• Liquid scattering

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- SAXS review

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Homework Assignment #04: Chapter 4: 2, 4, 6, 7, 10 due Monday, October 24, 2016

Ordered 2D crystal

Amorphous solid or liquid





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C. Segre (IIT)

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$$\mathcal{I}^{SRO}(ec{Q}) = \mathcal{N}f(ec{Q})^2 + \mathcal{N}f(ec{Q})^2 \int_0^\infty 4\pi r^2 \left[
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$\mathsf{S}(\mathsf{Q})$ - the liquid structure factor

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We can rewrite the structure factor equation

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Which is the sine Fourier Transform of the deviation of the atomic density from its average, $\mathcal{H}(r) = 4\pi r [g(r) - 1]$

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The relation between radial distribution function and structure factor can be extended to multi-component systems where $g(r) \rightarrow g_{ij}(r)$ and $S(Q) \rightarrow S_{ij}(Q)$.

Measurement of the liquid structure factor of molten metals have shown that there is short range order which leads to the phenomenon of supercooling.



C. Segre (IIT)

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This indicates the presence of icosahedral clusters which inhibit crystallization.





"Difference in Icosahedral Short-Range Order in Early and Late Transition Metal Liquids", G.W. Lee et al. *Phys. Rev. Lett* **93**, 037802 (2004).

C. Segre (IIT)

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= $\left| \int_{V} \rho_{sl} e^{i\vec{Q}\cdot\vec{r}} dV \right|^2$

Recall that there was an additional term in the scattering intensity which becomes important at small Q.

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Where we have assumed sufficient averaging and introduced $\rho_{sl} = f \rho_{at}$. This final expression looks just like an atomic form factor but the charge density that we consider here is on a much longer length scale than an atom.

The SAXS experiment



The simplest case is for a dilute solution of non-interacting molecules.

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If we introduce the single-particle form factor $\mathcal{F}(\vec{Q})$: $\mathcal{F}(\vec{Q}) = \frac{1}{V_p} \int_{V_p} e^{i\vec{Q}\cdot\vec{r}} dV_p$ $I^{SAXS}(\vec{Q}) = \Delta \rho^2 V_p^2 |\mathcal{F}(\vec{Q})|^2$

Where $\Delta \rho = (\rho_{sl,p} - \rho_{sl,0})$, and the form factor depends on the morphology of the particle (size and shape).

$$\mathcal{F}(Q) = \frac{1}{V_p} \int_0^R \int_0^{2\pi} \int_0^{\pi} e^{iQr\cos\theta} r^2 \sin\theta \, d\theta \, d\phi \, dr$$

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$$= 3 \left[\frac{\sin(QR) - QR\cos(QR)}{Q^3 R^3} \right]$$

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PHYS 570 - Fall 2016

September 05, 2016 11 / 17

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PHYS 570 - Fall 2016

September 05, 2016 12 / 17
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In the long wavelength limit $QR \rightarrow 0$ we can approximate the scattering factor with the first terms of the sum

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September 05, 2016 17 / 17
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