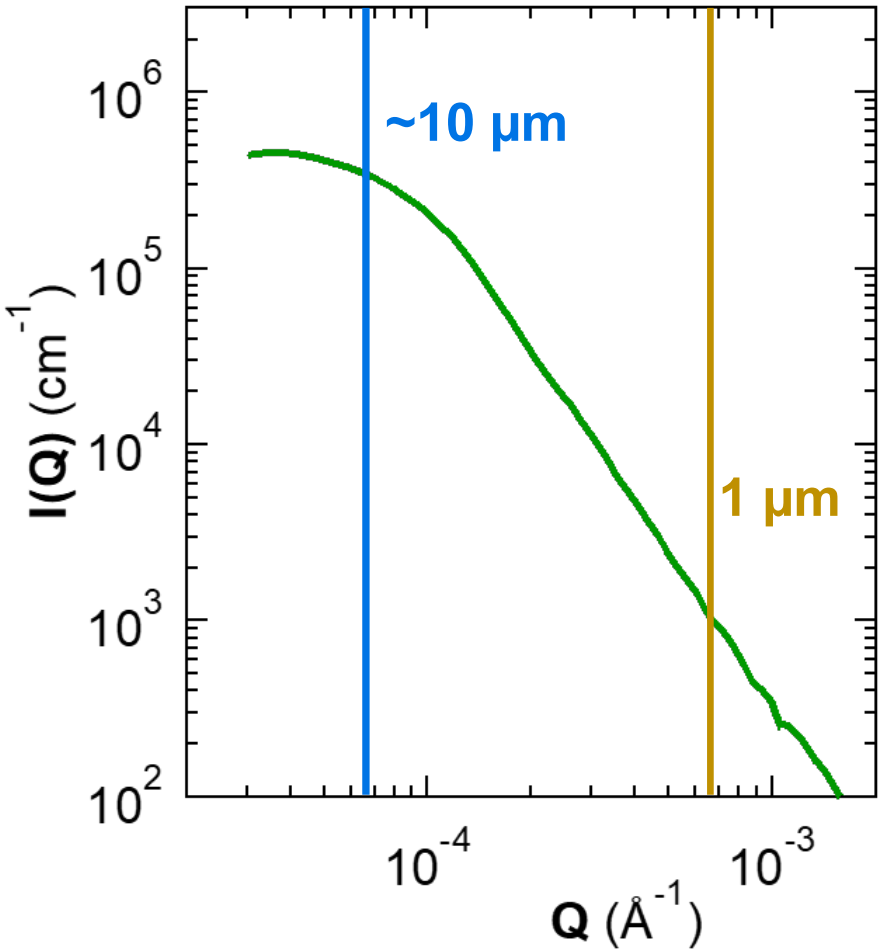
Background Information

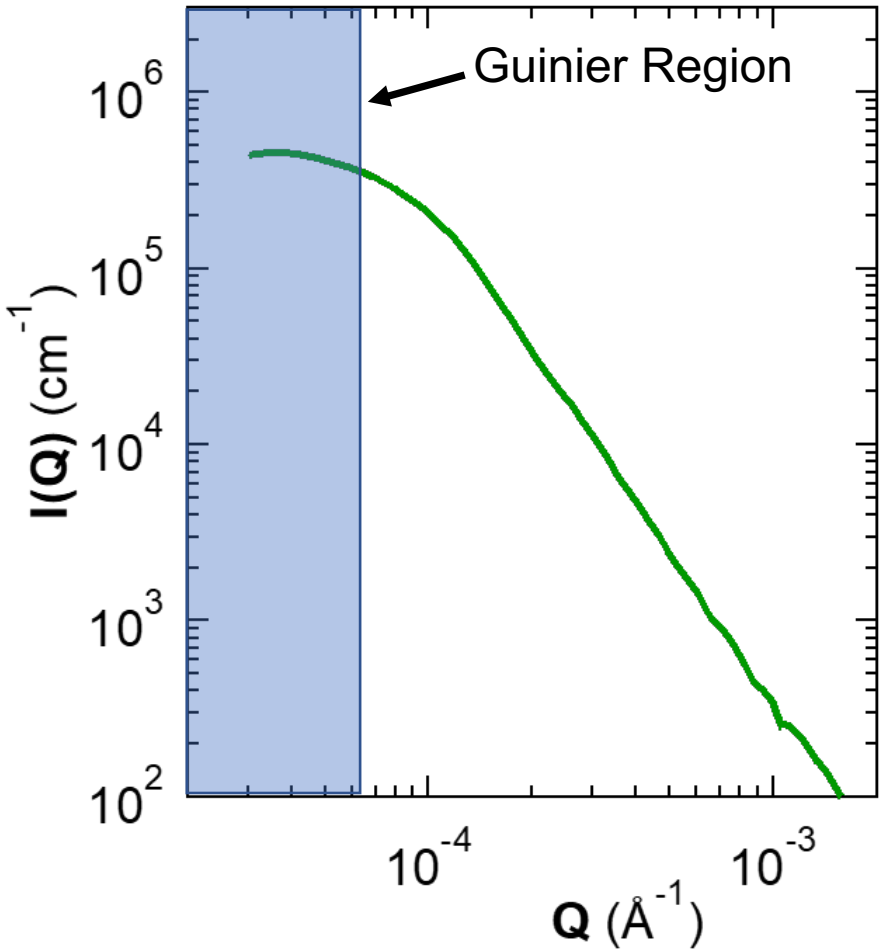
Small Angle Scattering is a powerful technique for investigating large scale particles or structures

larger structures ⟷ *smaller structures*



- High Q
  - Smaller length scales
  - Shape of individual particles
- Low Q
  - Larger length scales
  - Plateau or peak
  - Overall size and structure

