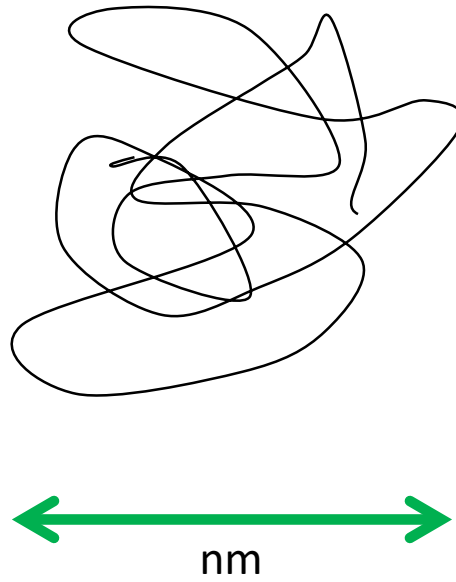


Effect of Nanoparticle Architecture on Mechanical Properties of Polymer Composites

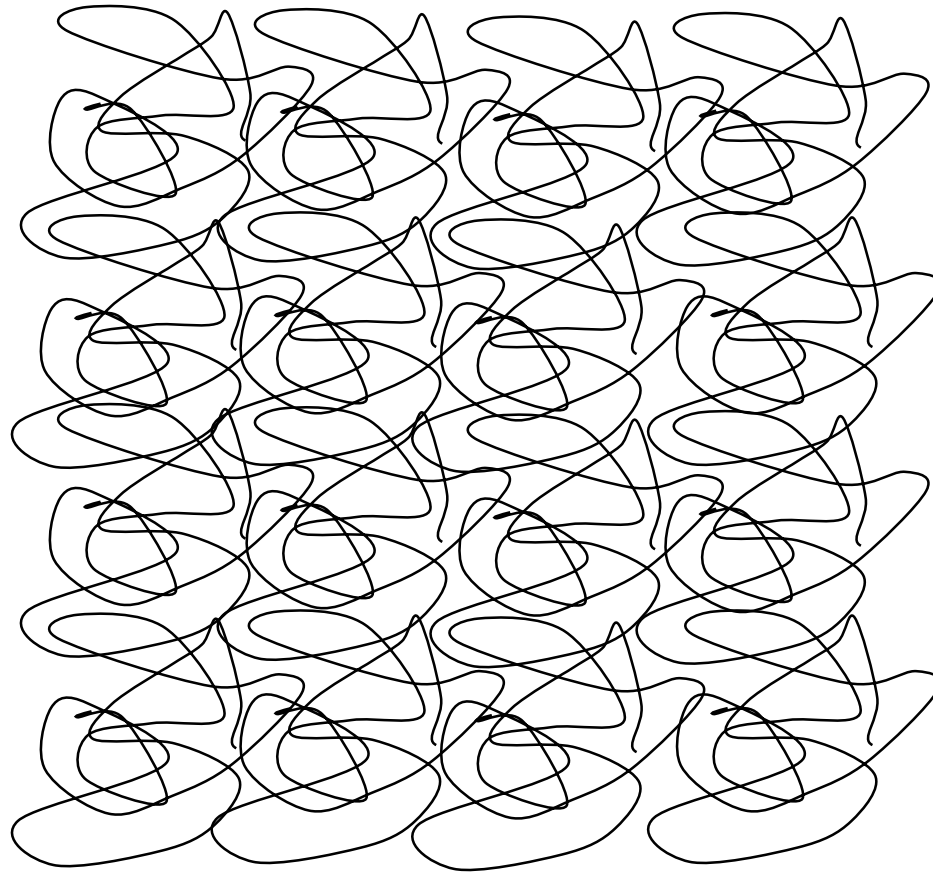
Madeleine Pasco



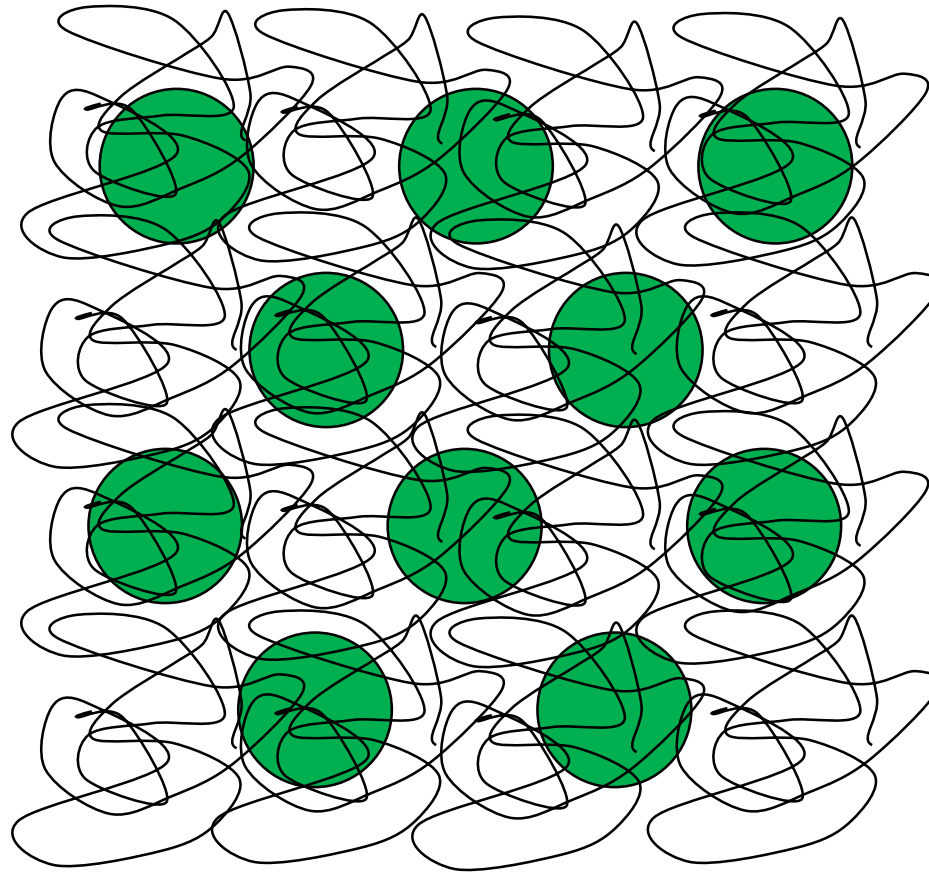
What is a nanocomposite polymer?



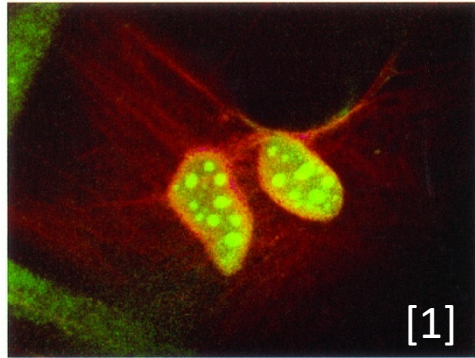
What is a nanocomposite polymer?



What is a nanocomposite polymer?

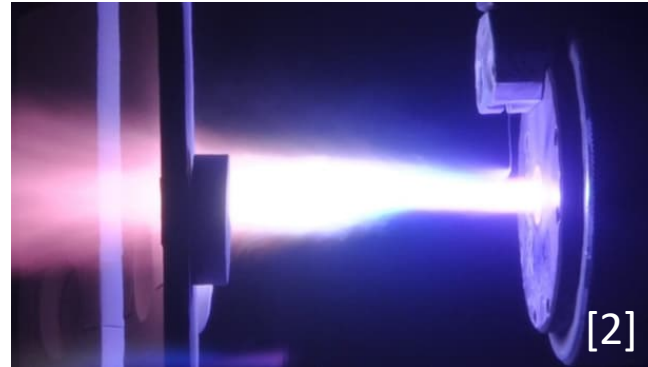


Nanoparticles and nanoparticle-polymer composites have a wide variety of uses and come in a range of shapes and sizes.



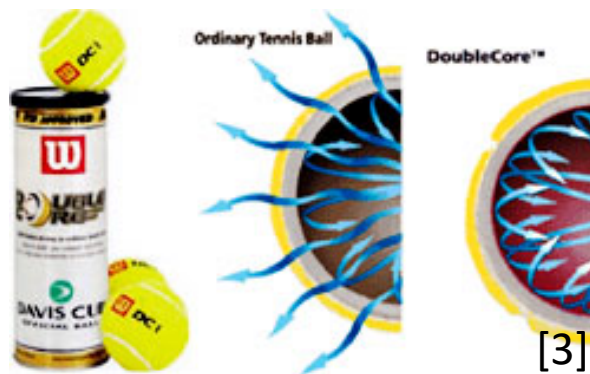
[1]

Biological uses



[2]

Engine coating



[3]

Tennis balls



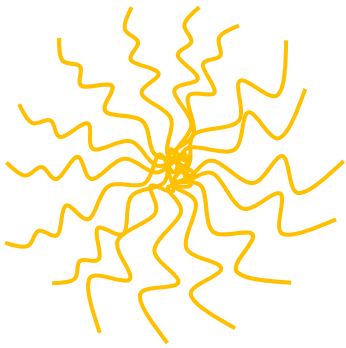
[3]

Deep-penetrating skin cream

[1] M. Bruchez, M. Moronne, P. Gin, S. Weiss, A. Alivisatos. (1998). "Semiconductor Nanocrystals as Fluorescent Biological Labels." *Science*. [2] B. Coxworth. (2014). "Nanoparticle coating could let aircraft engines last three times longer." *Gizmag*. [3] R. Paul. (2003). "The Top Ten Nanotech Products of 2003." *Forbes*.

Certain commercial equipment, instruments, or materials are identified in this paper to foster understanding. Such identification does not imply recommendation or endorsement by the National Institute of Standards and Technology, nor does it imply that the materials or equipment identified are necessarily the best available for the purpose.

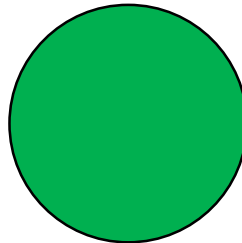
Nanoparticles come in a variety of sizes and shapes. We focused on spherical morphologies.



