Today's Outline - October 24, 2016

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Homework Assignment #05:
Chapter 5: 1, 3, 7, 9, 10
due Wednesday, November 02, 2016

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No class on Wednesday, November 9, 2016

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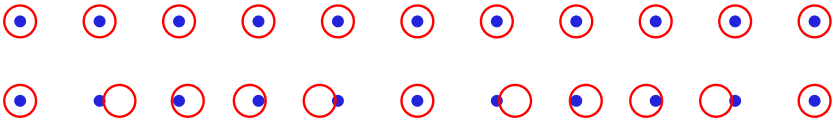

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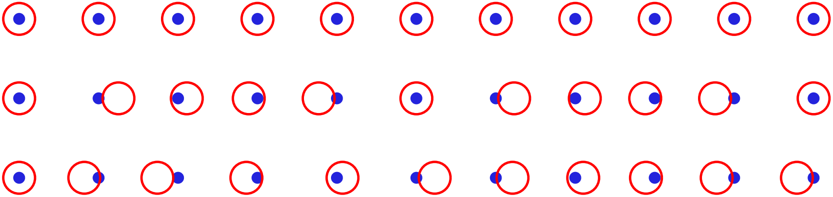

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the diffraction pattern has main Bragg peaks plus satellite peaks

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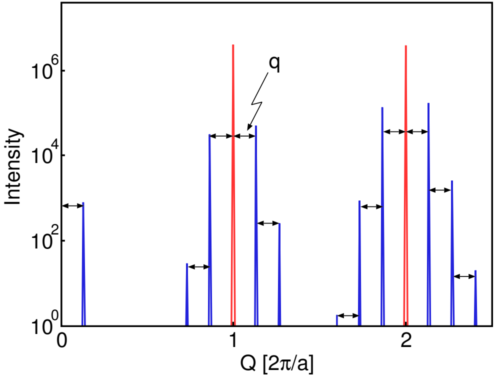

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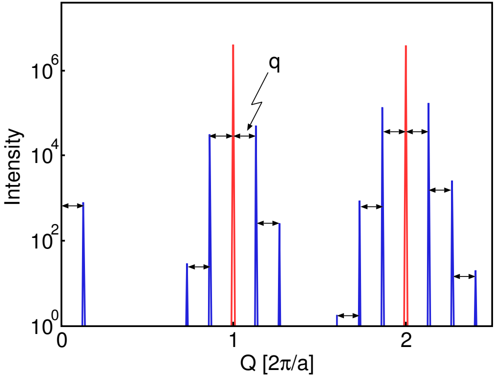

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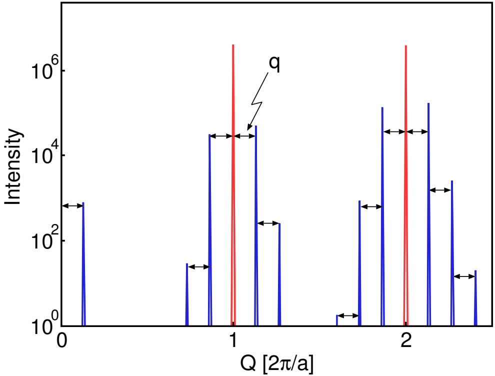
If the modulation of the structure is a multiple of the lattice parameter, the modulation is simply a superlattice and the actual lattice parameter will be changed.



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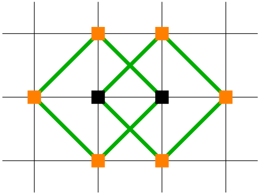

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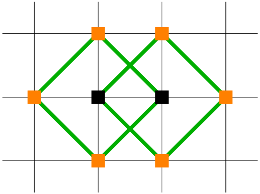

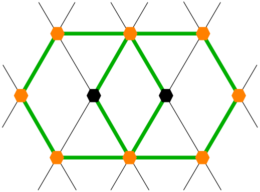

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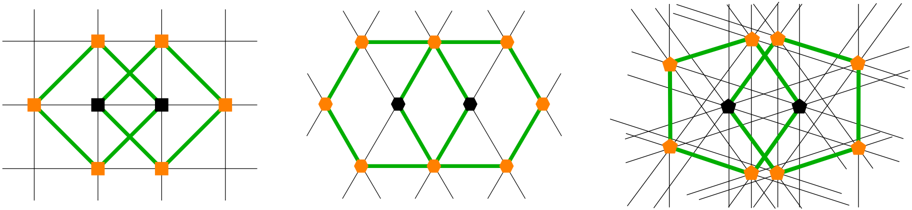