Guinier analysis is a shape independent method for analyzing data

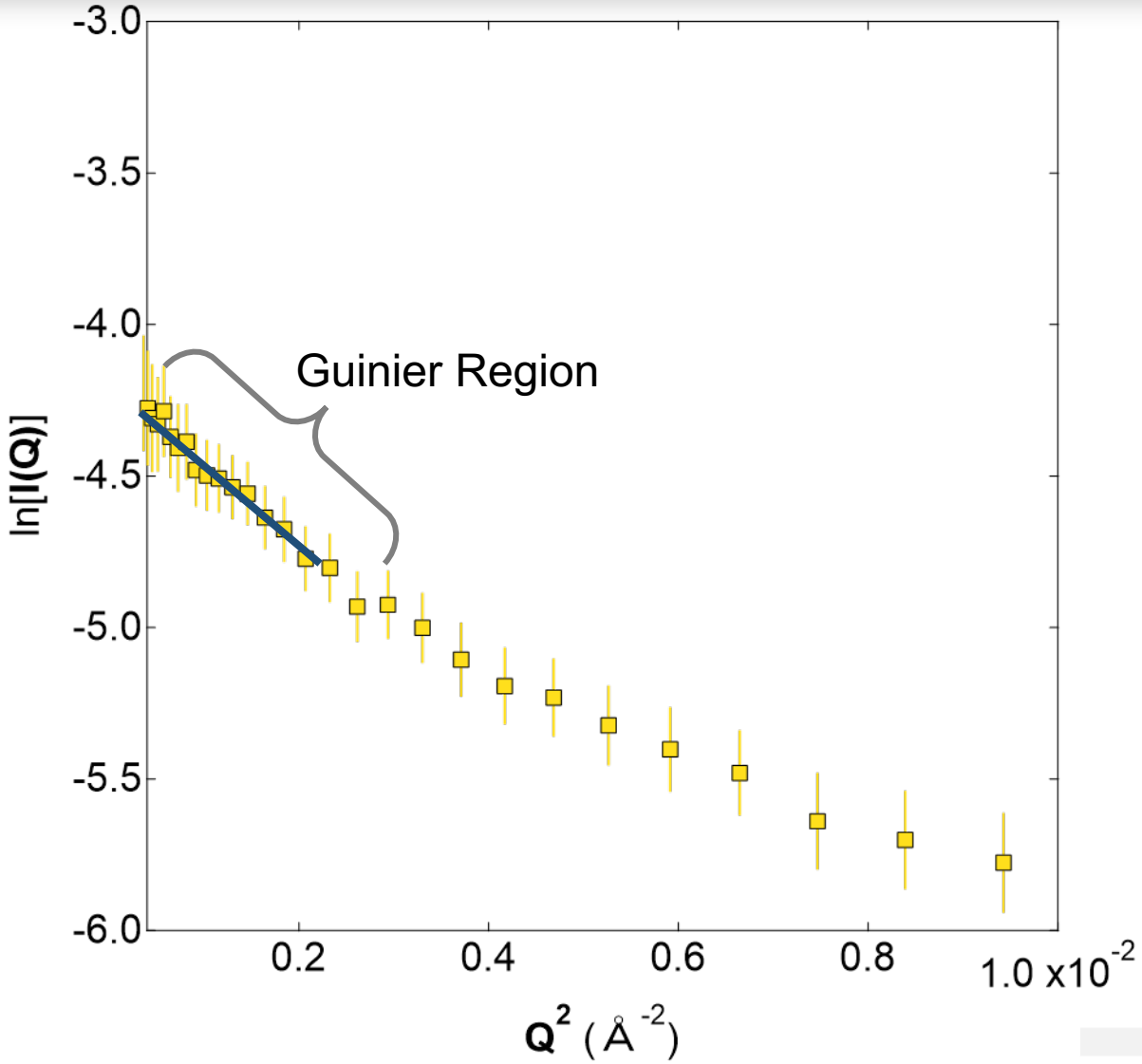


Radius of gyration, R_g

Guinier approximation

$$I(Q) - I_{bgd} = I_0 e^{\frac{-1}{3}R_g^2 Q^2}$$

Guinier plot $\ln[I(Q)]$ vs Q^2



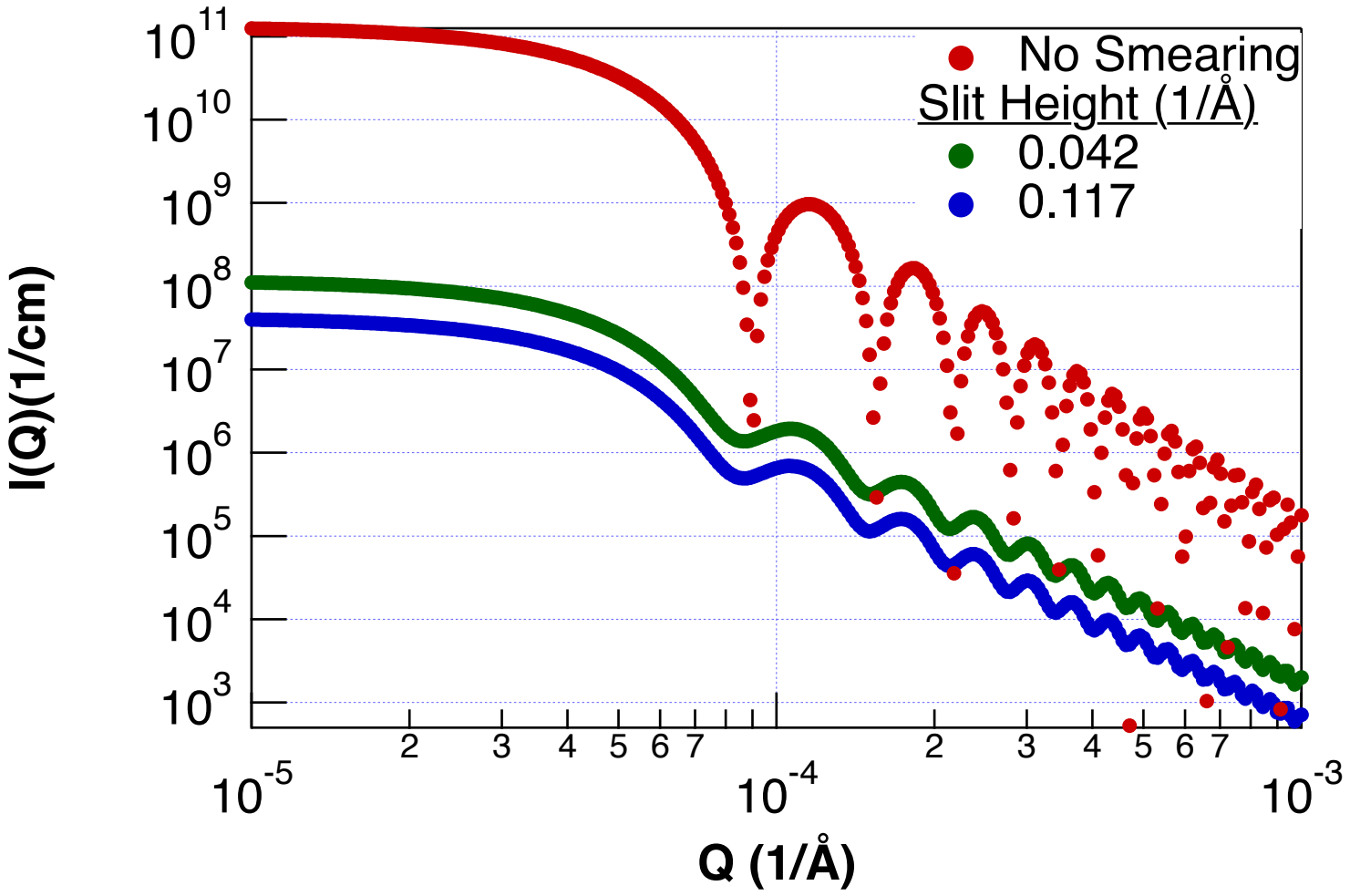
$$I(Q) - I_{bgd} = I_0 e^{\frac{-1}{3}R_g^2 Q^2}$$

$$\ln\left[I(Q) - I_{bgd}\right] = \ln I_0 - \frac{1}{3}R_g^2 Q^2$$

$$Slope = -\frac{1}{3}R_g^2$$

$$Intercept = \ln[I_0]$$

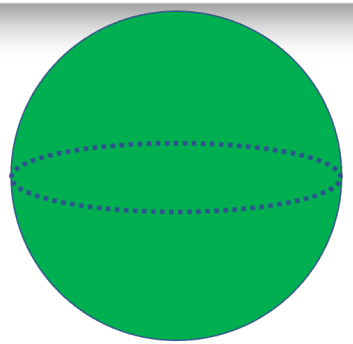
Slit-smearing is an instrument geometry effect



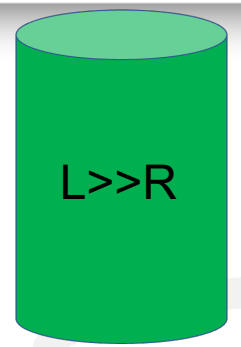
- Slit geometry enables access to very low Q values
  - USAXS
  - USANS
- Slit geometry causes an effect known as slit-smearing

Approach to evaluating Guinier analysis on slit-smeared data

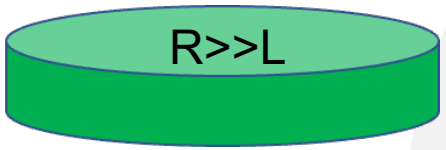
- Guinier analysis is a useful tool for understanding scattering data
- Slit-smearing causes distortions to data that can influence results from a Guinier fit
- We simulated data from four generic shapes with and without slit-smearing
- Performed Guinier analysis on both data sets and compared fit results and true values defined in the simulation



$$R_g = \sqrt{\frac{3}{5}}R$$



$$R_g = \sqrt{\frac{L^2}{12} + \frac{R^2}{2}}$$



$$R_g = \sqrt{\frac{L^2}{12} + \frac{R^2}{2}}$$

$$R_g = \frac{1}{6}Nb^2$$

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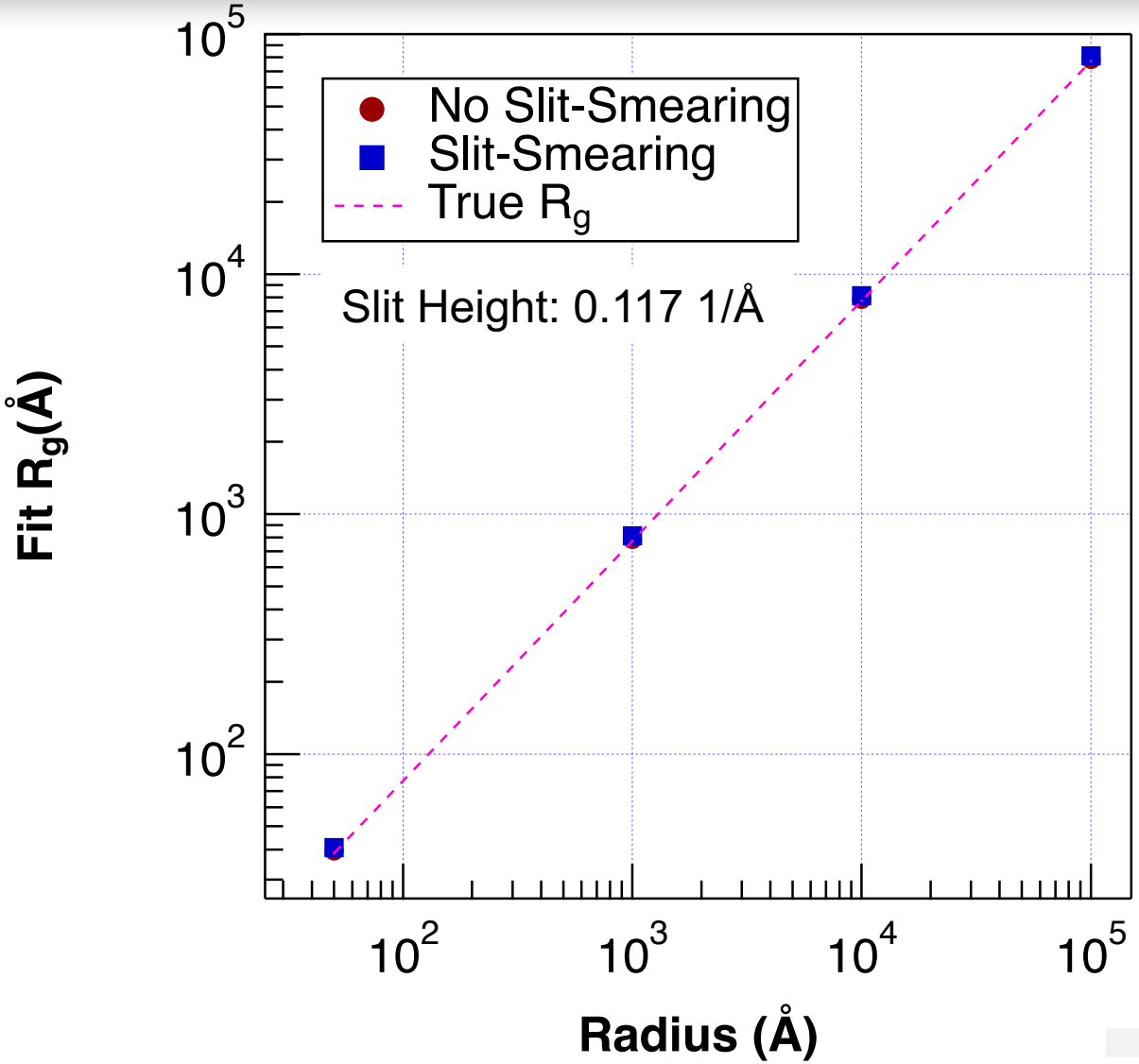
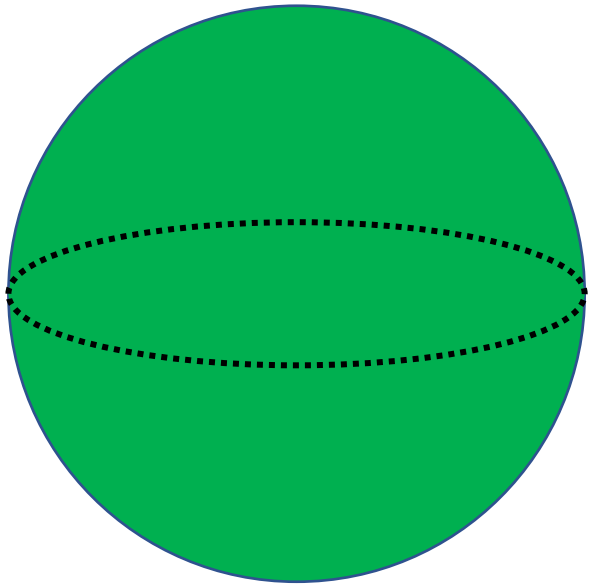
Results