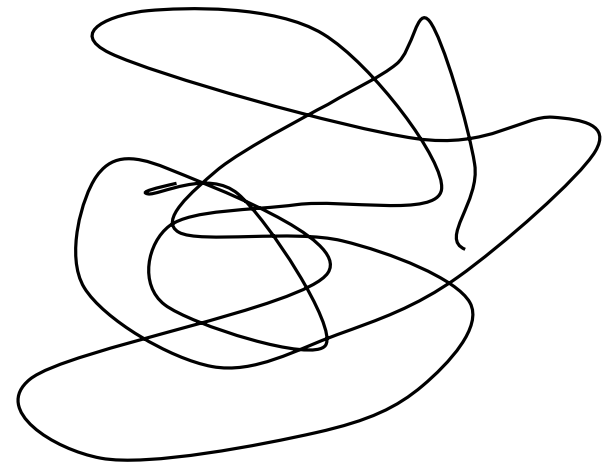
Star PMMA
312 kg/mol



Linear PMMA
100 kg/mol

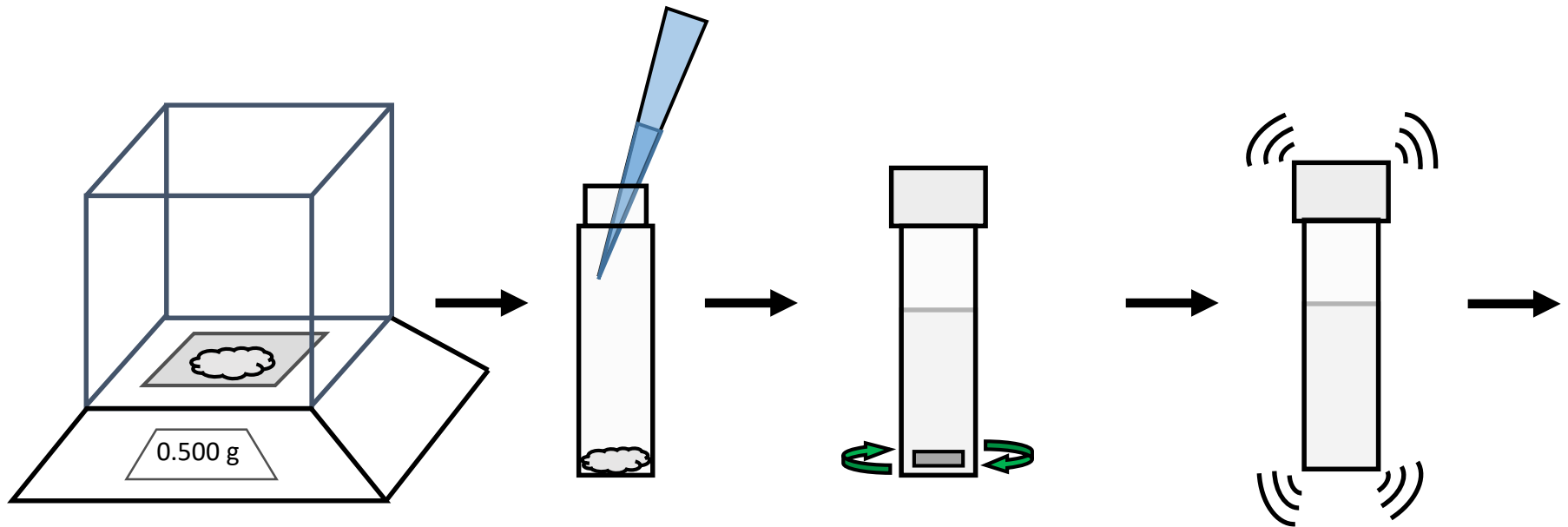


Silica
13 nm diameter

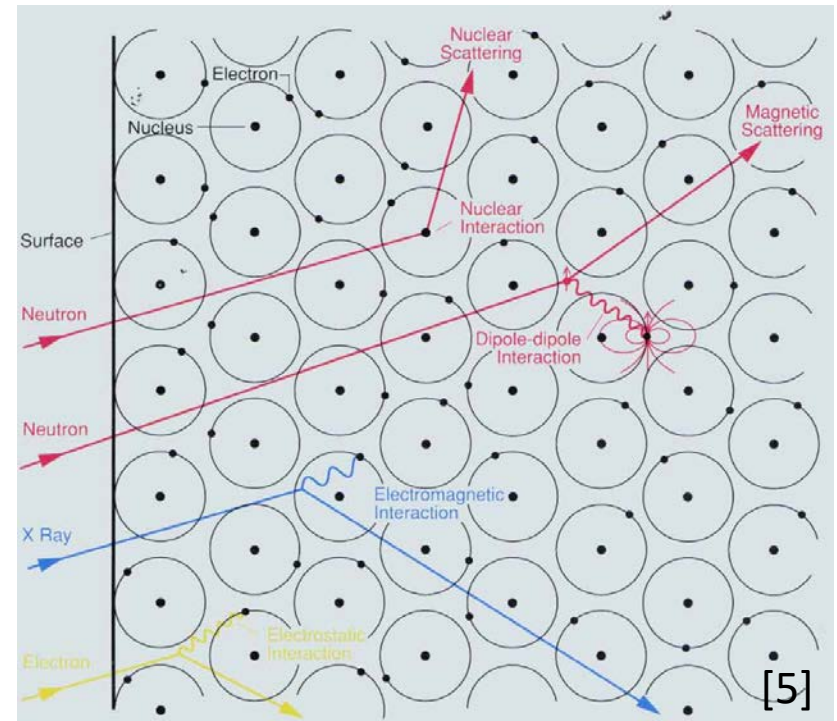
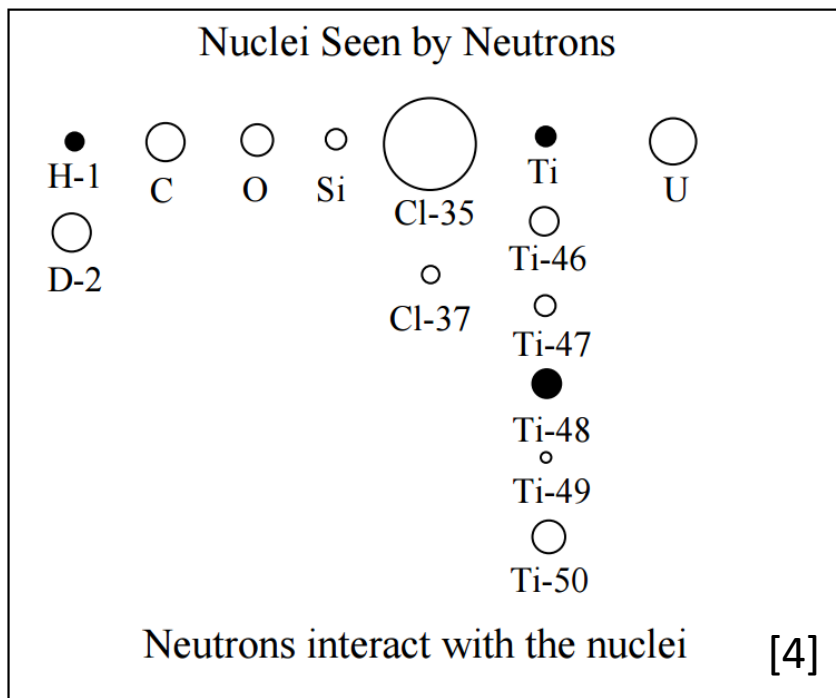
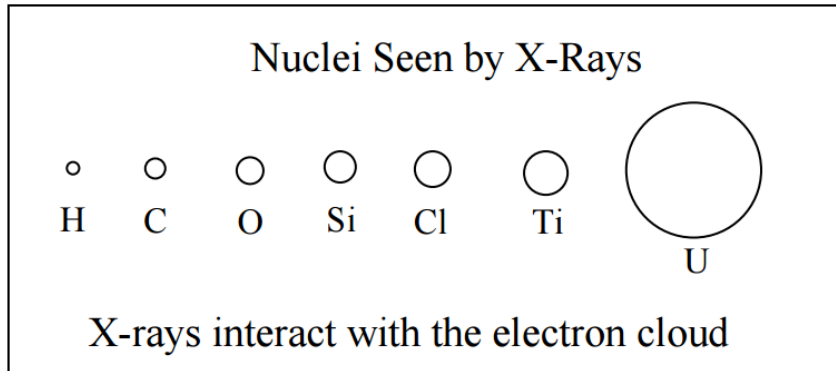


PEO
200 kg/mol

Samples are prepared to get an even distribution of nanoparticle in polymer.

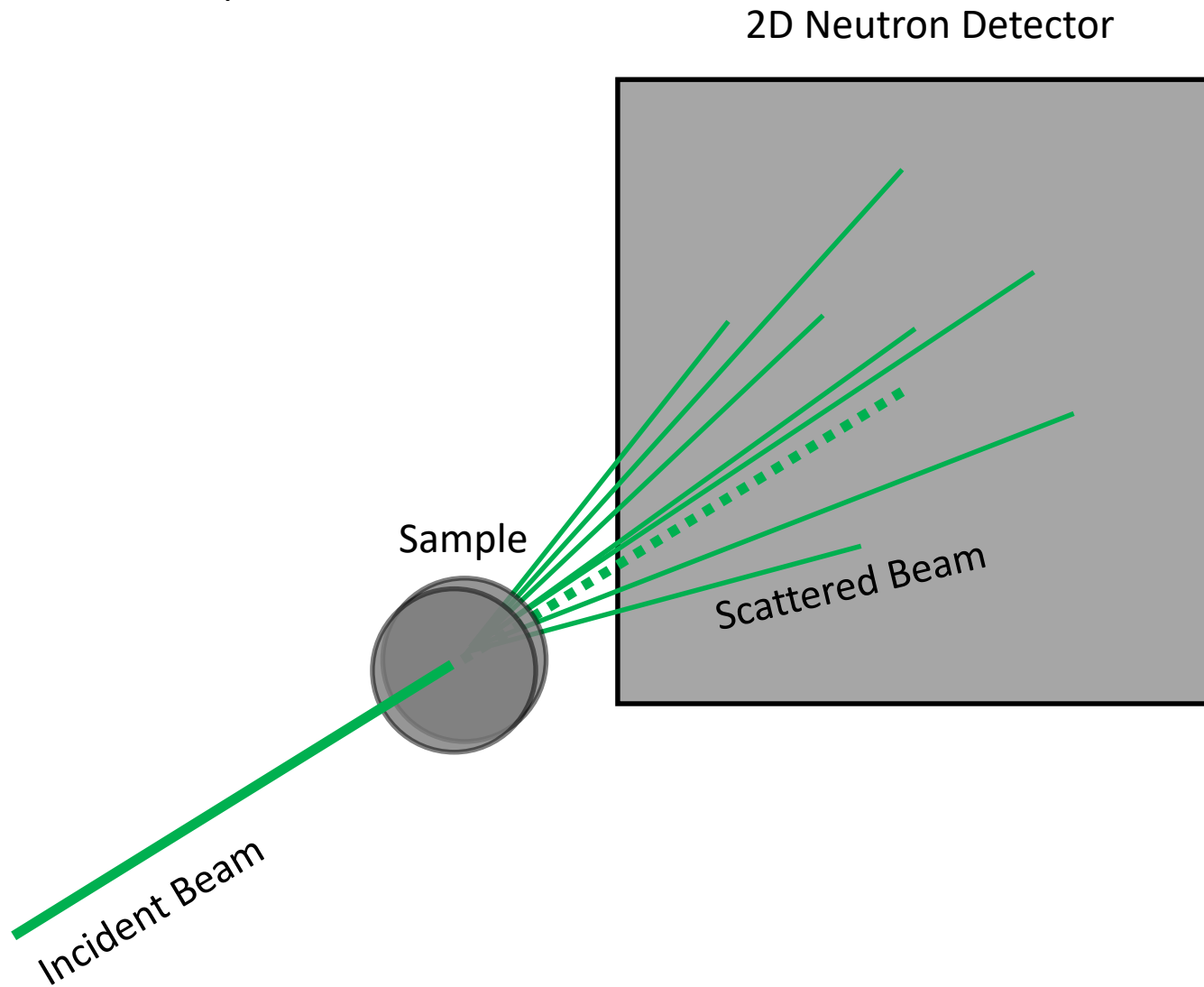


Neutrons interact with the nuclei of atoms and so are able to detect lighter atoms than can X-rays, as well as detect differences between isotopes.