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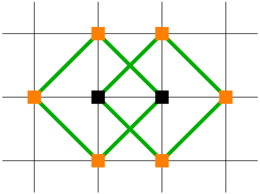

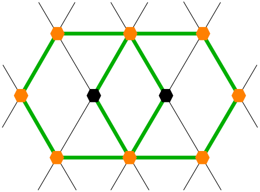

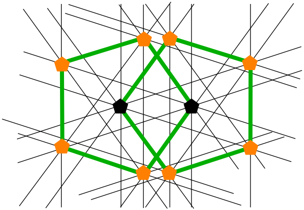

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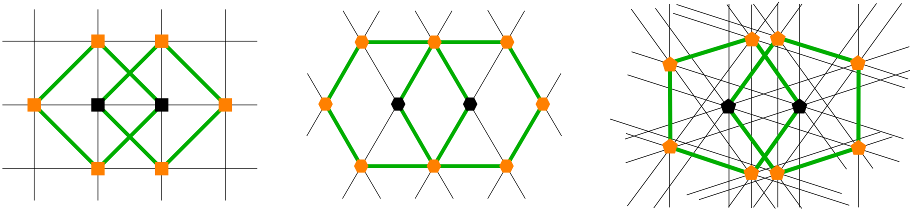

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In 2011 Shechtman was awarded the Nobel Prize in Chemistry

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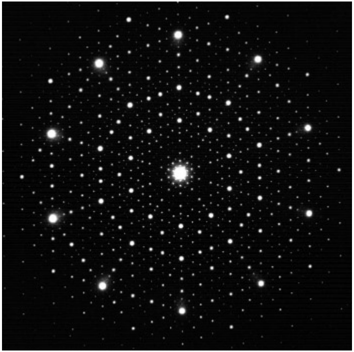
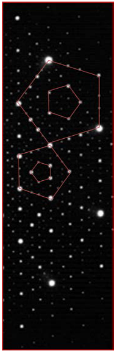
The electron micrographs show that there must be long range order to be able to get such sharp diffraction peaks





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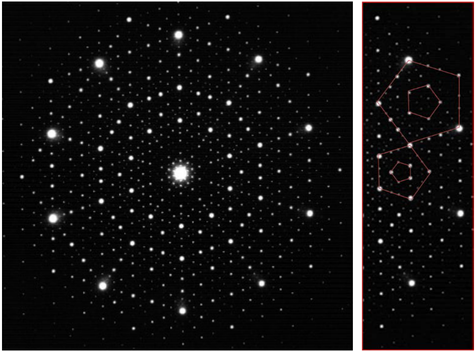

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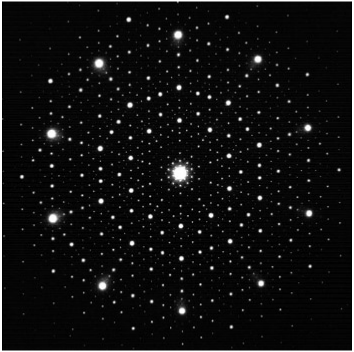

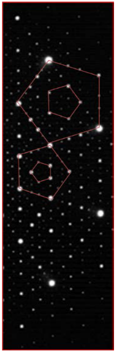

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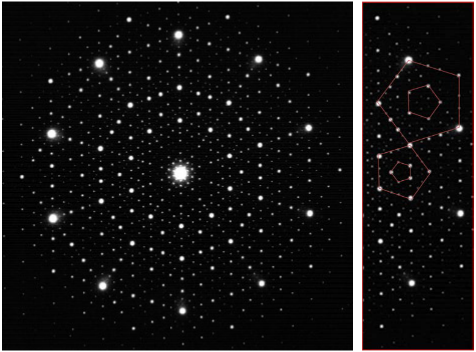

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Other groups have discovered stable icosahedral phases with three and two elements.

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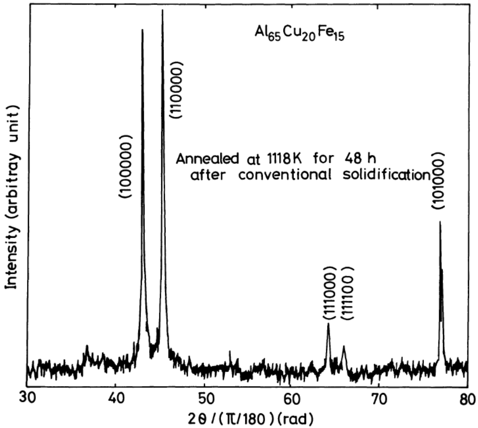

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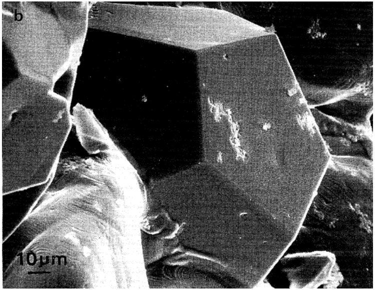

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Lattice Vibrations

Atoms on a lattice are not rigid but vibrate. There is zero-point motion as well as thermal motion. These vibrations influence the x-ray scattering.