Good agreement between fit R_g and true R_g for spherical model

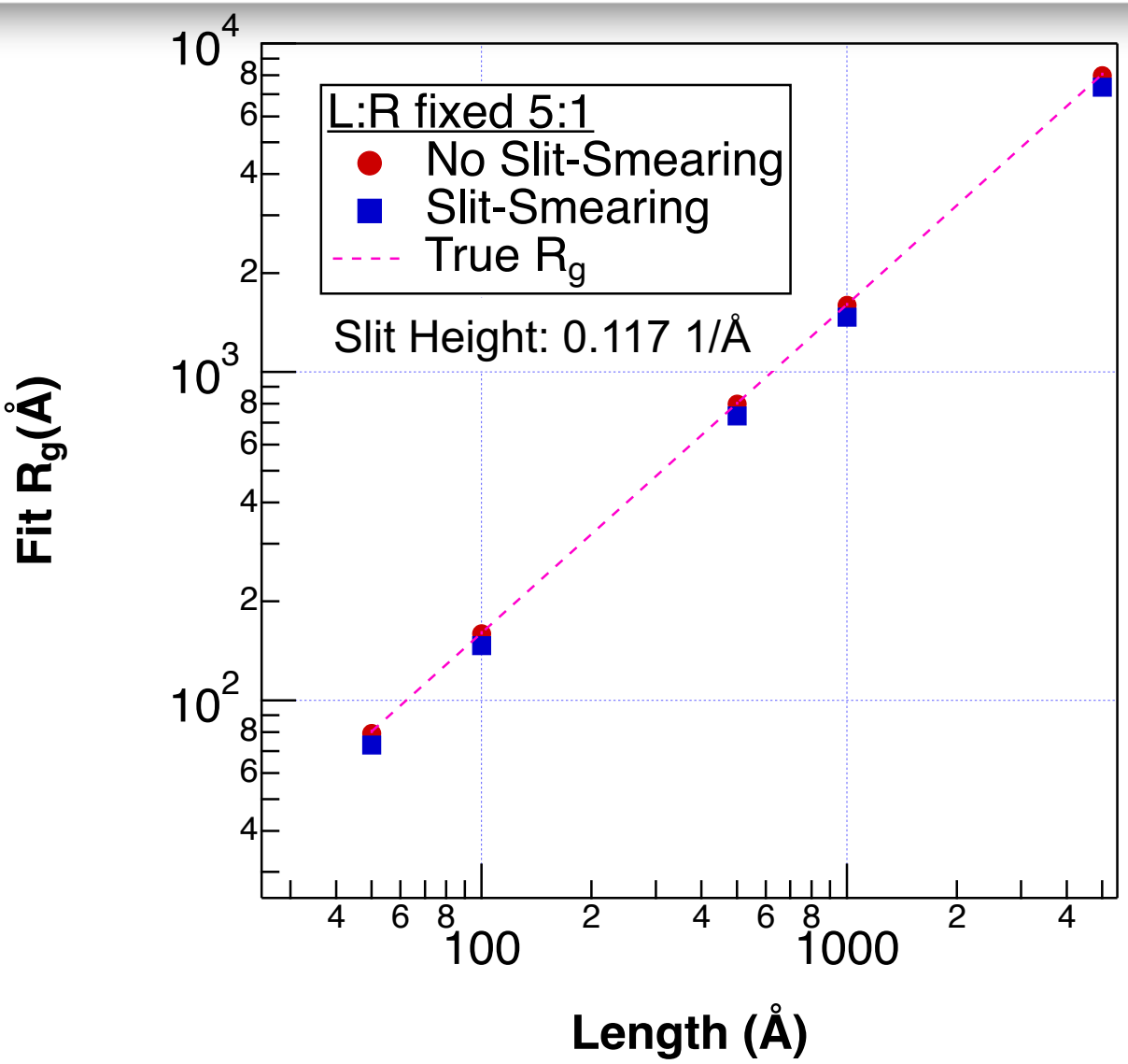


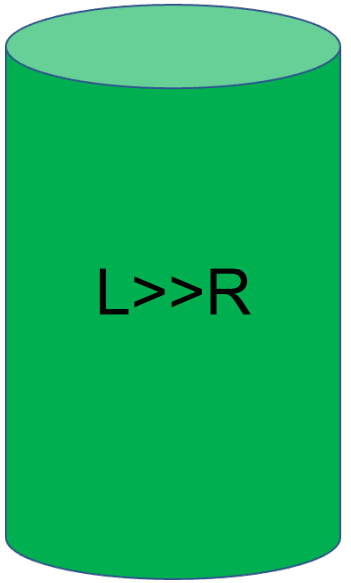


$$R_g = \sqrt{\frac{3}{5}}R$$

- Slit-smeared data seems to show good agreement
- Error between 1% – 5%

Cylinder seems to have good agreement between fit R_g and true R_g with small aspect ratio