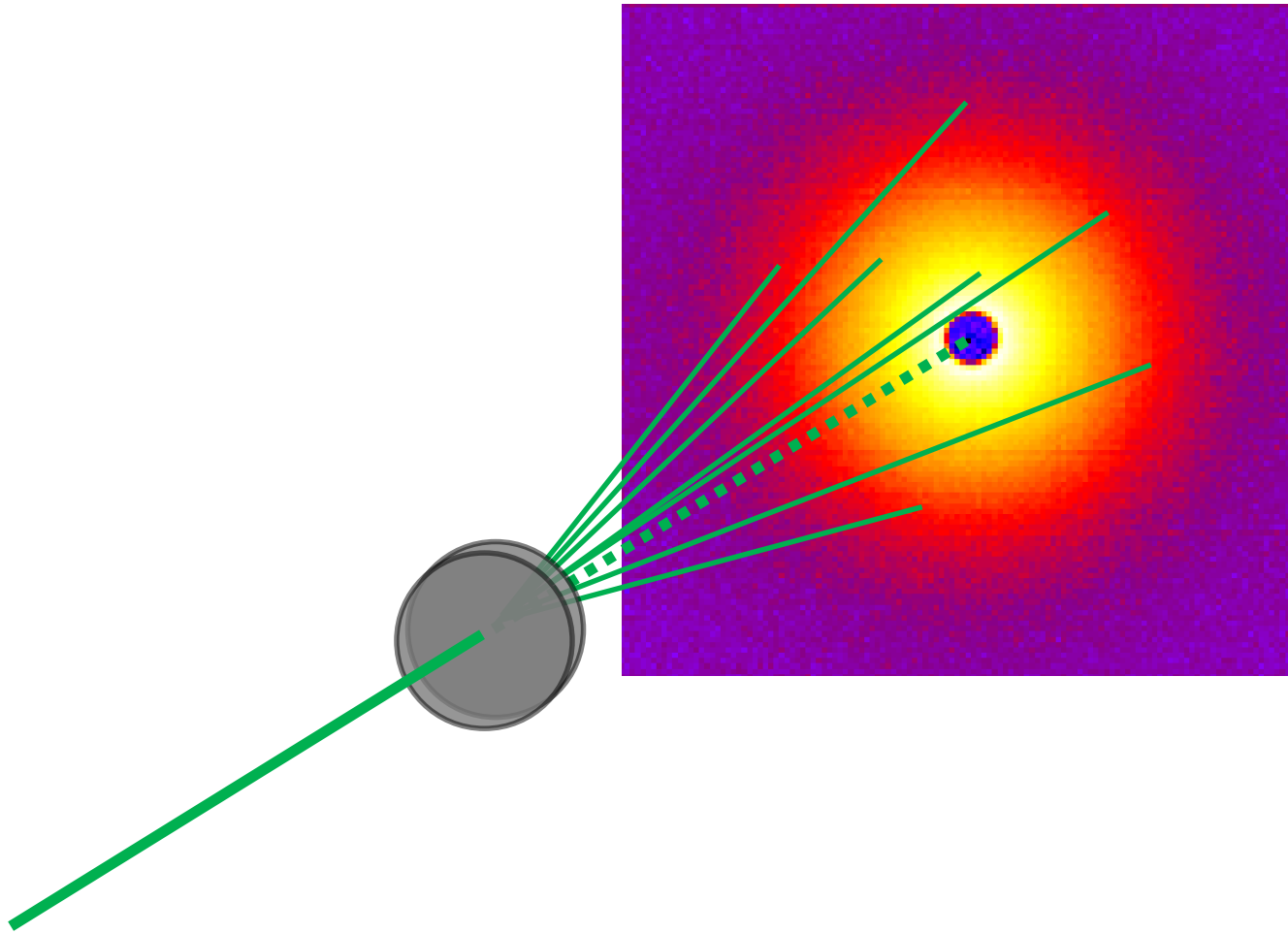


[4] National Institute of Standards and Technology. (2015). "The SANS Toolbox." *NIST Center for Neutron Research*. [5] R. Pynn. "Neutron Scattering: A Primer." *Los Alamos Neutron Science Center*.

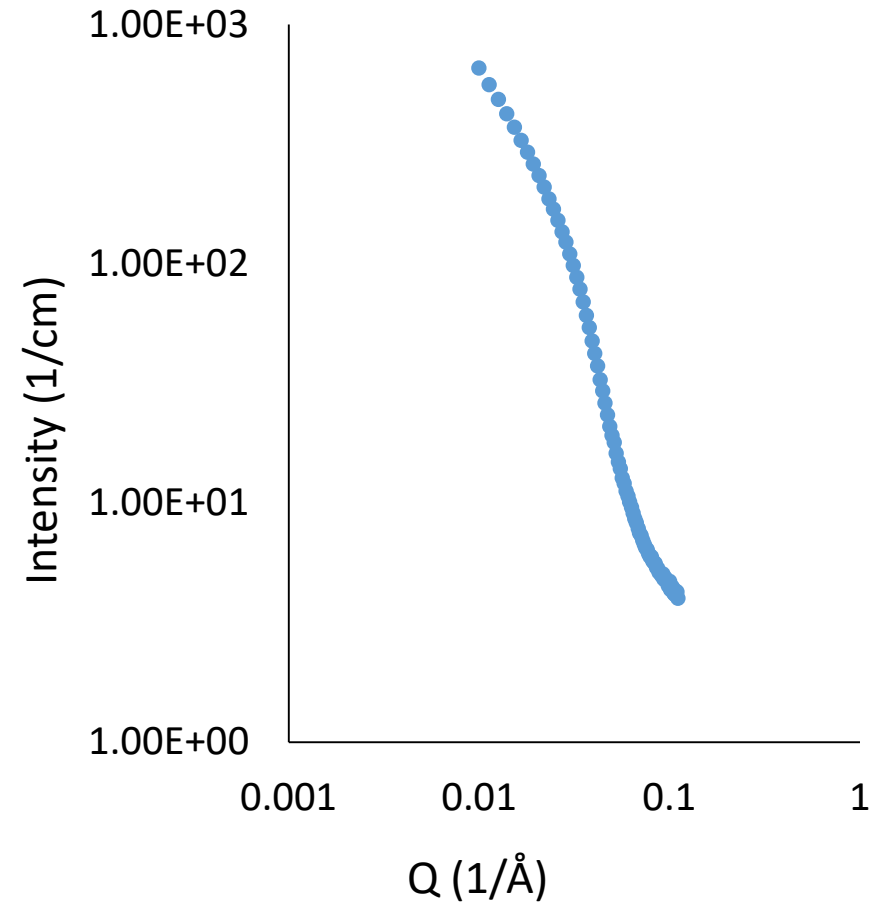
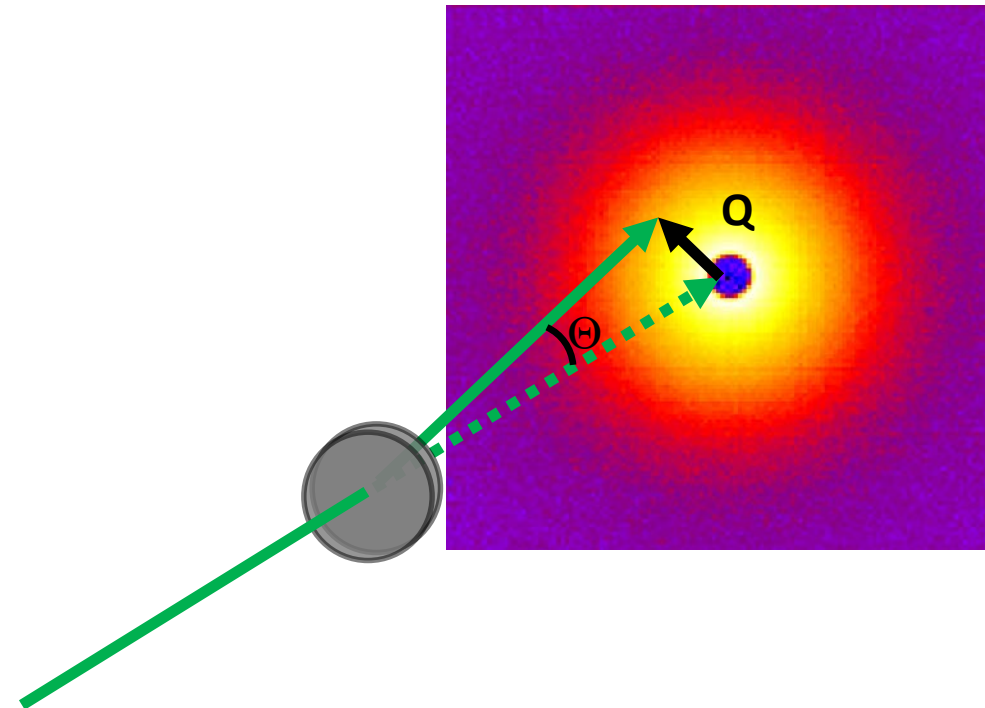
Small-angle neutron scattering (SANS) was used to measure size and distribution of particles in the samples.



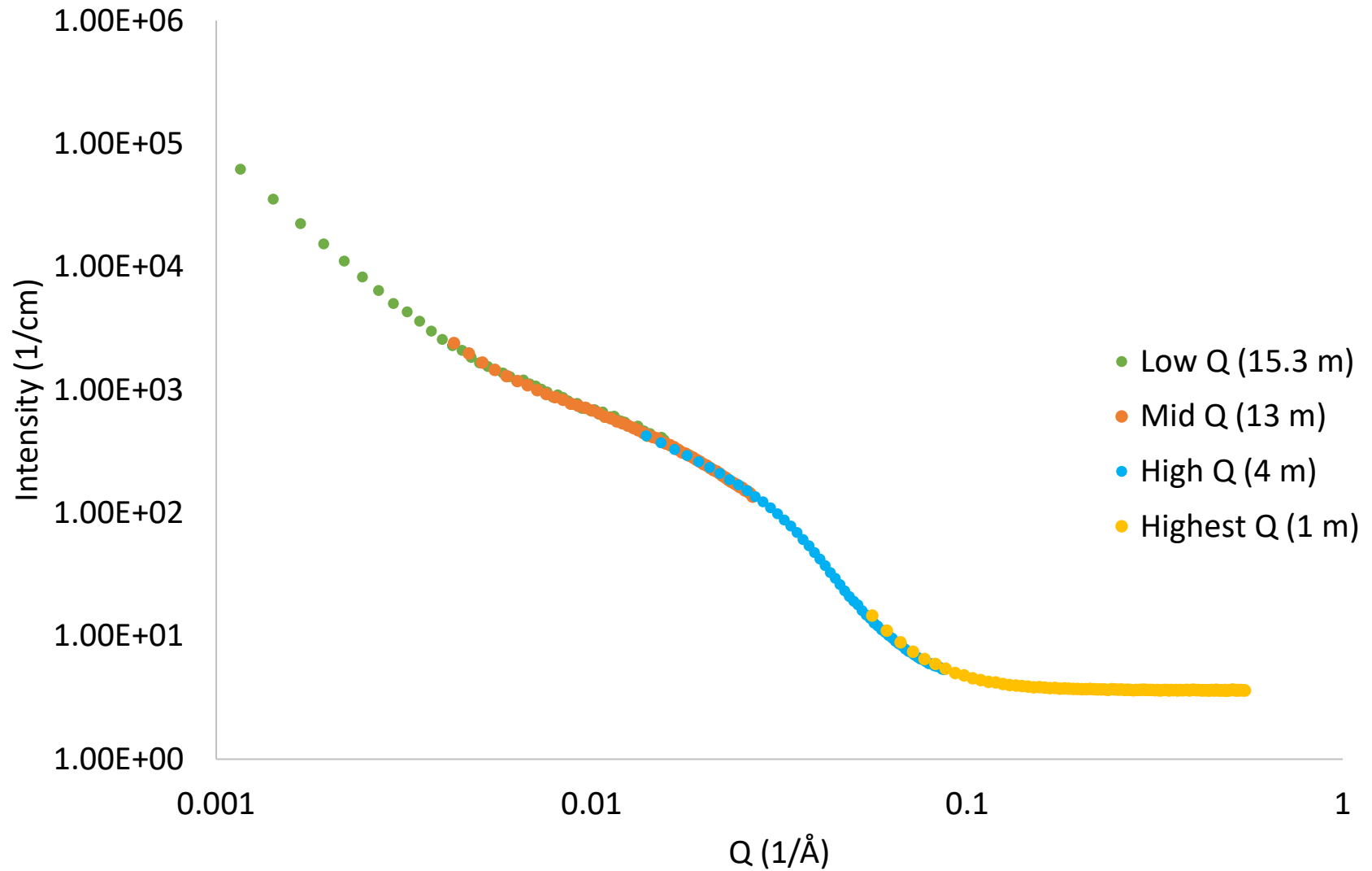
Small-angle neutron scattering (SANS) was used to measure size and distribution of particles in the samples.