For a 1D lattice, we replace the position of the atom with its *instantaneous* position, $\vec{R}_n + \vec{u}_n$ where $\vec{u}_n$ is the displacement from the equilibrium position, $\vec{R}_n$. Computing the intensity:

$$I = \left\langle \sum_m f(\vec{Q}) e^{i\vec{Q}\cdot(\vec{R}_m+\vec{u}_m)} \sum_n f^*(\vec{Q}) e^{-i\vec{Q}\cdot(\vec{R}_n+\vec{u}_n)} \right\rangle$$
$$= \sum_m \sum_n f(\vec{Q}) f^*(\vec{Q}) e^{i\vec{Q}\cdot(\vec{R}_m-\vec{R}_n)} \left\langle e^{i\vec{Q}\cdot(\vec{u}_m-\vec{u}_n)} \right\rangle$$

The last term is a time average which can be simplified using the Baker-Hausdorff theorem, $\left\langle e^{ix} \right\rangle = e^{-\langle x^2 \rangle/2}$

$$\left\langle e^{i\vec{Q}\cdot(\vec{u}_m-\vec{u}_n)} \right\rangle = \left\langle e^{iQ(u_{Qm}-u_{Qn})} \right\rangle = e^{-\langle Q^2 (u_{Qm}-u_{Qn})^2 \rangle/2}$$

Lattice Vibrations

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The second term is the Thermal Diffuse Scattering and actually increases with mean squared displacement.

Thermal Diffuse Scattering

$$I^{TDS} = \sum_m \sum_n f(\vec{Q})e^{-M} e^{i\vec{Q}\cdot\vec{R}_m} f^*(\vec{Q})e^{-M} e^{-i\vec{Q}\cdot\vec{R}_n} \left[e^{Q^2\langle u_{Qm} u_{Qn}\rangle} - 1 \right]$$

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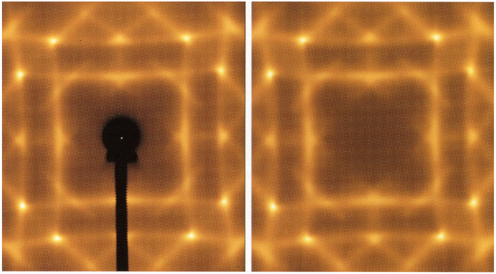

incident beam along (100)

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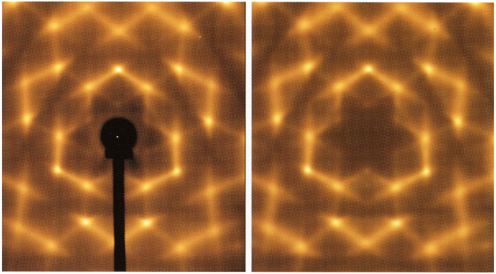

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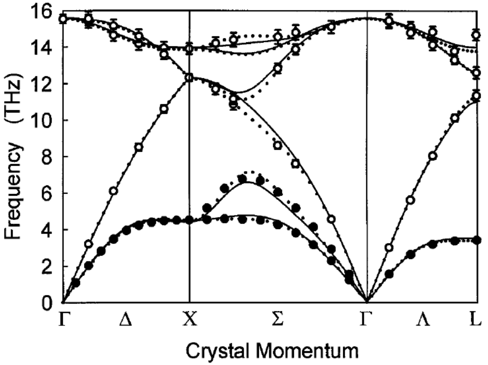

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In general, Debye-Waller factors can be anisotropic

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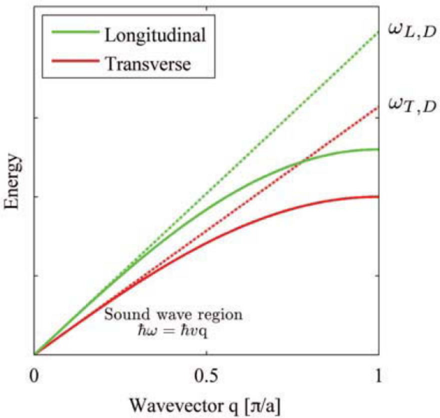