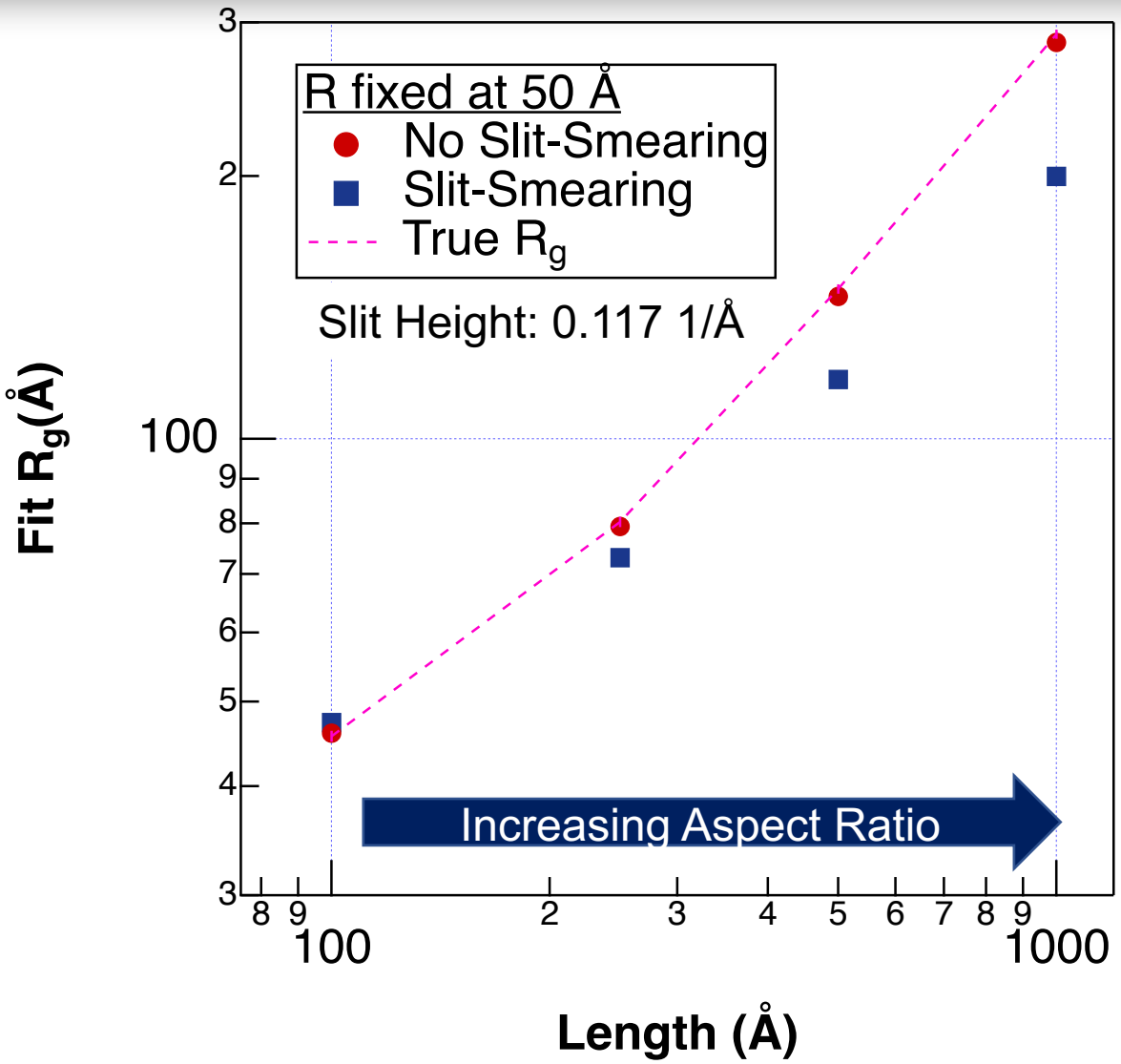


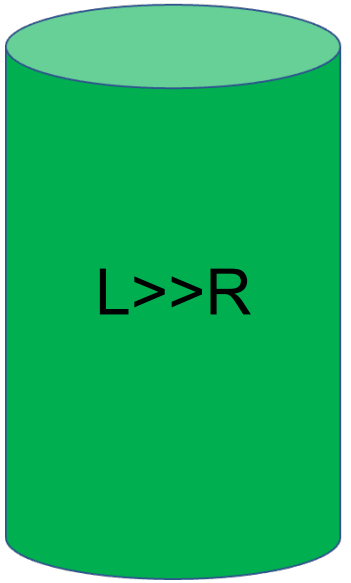


$$R_g = \sqrt{\frac{L^2}{12} + \frac{R^2}{2}}$$

- Fit results seem to have good agreement
- Error under 10%

Cylinder model has increasing deviation between fit R_g and true R_g value as aspect ratio increases