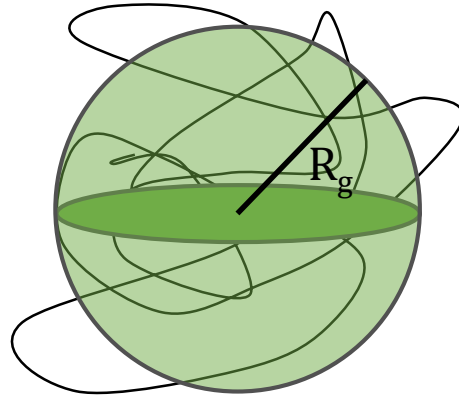
The vector difference between the incident beam and the scatter beam is called “Q”. Isotropic scattering allows us to take a circular average of intensity as a function of Q.



Stitching together data across Q-ranges reveals the behavior of the samples over a large length scale.



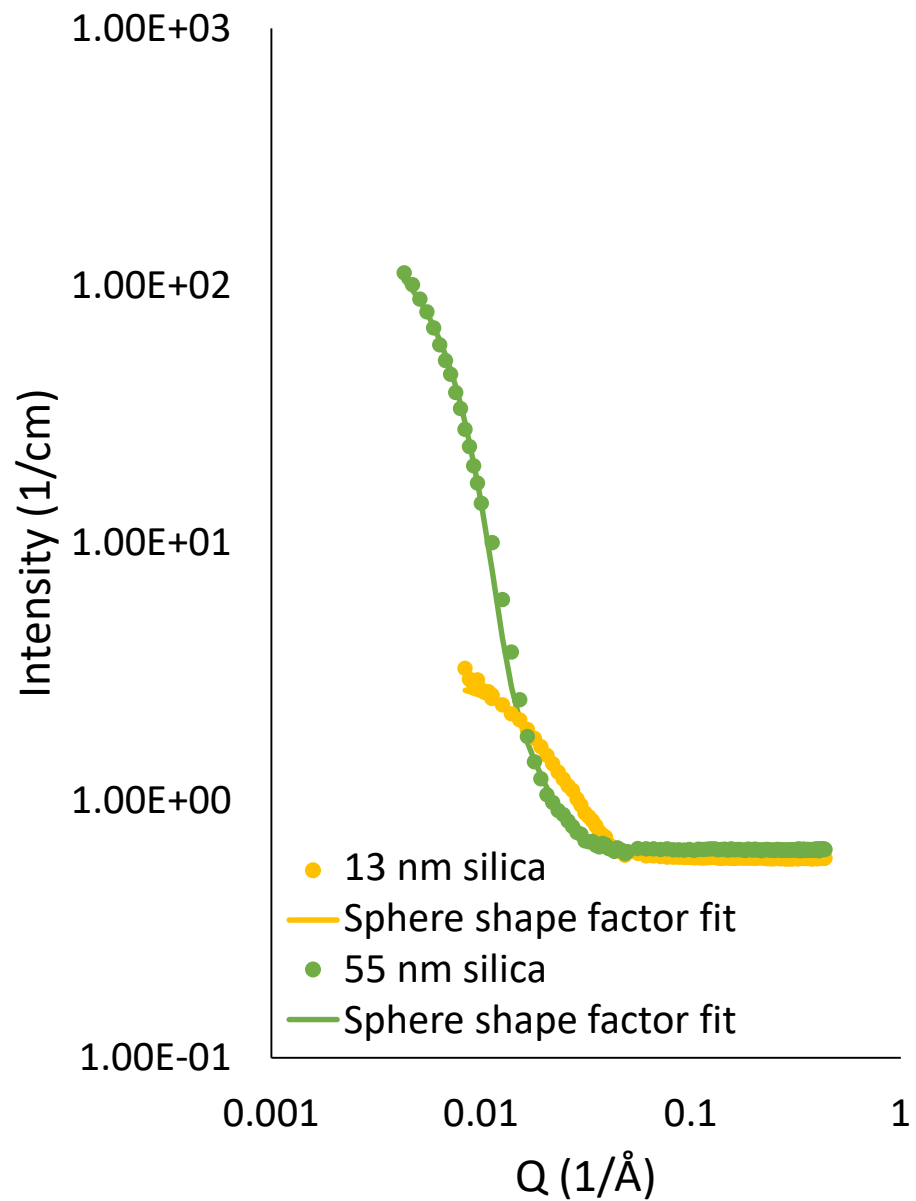
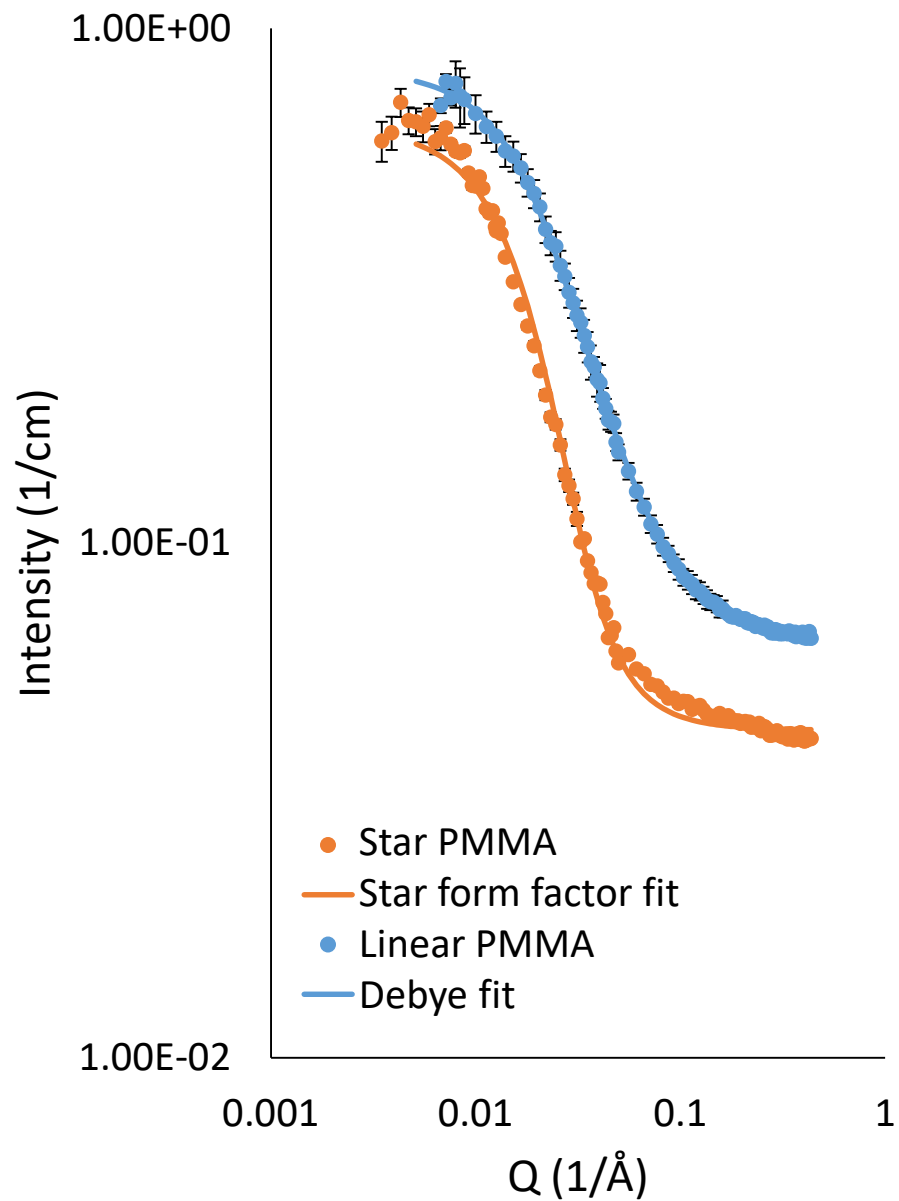
Star radius can be calculated from the linear radius of gyration



$$R_{g,\text{linear}} = \sqrt{\left(\frac{R_0^2}{M} * M\right) * \frac{1}{6}}$$

<u>Particle</u>	<u>Molecular Weight</u>	<u>Calculated Radius</u>
13 nm Silica		6.5 nm
55 nm Silica		27.5 nm
Linear PMMA	100 kg/mol	8.06 nm
Star PMMA	312 kg/mol	6.17 nm

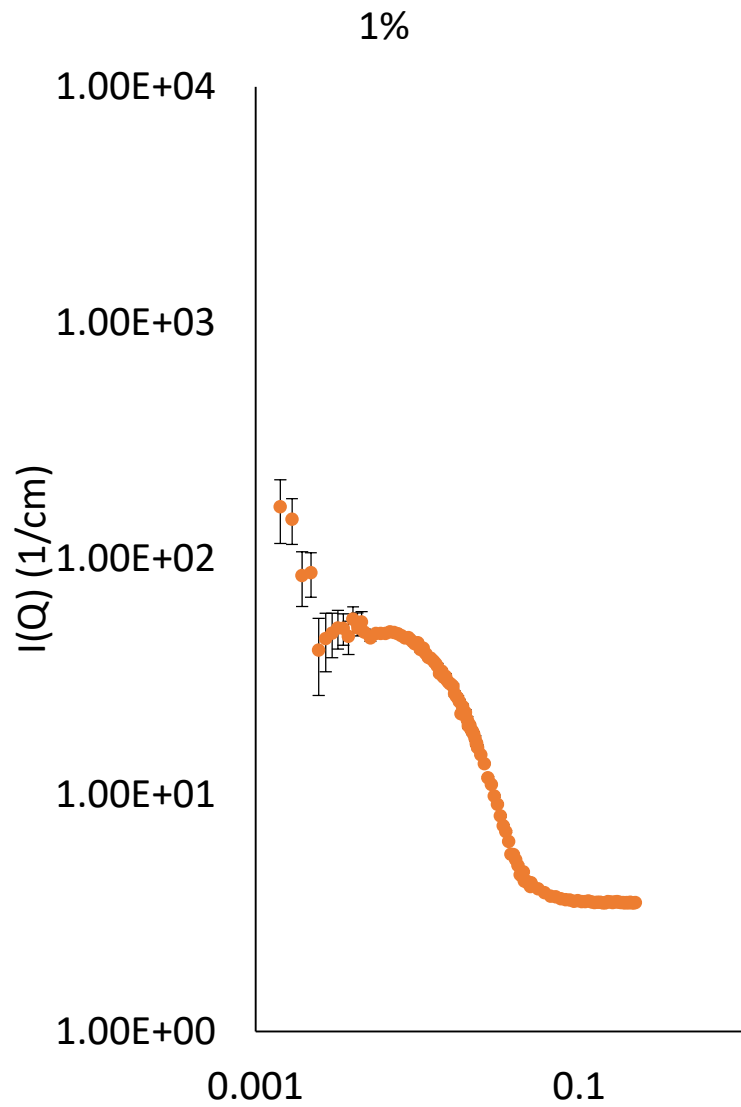
First we measured dilute solutions of nanoparticles without polymer.