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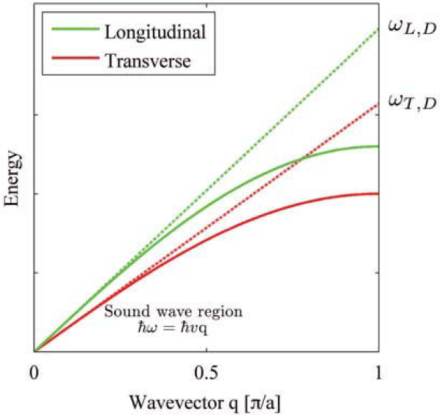

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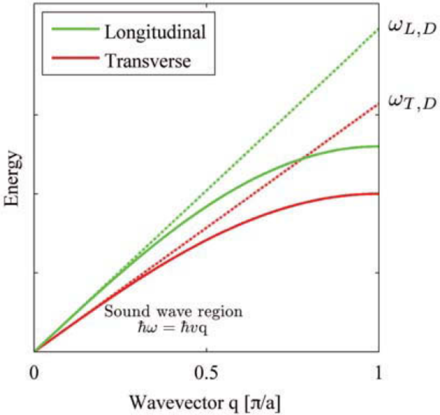

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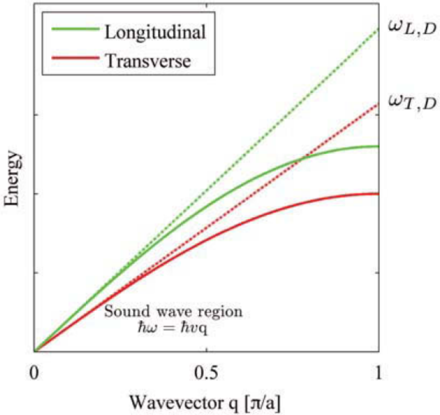

$$B_T[\text{Å}^2] = \frac{11492\text{T[K]}}{\text{A}\Theta^2[\text{K}^2]}\phi(\Theta/\text{T}) + \frac{2873}{\text{A}\Theta[\text{K}]}$$

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C*	12	2230	0.11	0.11	0.12
Al	27	428	0.25	0.30	0.72
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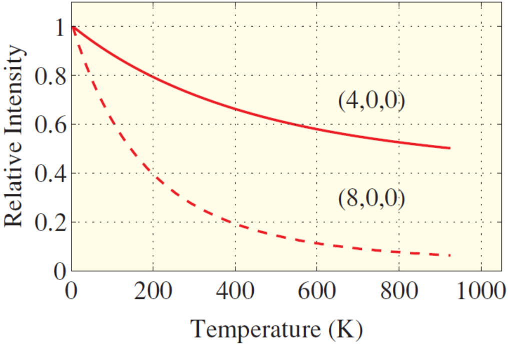
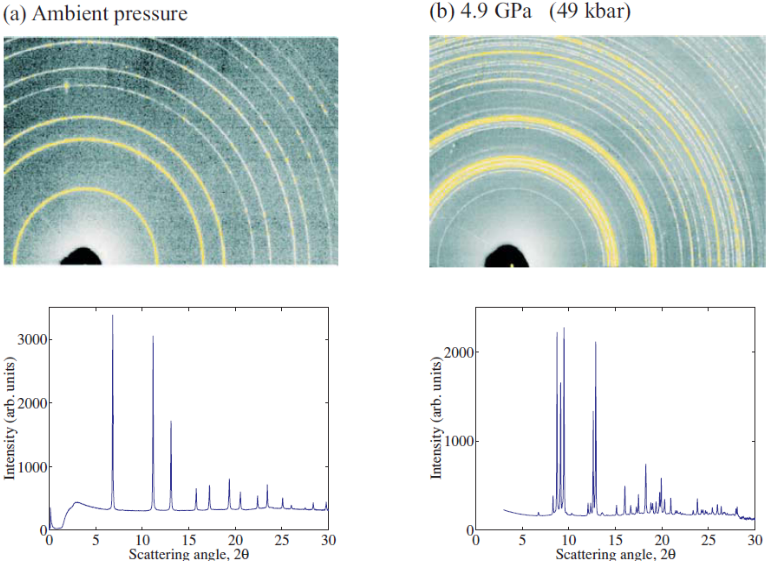