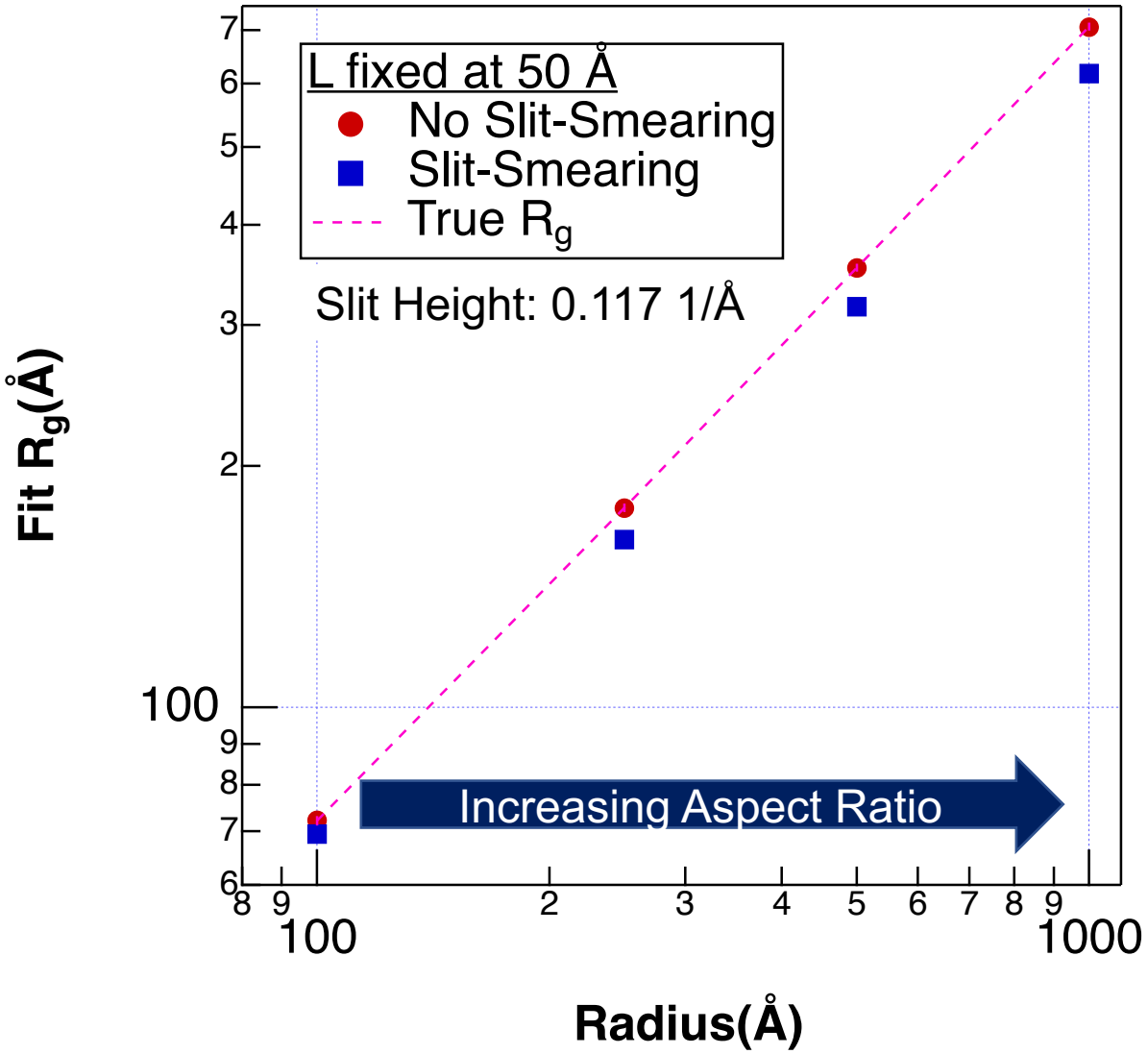


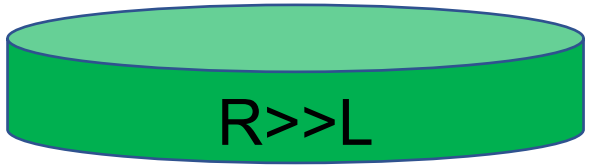


$$R_g = \sqrt{\frac{L^2}{12} + \frac{R^2}{2}}$$

- Larger aspect ratios show more deviation
- Error between 15% – 20%

Disc model has similar trends as cylinder but with less overall error

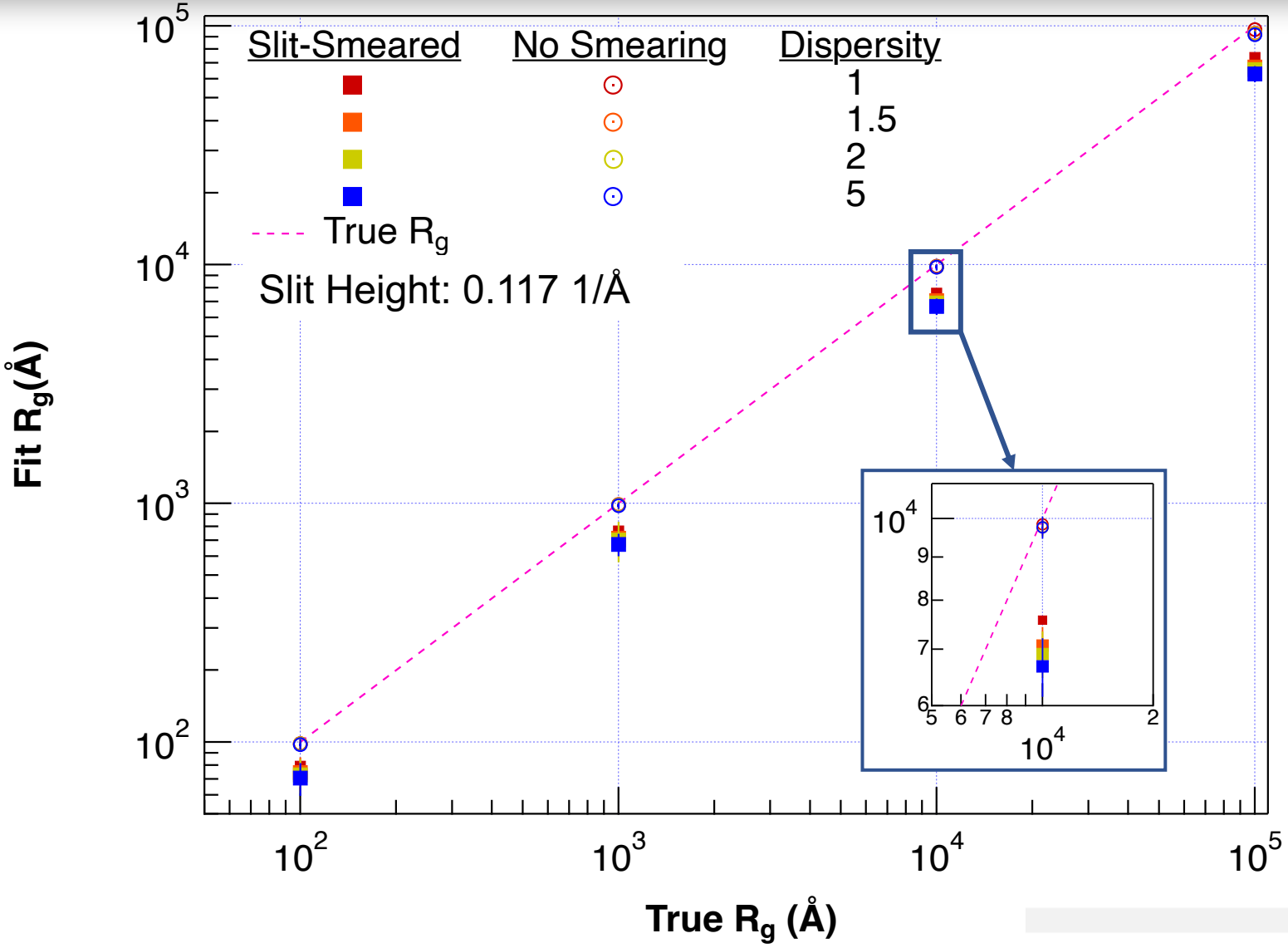


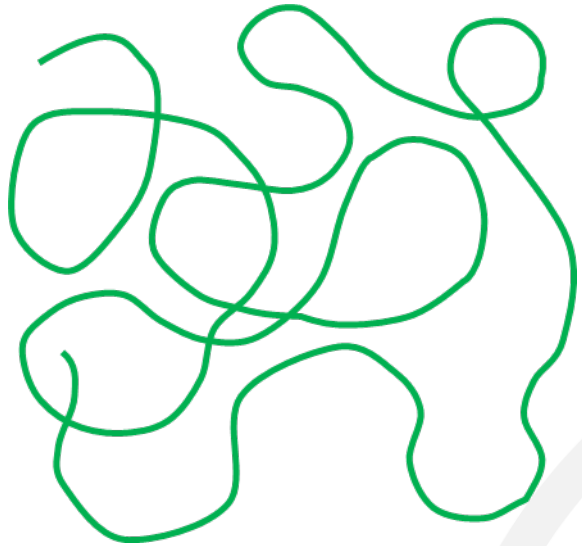


$$R_g = \sqrt{\frac{L^2}{12} + \frac{R^2}{2}}$$

- Observed similar trend as cylinder but less deviation
- Error under 10%

Polymer chain has largest deviation between fit R_g and true R_g out of all models tested





$$R_g = \frac{1}{6} N b^2$$

- Large deviation in results
- Increasing deviation as dispersity increases

Conclusions

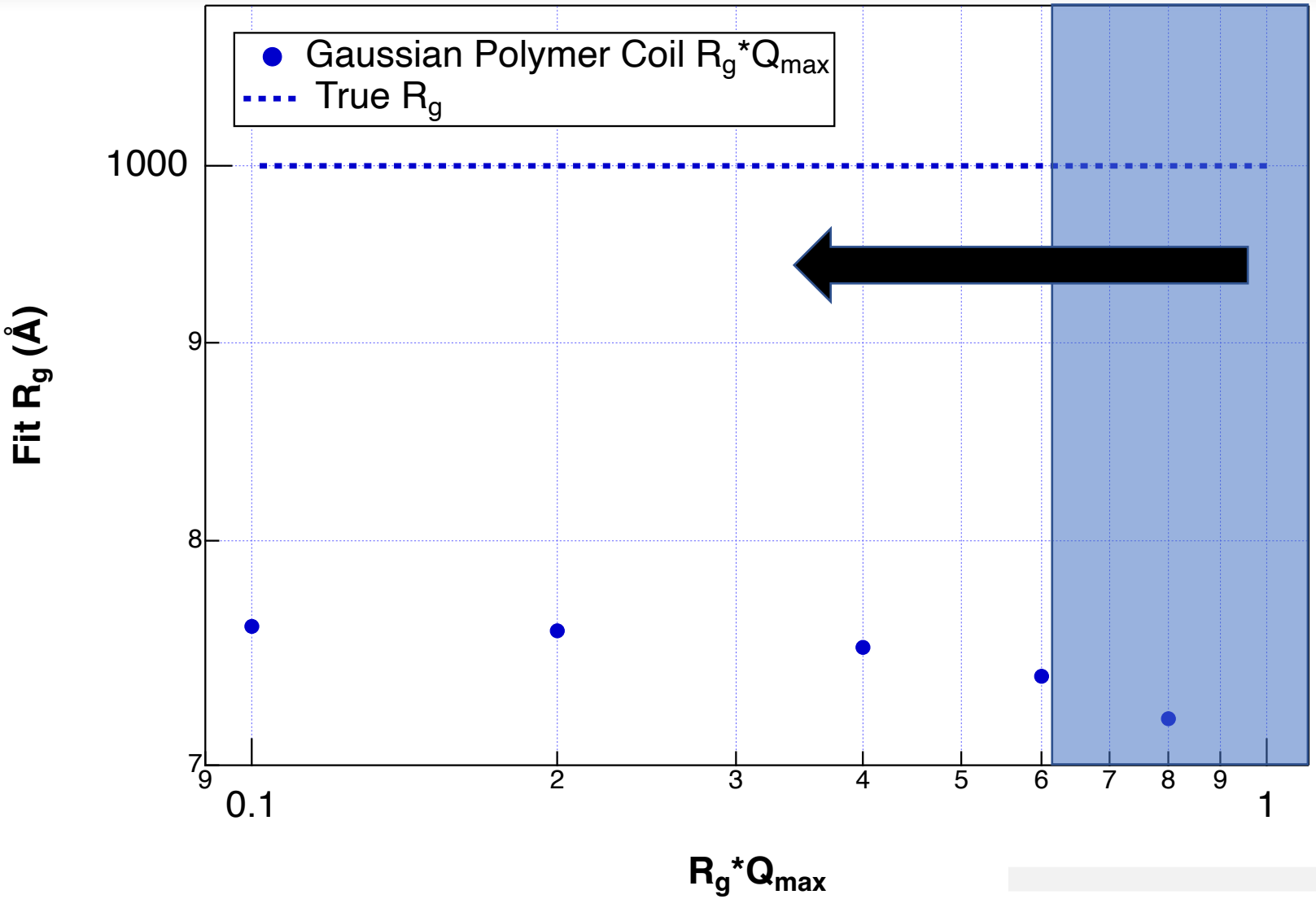
- Evaluated Guinier analysis for slit-smeared data
- Slit-smearing distorts sphere Guinier results the least
- More complex shapes show greater effect of smearing
- Guinier analysis is not ruled out for slit-smeared data, but if using more complex shapes, should be used with caution

Acknowledgements

- Thanks to Rachel Ford, Yun Liu, Julie Borchers, Joe Dura, Susana Teixeira, and all students for a great SURF 2022
- SASView (https://www.sasview.org/)

Backup Slides (Just in case but not used in presentation)

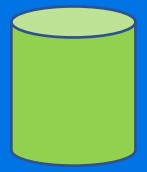
Shrinking Guinier region shows only slight improvement to cylinder with large aspect ratio.