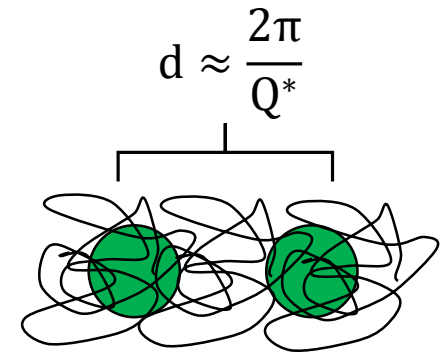
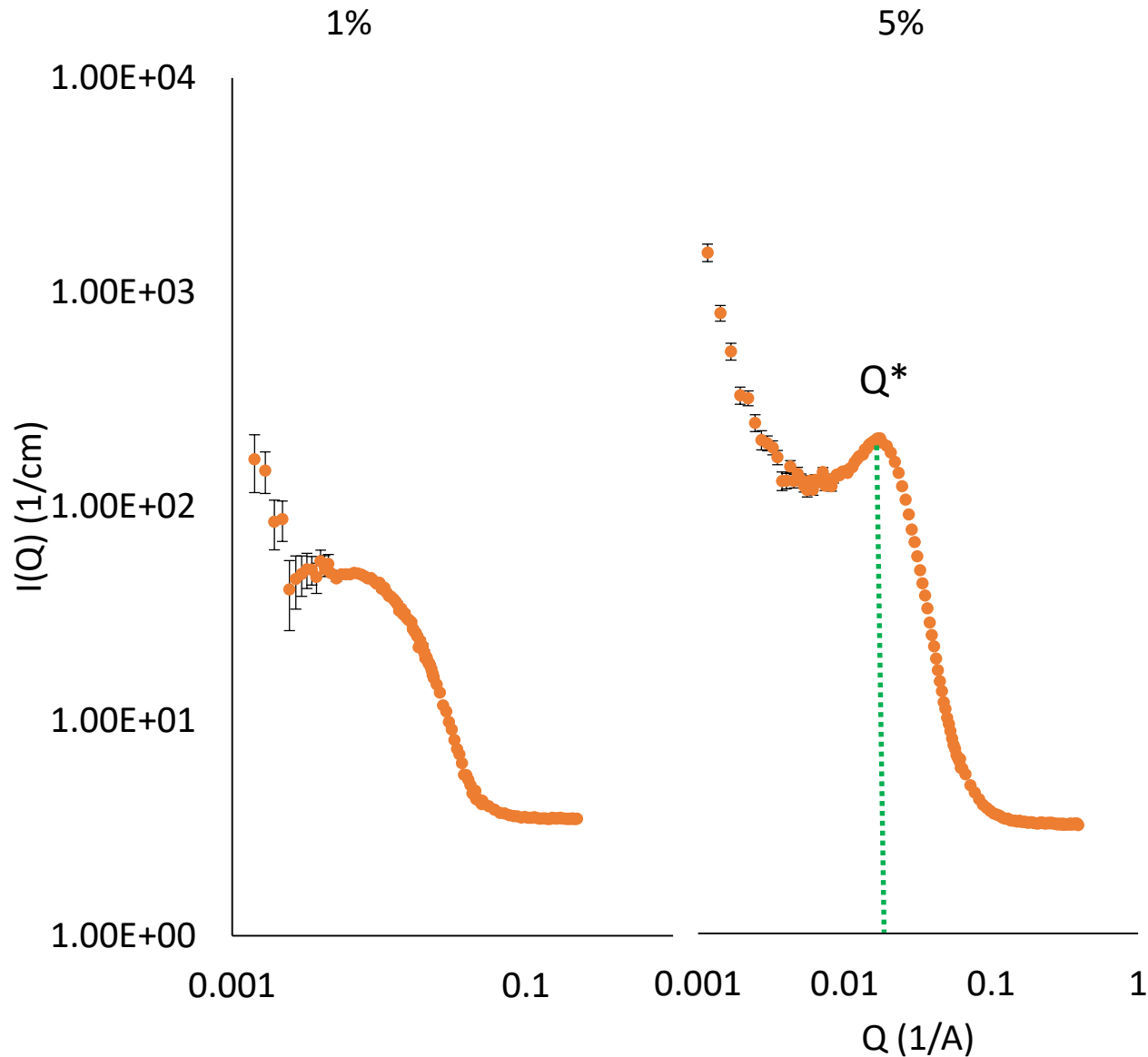
Comparison of theoretical size, size alone, and size in polymer.

<u>Particle</u>	<u>Molecular Weight</u>	<u>Theoretical Radius</u>	<u>Radius in Solution</u>
13 nm Silica	-	6.5 nm	7.2 ± 0.03 nm
55 nm Silica	-	27.5 nm	24.6 ± 0.07 nm
Linear PMMA	100 kg/mol	8.06 nm	7.9 ± 0.05 nm
Star PMMA	312 kg/mol	6.17 nm	9.6 ± 1.1 nm

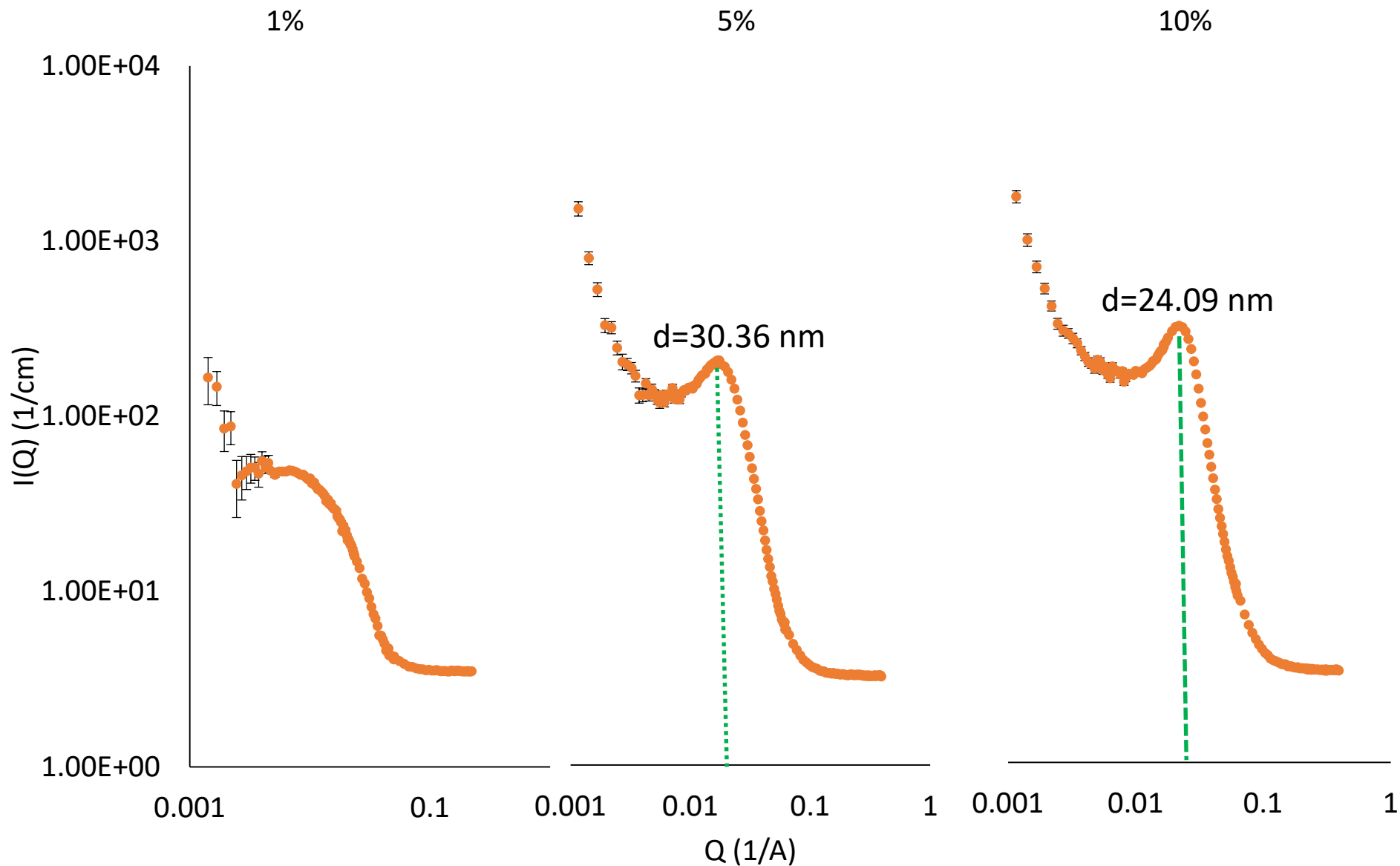
At 1% 13nm silica, the data shows the particles are spherical.



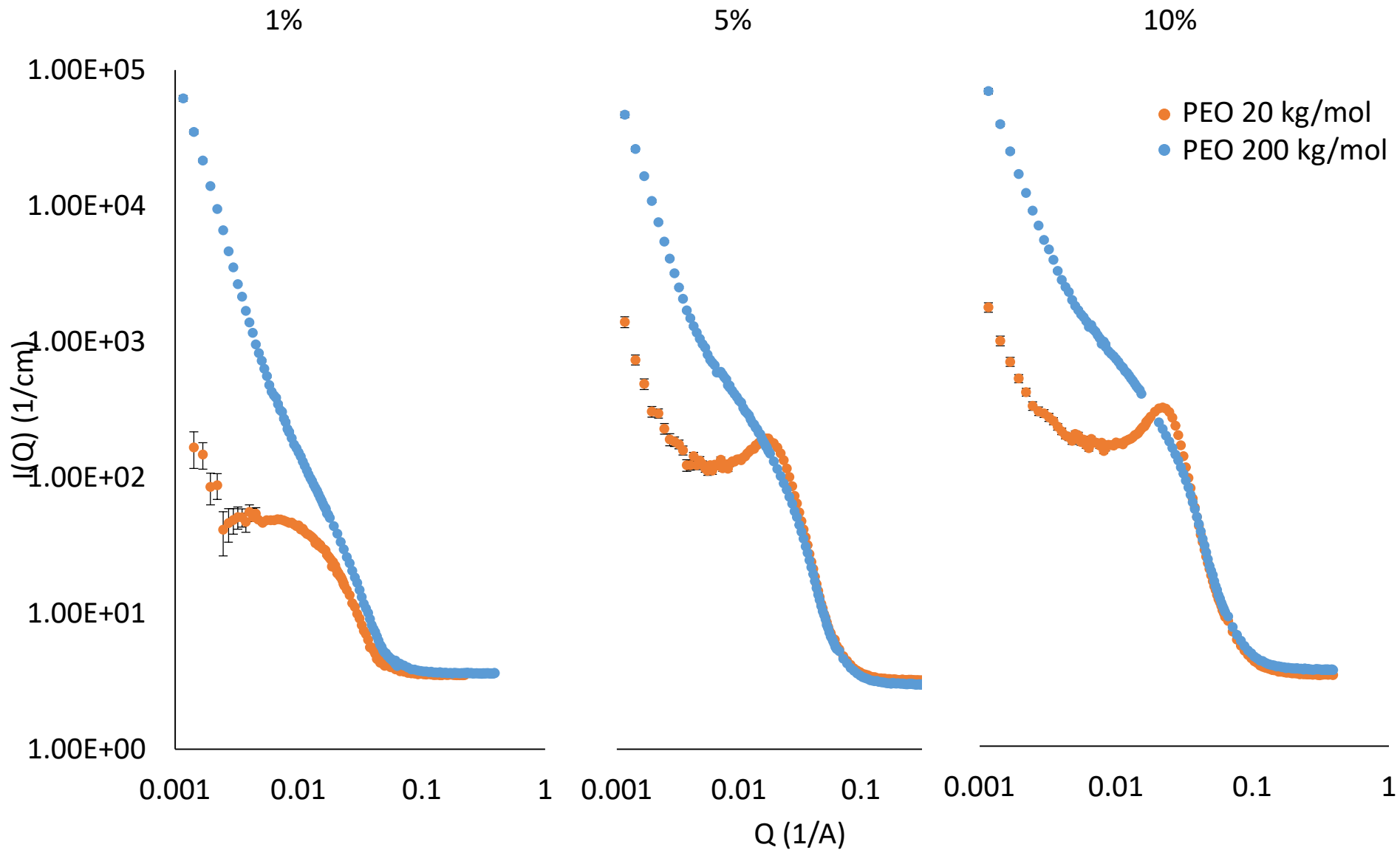
As silica concentration increases, a peak forms showing a uniform dispersal of particles in the polymer.