Powder diffraction



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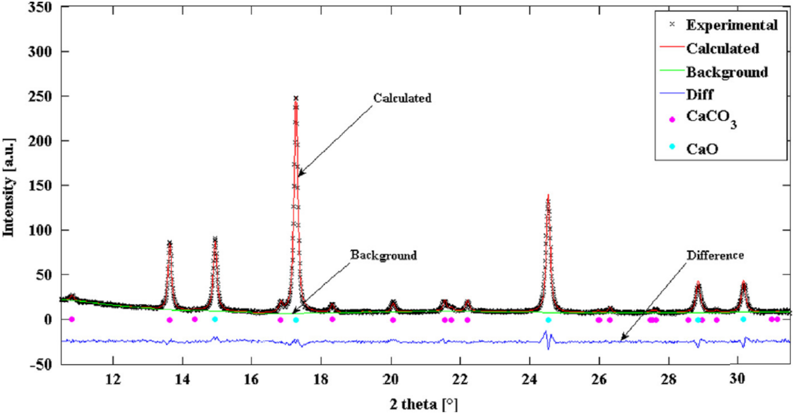

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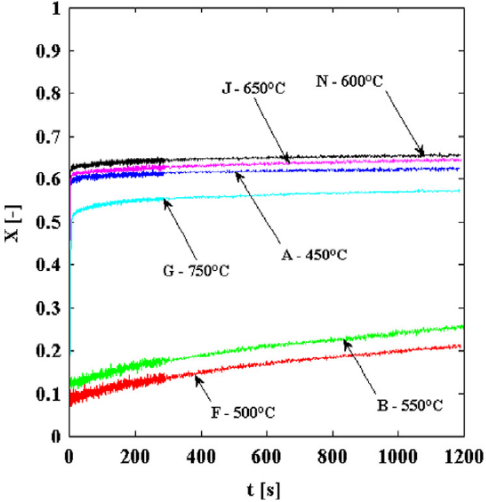
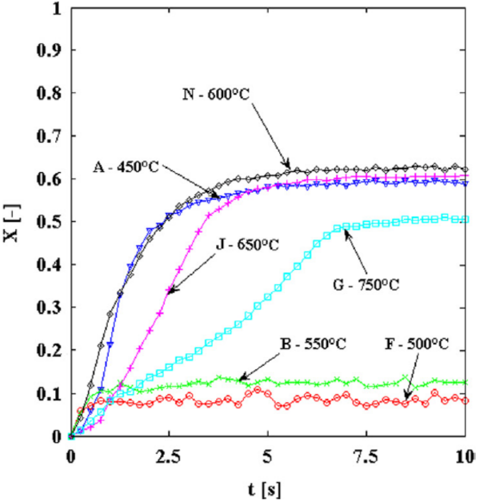
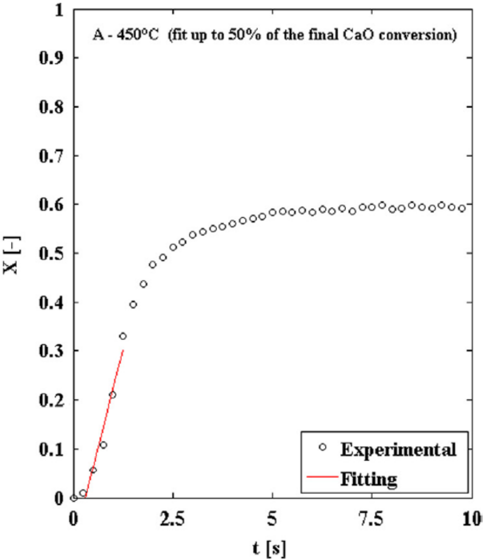


Final conversion fraction depends on temperature but also some other parameter (what?)

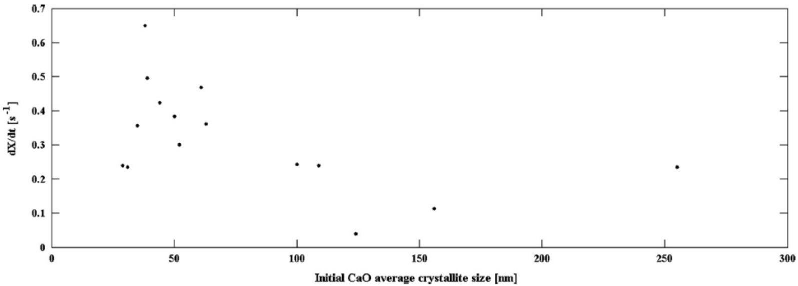


Reaction kinetics much faster than previously observed (0.28/s)

CaO-CaO_2 reaction kinetics



CaO-CaO_2 reaction kinetics



Initial crystallite size is one of the determining factors in inital rate of conversion and fraction converted.

CaO crystallite size can be related to porosity which is key to the conversion process.