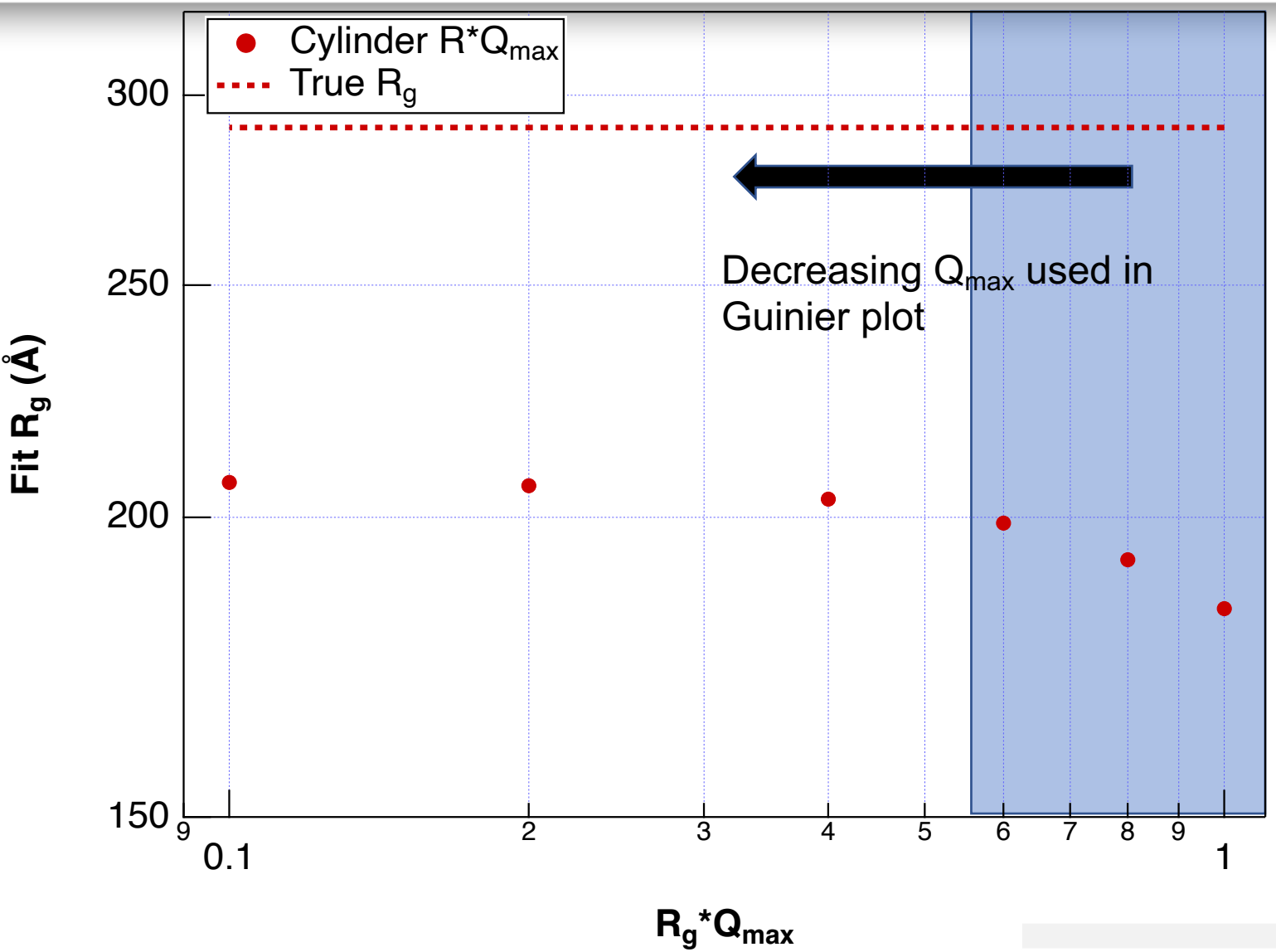


Percent Error: ~30% to ~24%

Decreasing Q_{max} used in Guinier plot

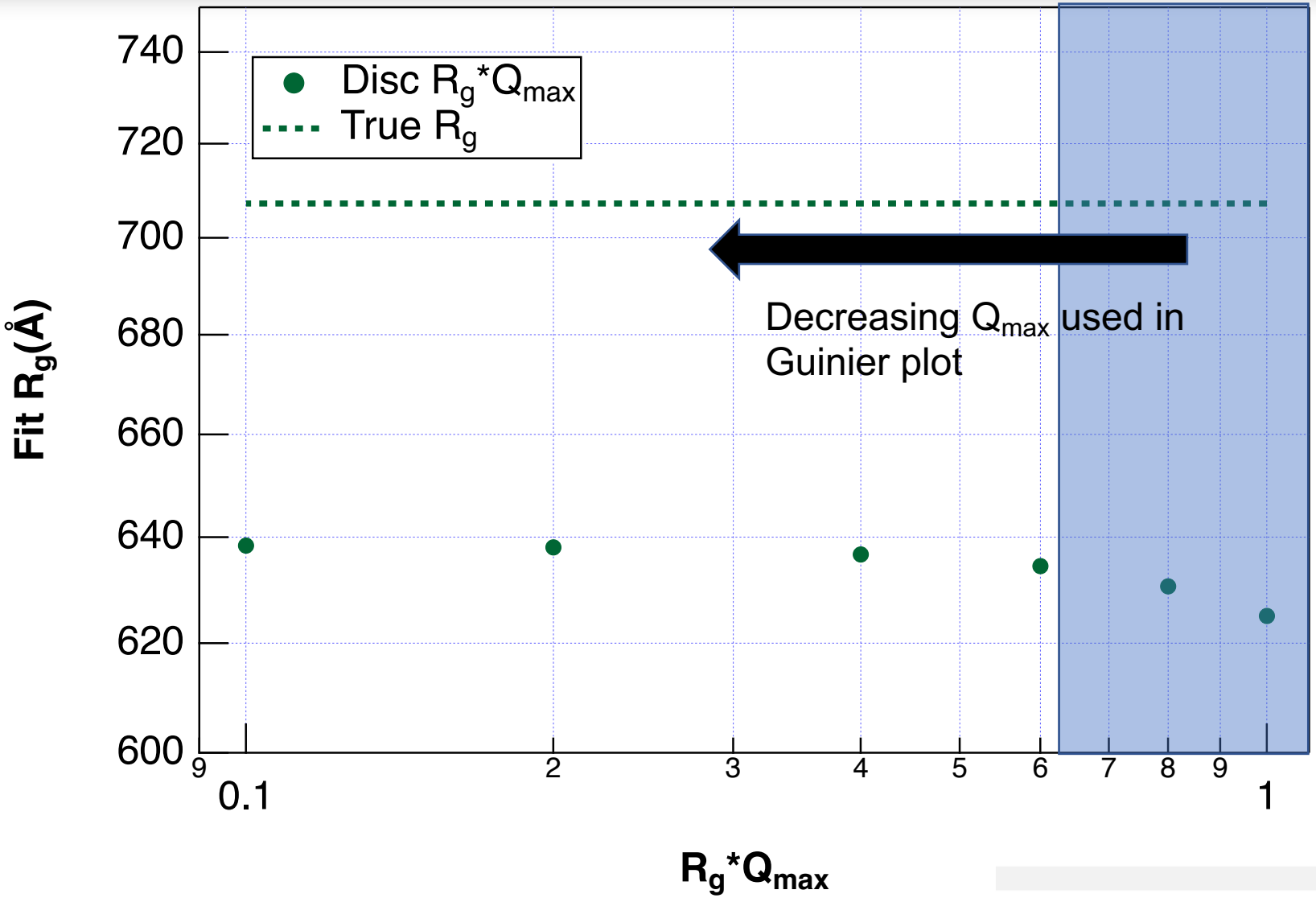
Shrinking Guinier shows only slight improvement to cylinder with large aspect ratio.





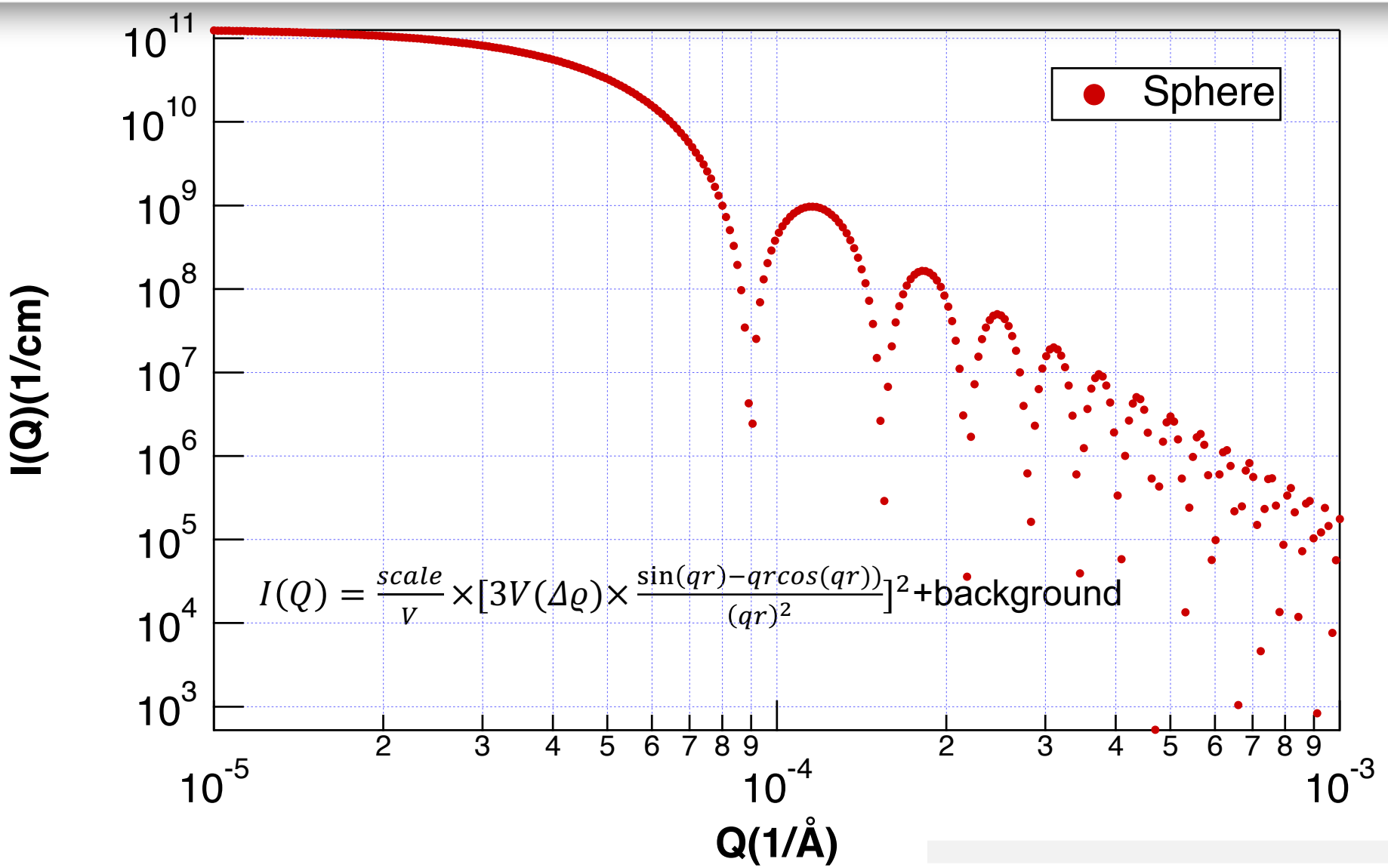
Percent Error: ~37% to ~31%

Shrinking Guinier allows disc with large aspect ratio to be within a reasonable percent error.