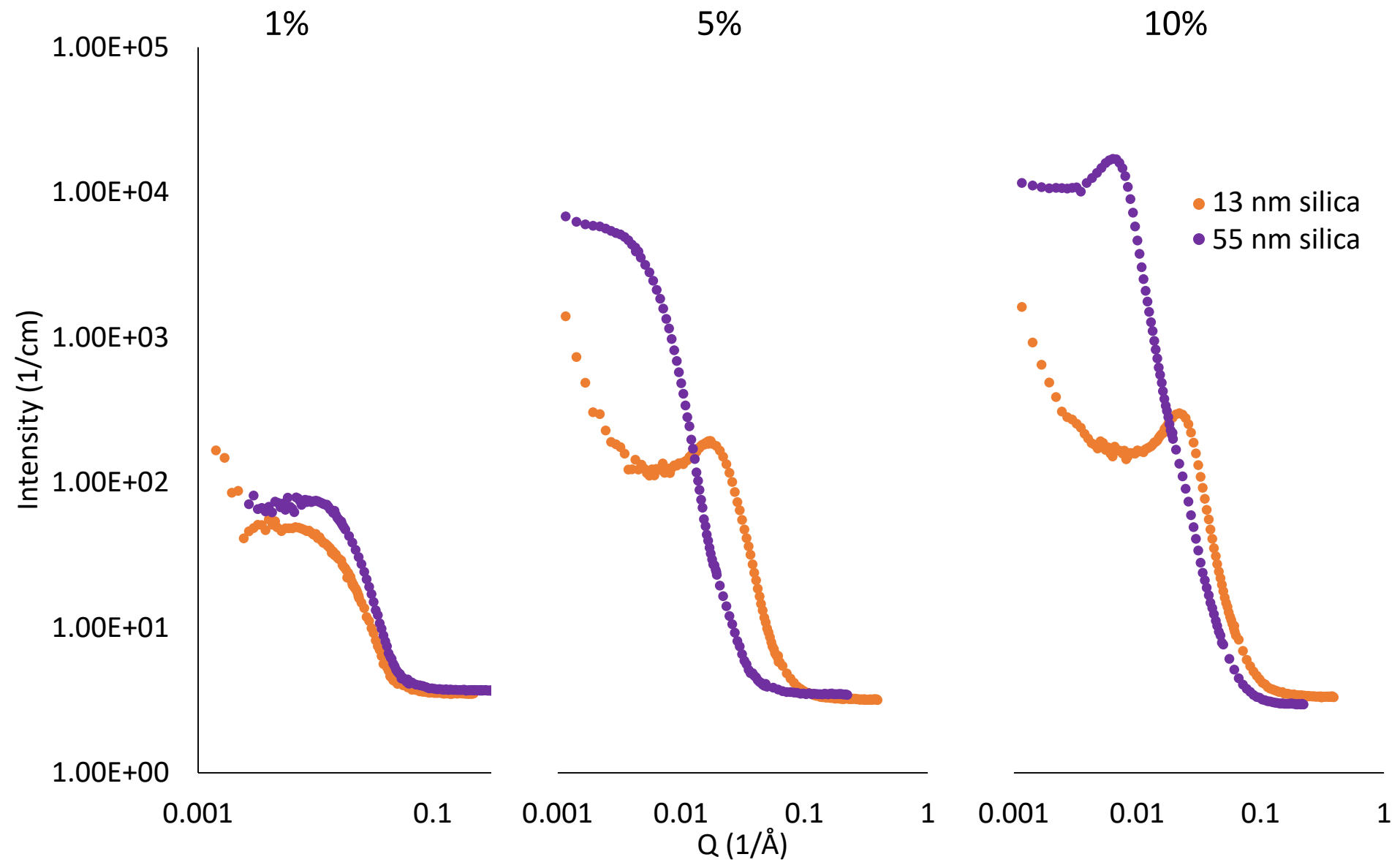
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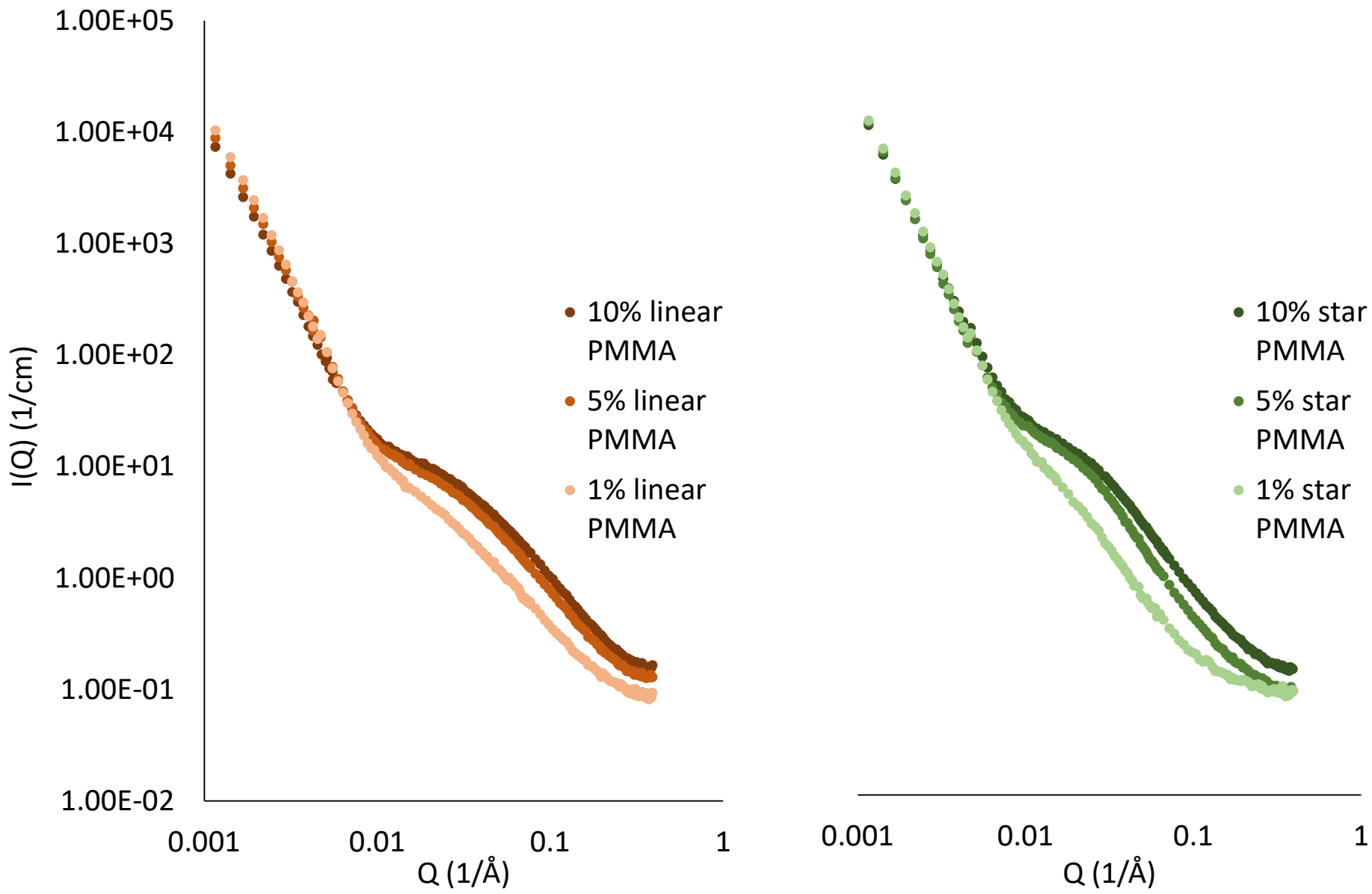
The 13 nm silica is more evenly dispersed in 20 kg/mol PEO than in 200 kg/mol PEO.



55 nm silica is not as well-dispersed as 13 nm silica at 5% concentration, but shows more uniform interface distance at 10%.



Linear and star PMMA did not differ greatly in dispersion or size over varying concentrations.



Rheology is the study of how a material flows.

Stress measured (stationary)

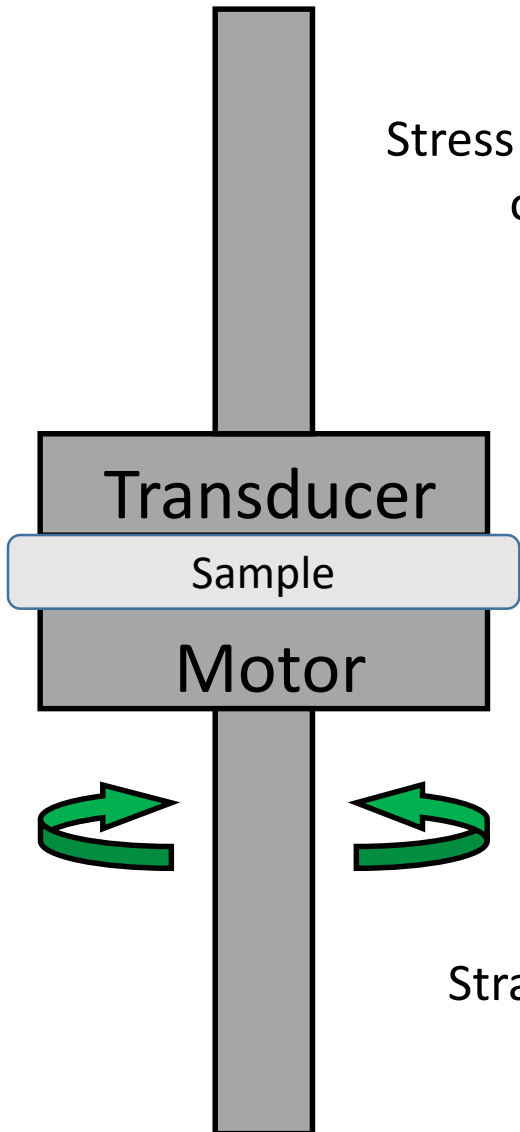
$$\sigma = \sigma_0 \sin(\omega t + \delta)$$