Percent Error: ~12% to ~10%

Spherical Model



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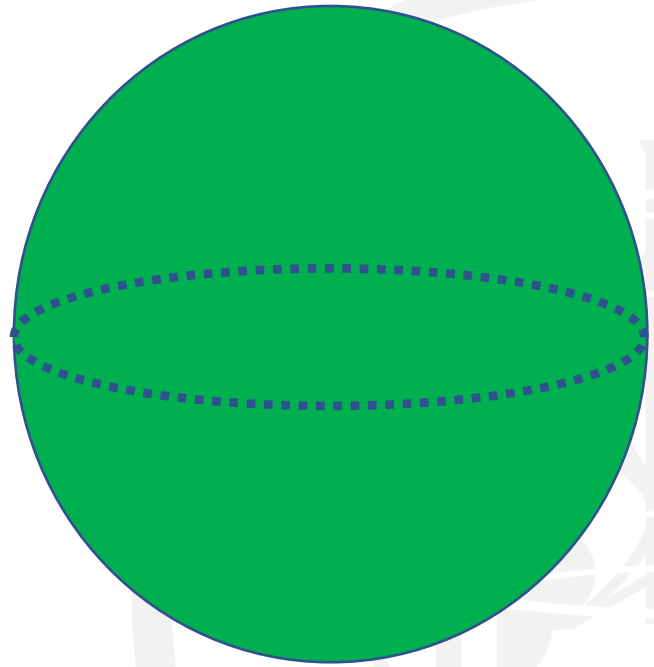
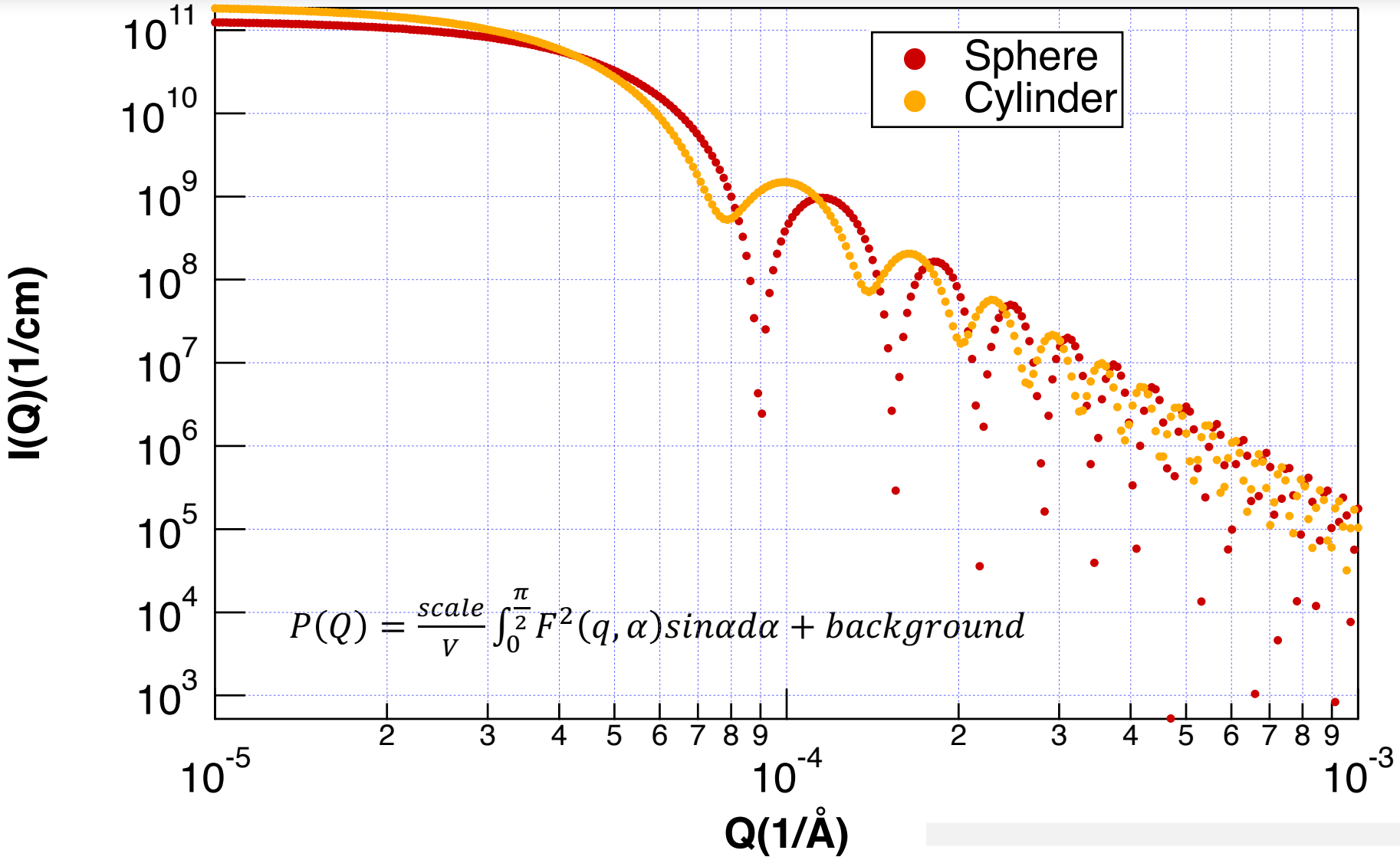
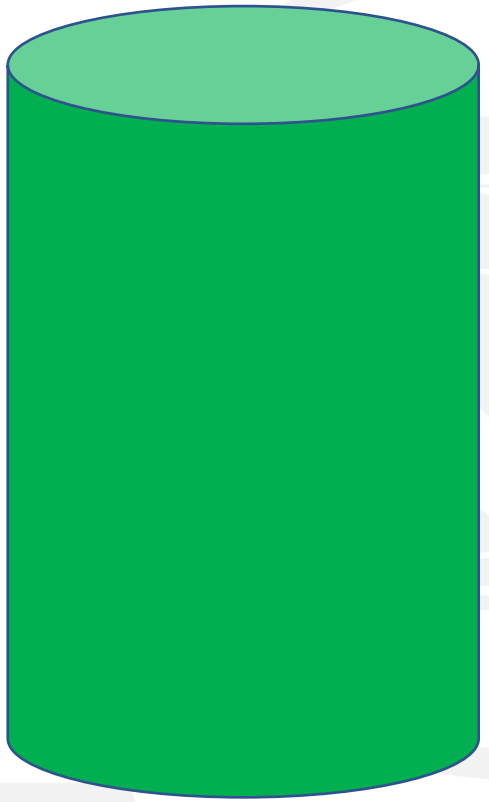