$$G' = \frac{\sigma_0}{\gamma_0} \cos(\delta)$$

Storage (Elastic) Modulus

$$G'' = \frac{\sigma_0}{\gamma_0} \sin(\delta)$$

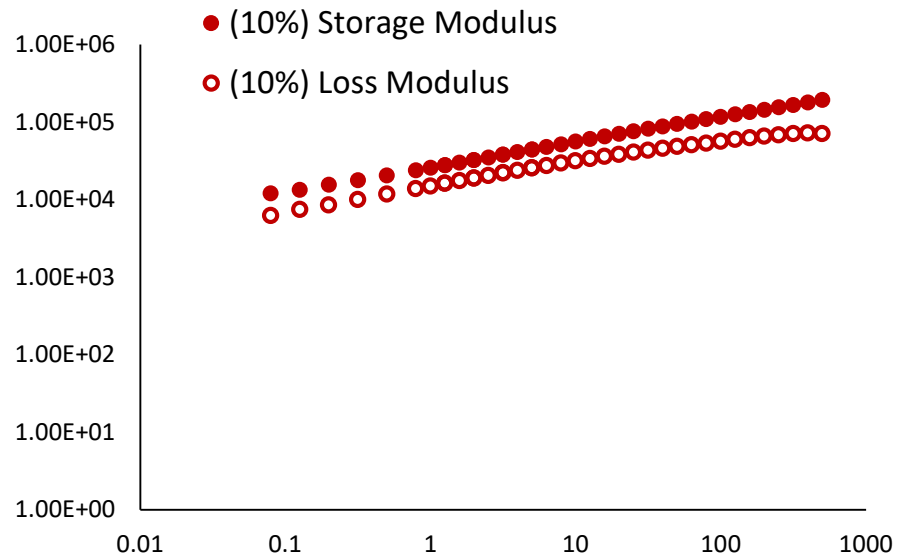
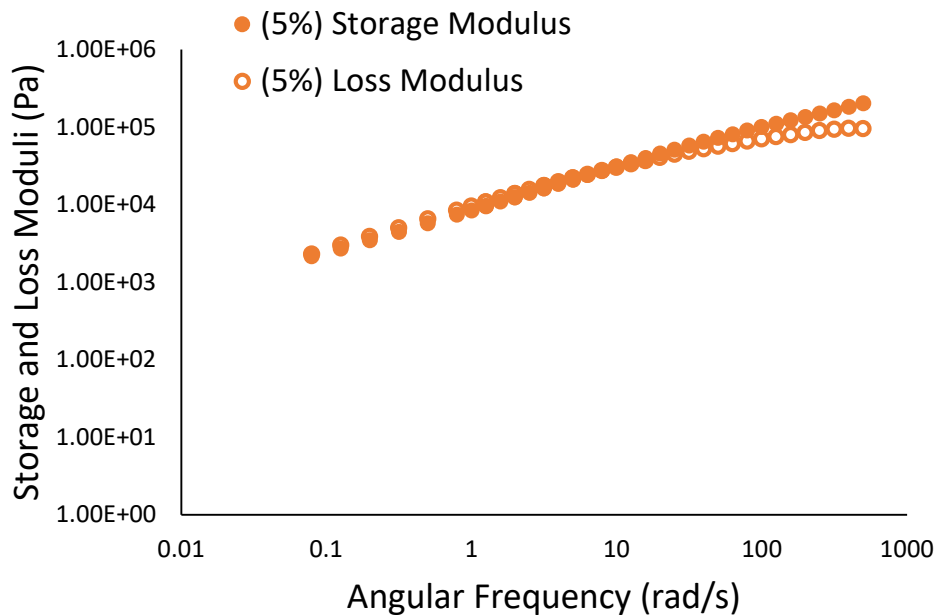
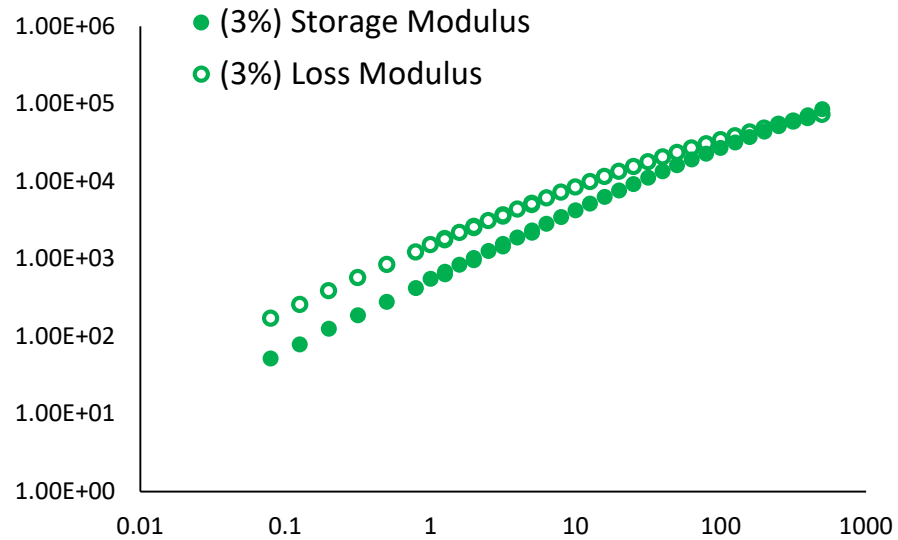
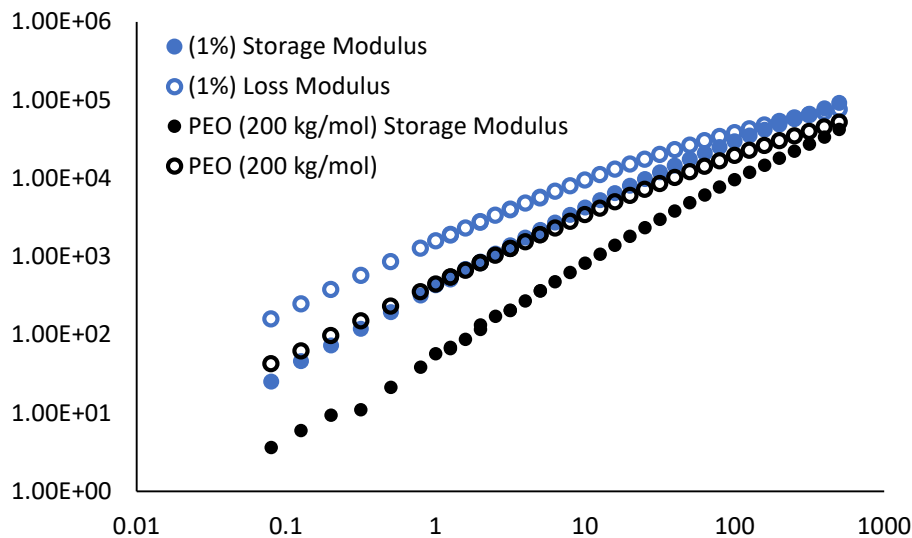
Loss (Viscous) Modulus



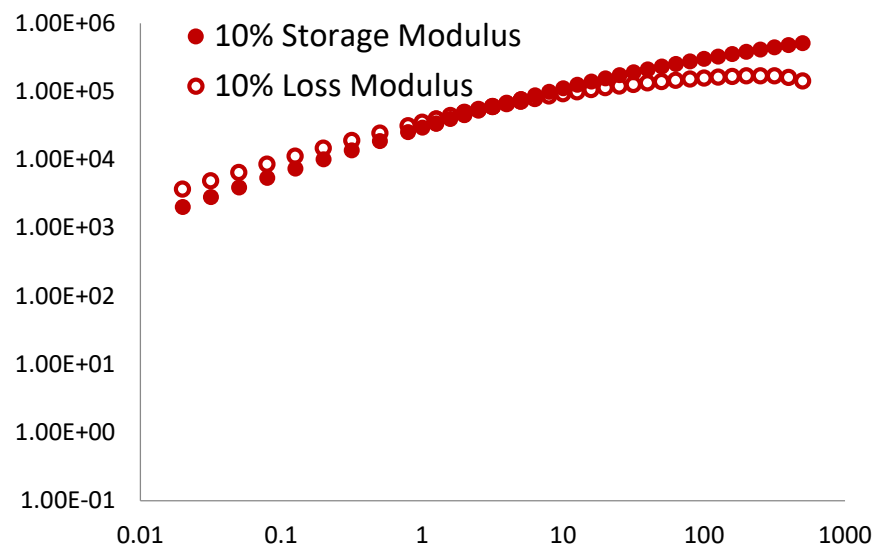
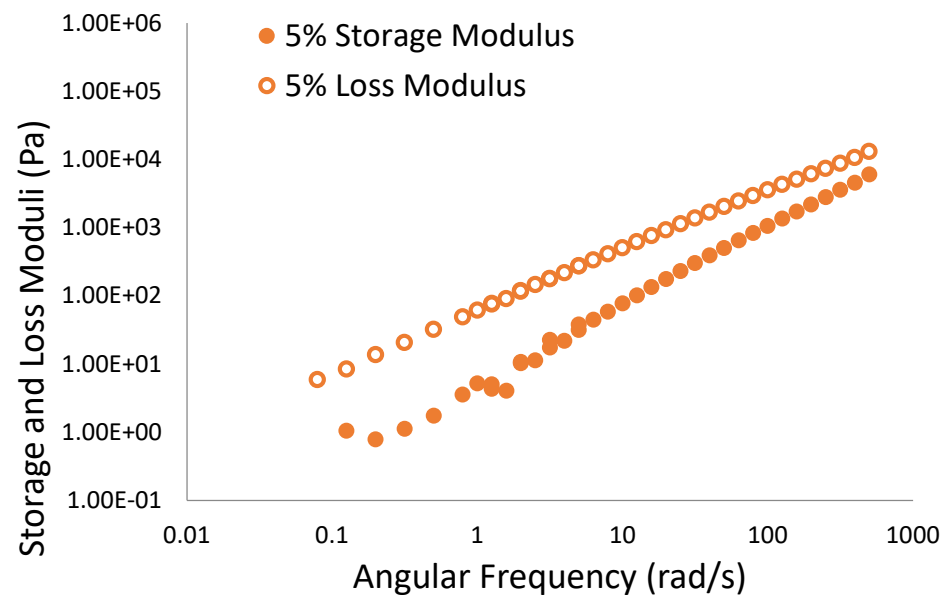
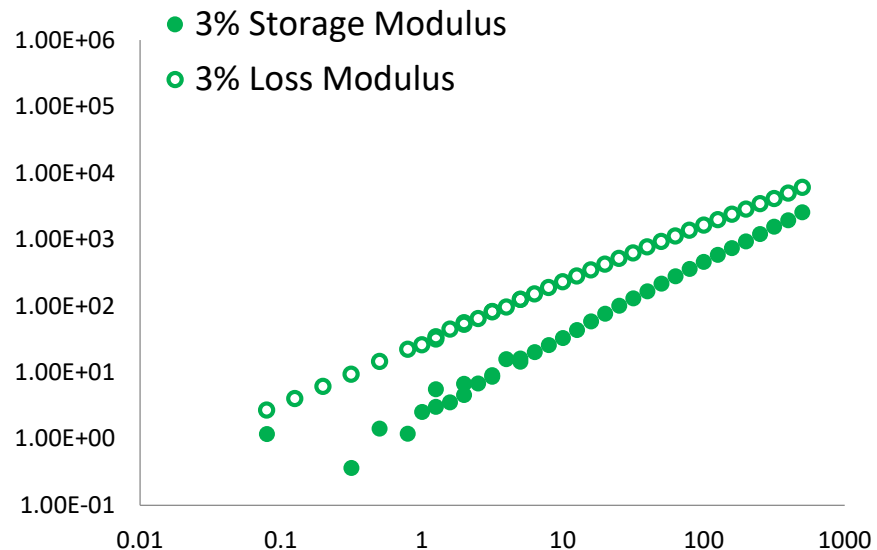
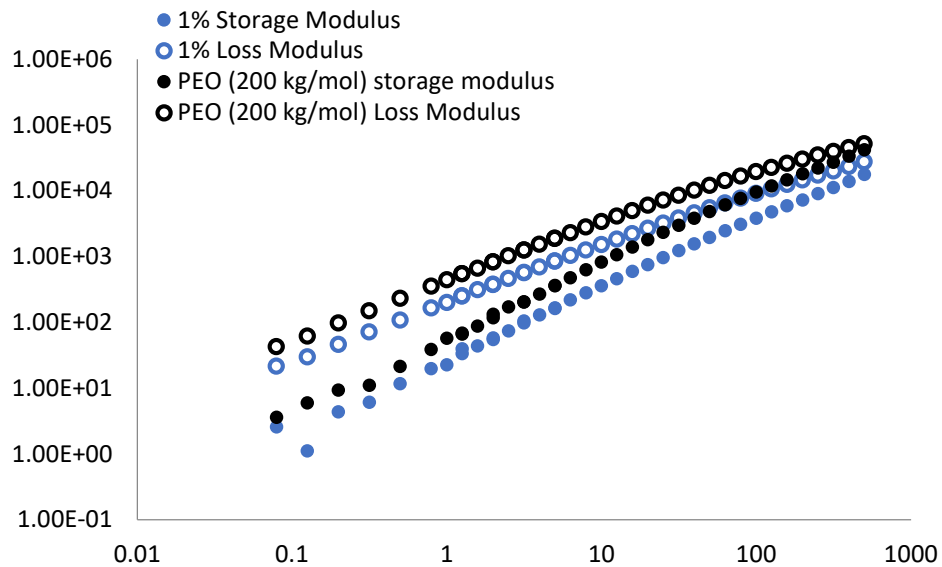
Strain applied (rotates)