Cylindrical Model

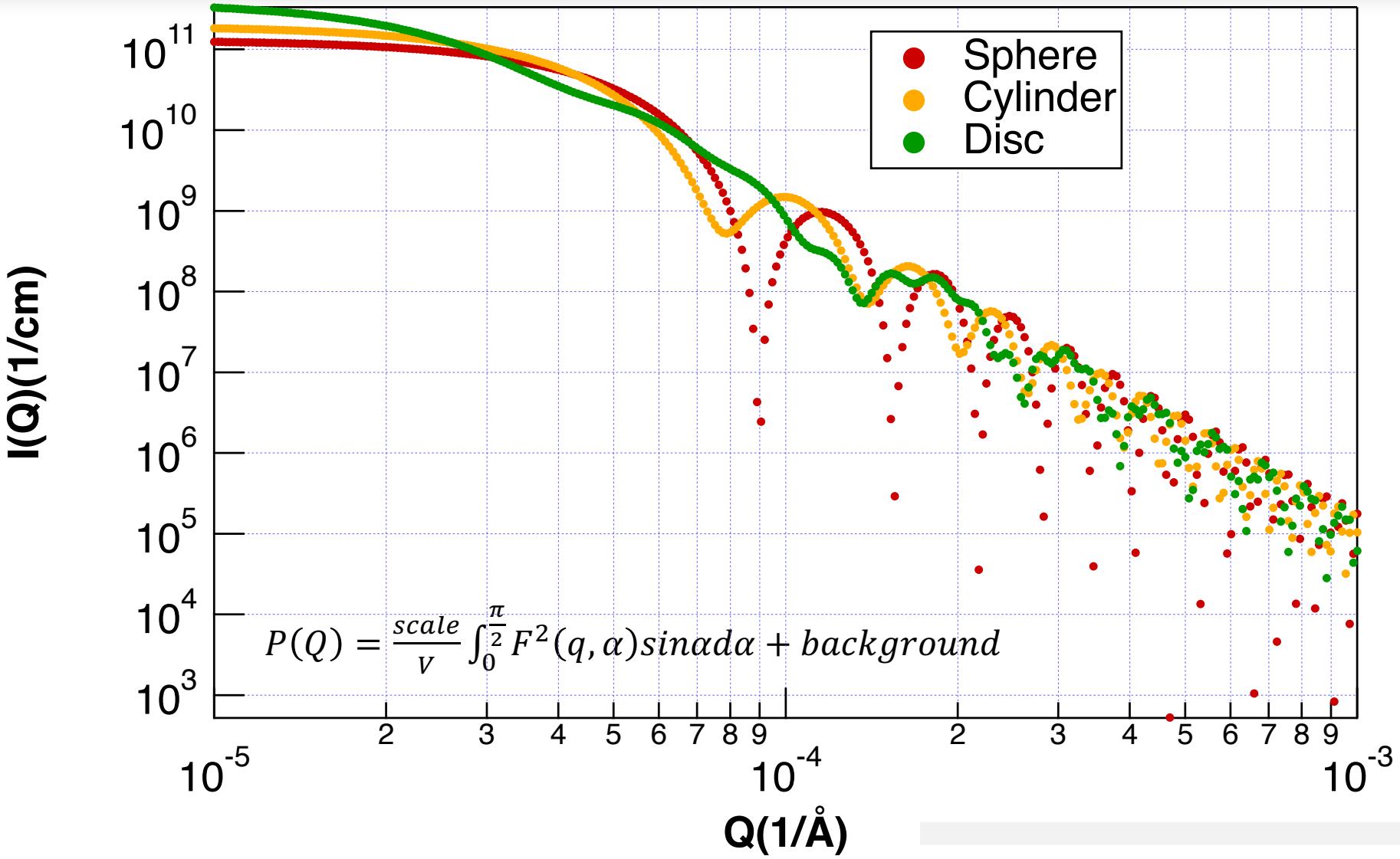


$$R_g = \sqrt{\frac{L^2}{12} + \frac{R^2}{2}}$$

$$L \gg R$$



Disc Model



$$R_g = \sqrt{\frac{L^2}{12} + \frac{R^2}{2}}$$

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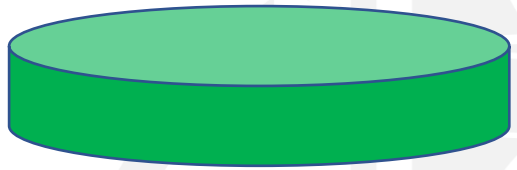
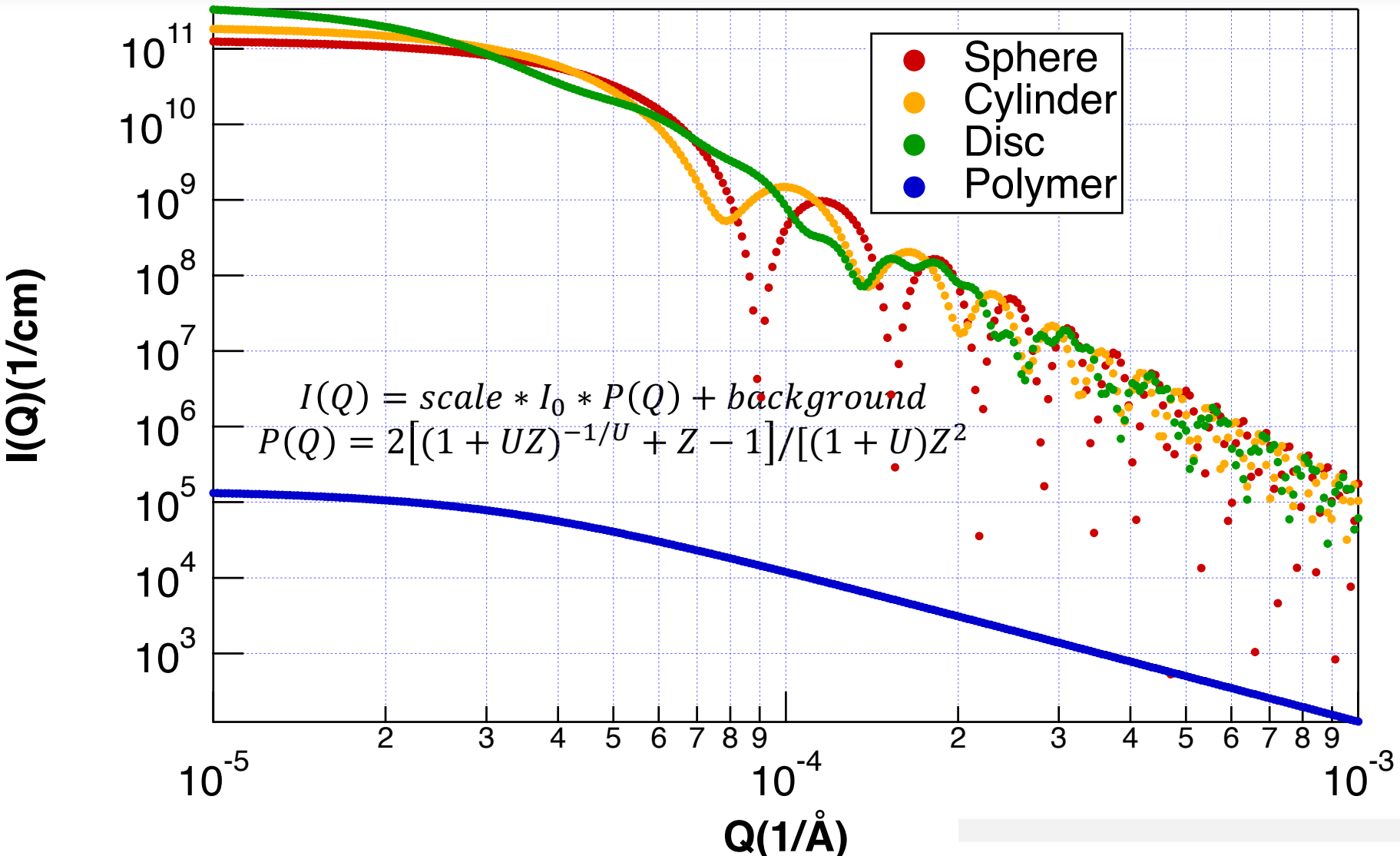
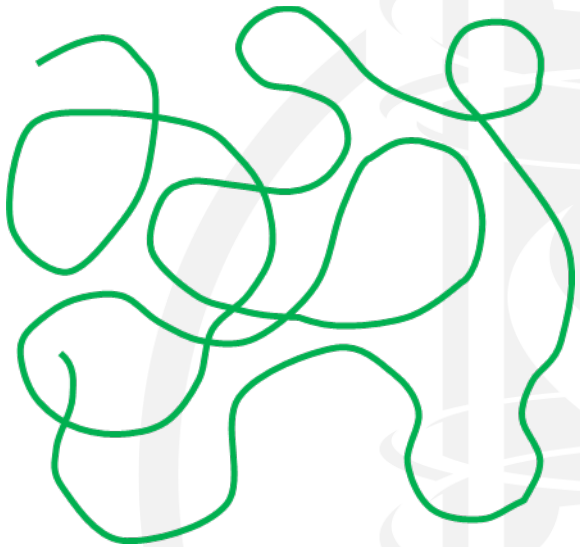


Gaussian Coil Polymer



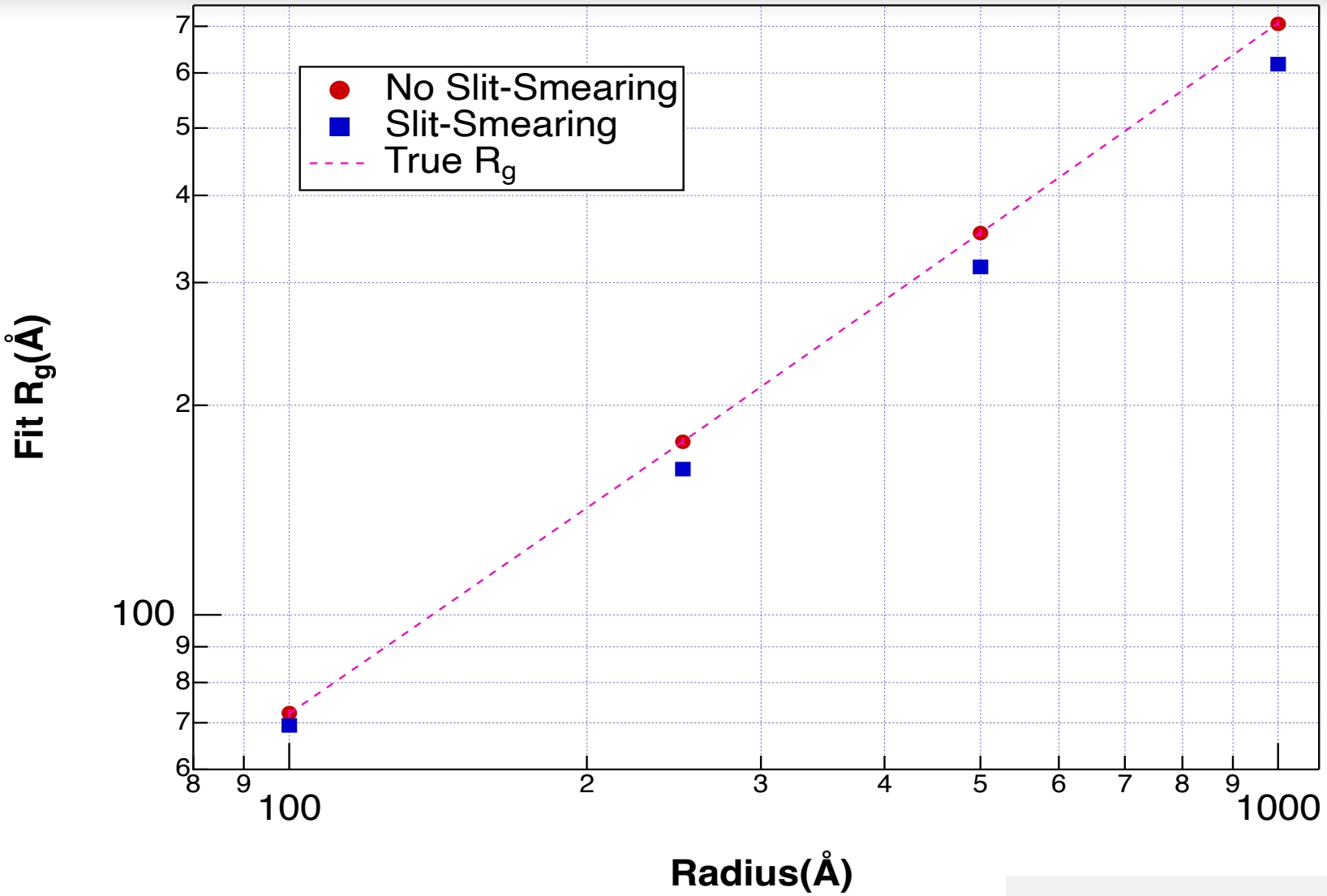
$$U = \left(\frac{M_w}{M_n}\right) - 1$$

$$V = M/(N_A\delta)$$



- Shrinking Guinier plot only slightly improves cylinder and Gaussian polymer coil deviation.

Disc model deviates from true R_g but the effect of slit-smearing is not as drastic in higher aspect ratios.



- Deviation increases as radius increases but the effect of the increasing radius is not as strong.

R>>L