$$\gamma = \gamma_0 \sin(\omega t)$$

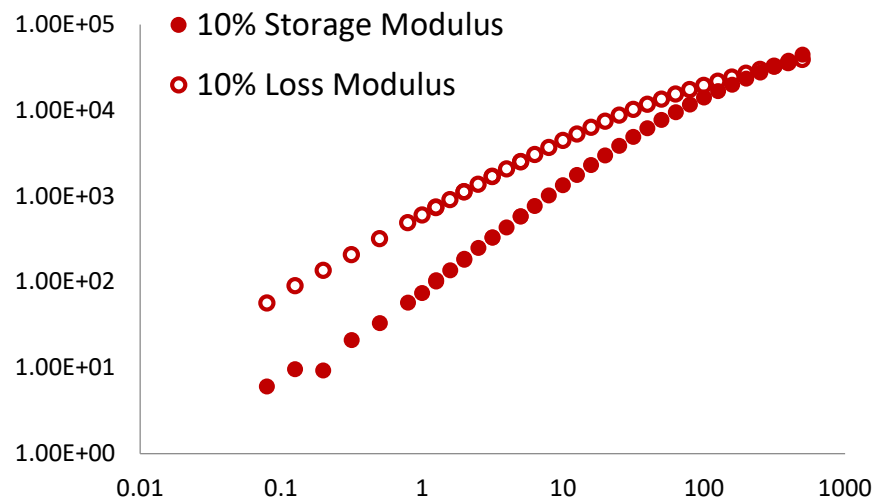
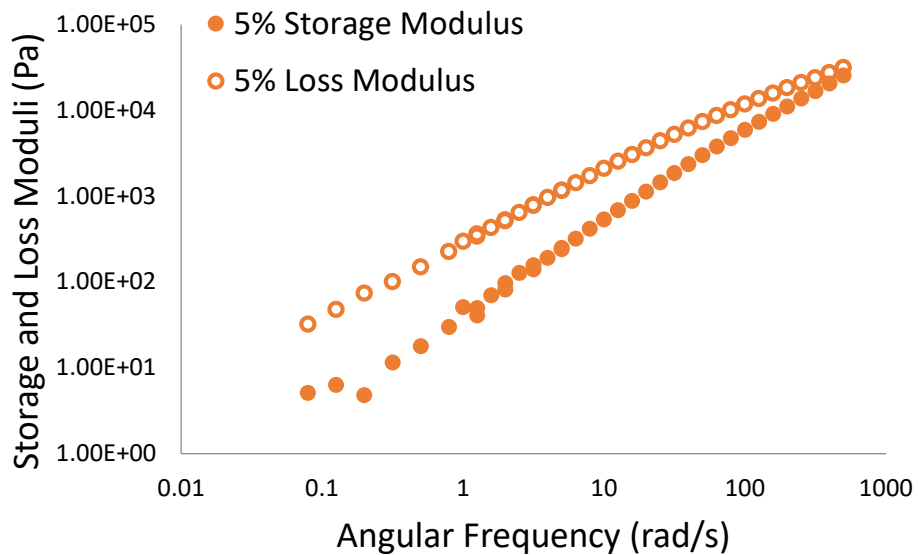
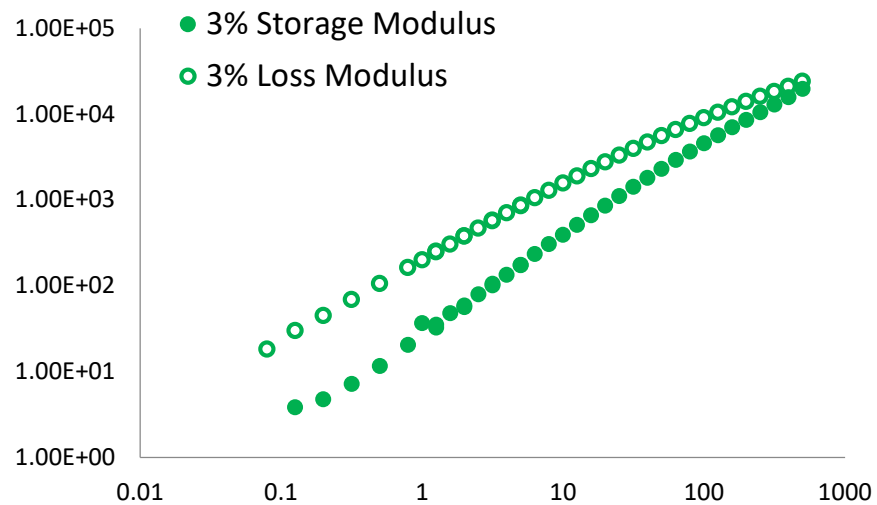
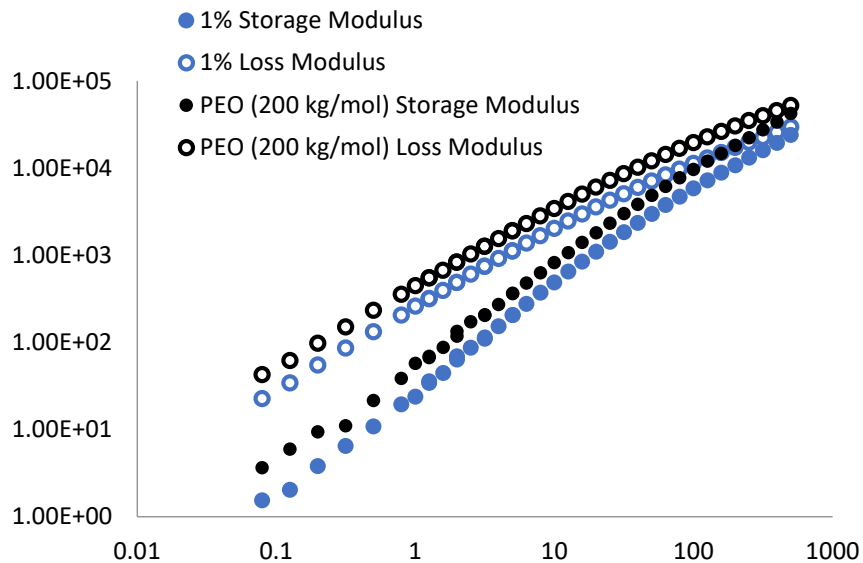
13 nm silica composite becomes more solid-like as nanoparticle concentration increases.



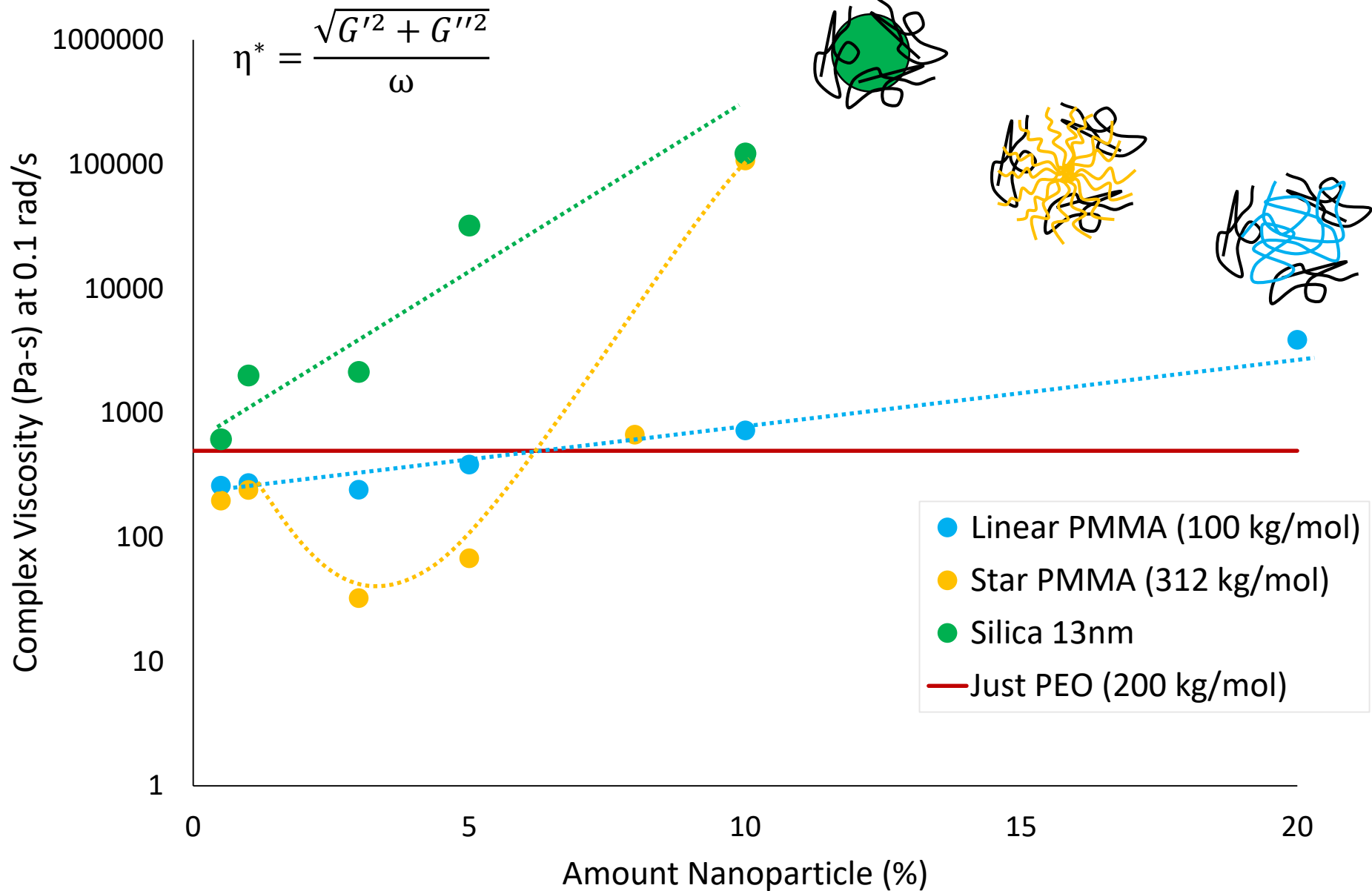
Star PMMA composite becomes more solid-like as nanoparticle concentration increases.



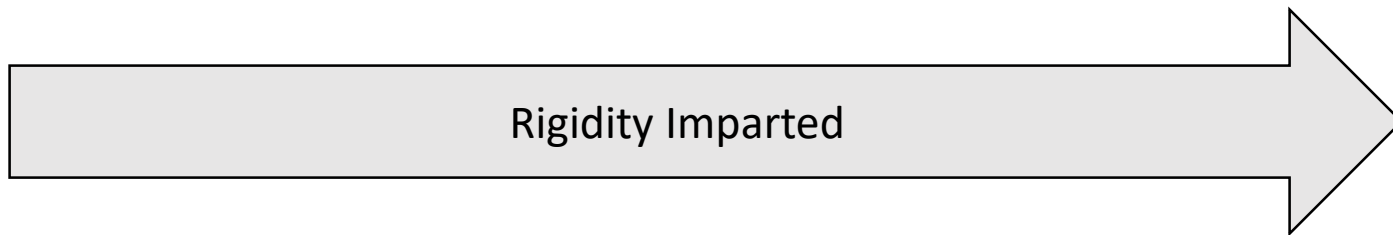
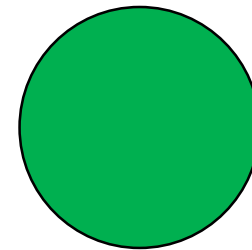
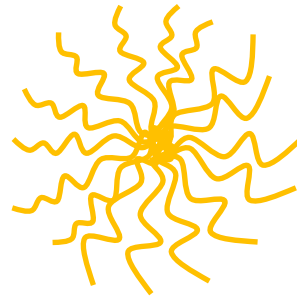
Linear PMMA does not become significantly more solid-like with increasing concentration.



Complex viscosity (η^*) of composite increases with increasing concentration of nanoparticle.



Composite rigidity increased with particle concentration and compactness.



Thank you!

Erkan Senses

Antonio Faraone

Michihiro Nagao

Javen Weston

NIST Center for Neutron Research

National Institute of Standards and Technology

National Science Foundation, Center for High Resolution Neutron Scattering