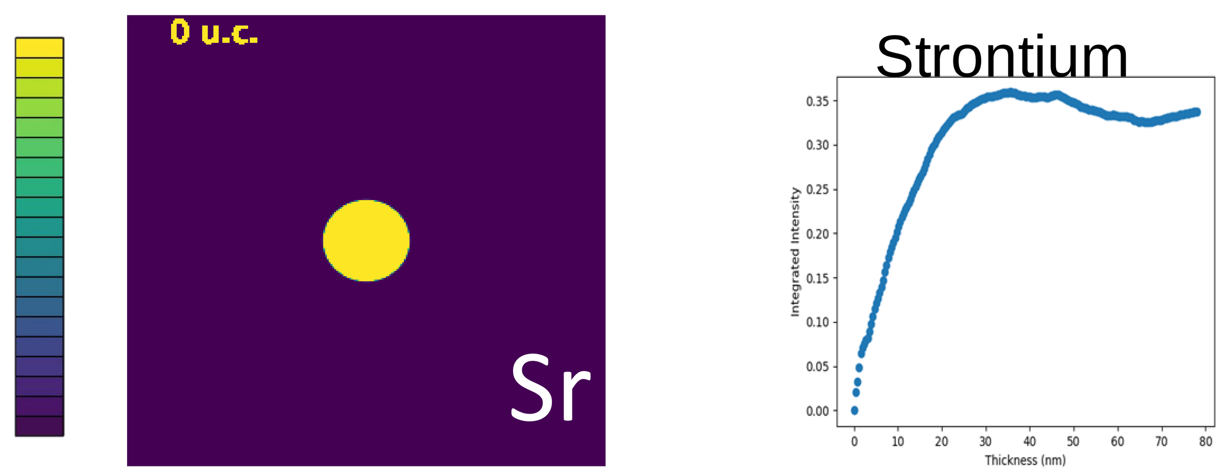
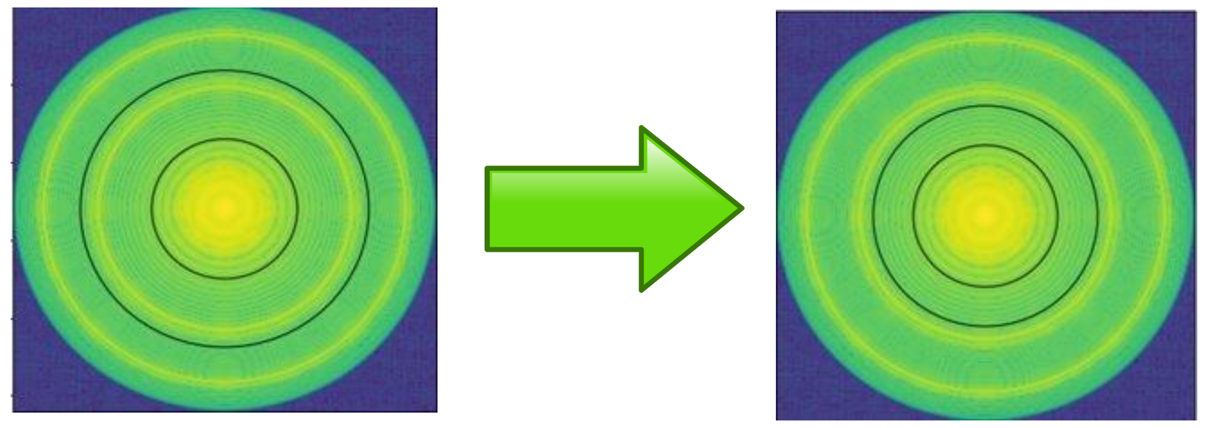
Abstract

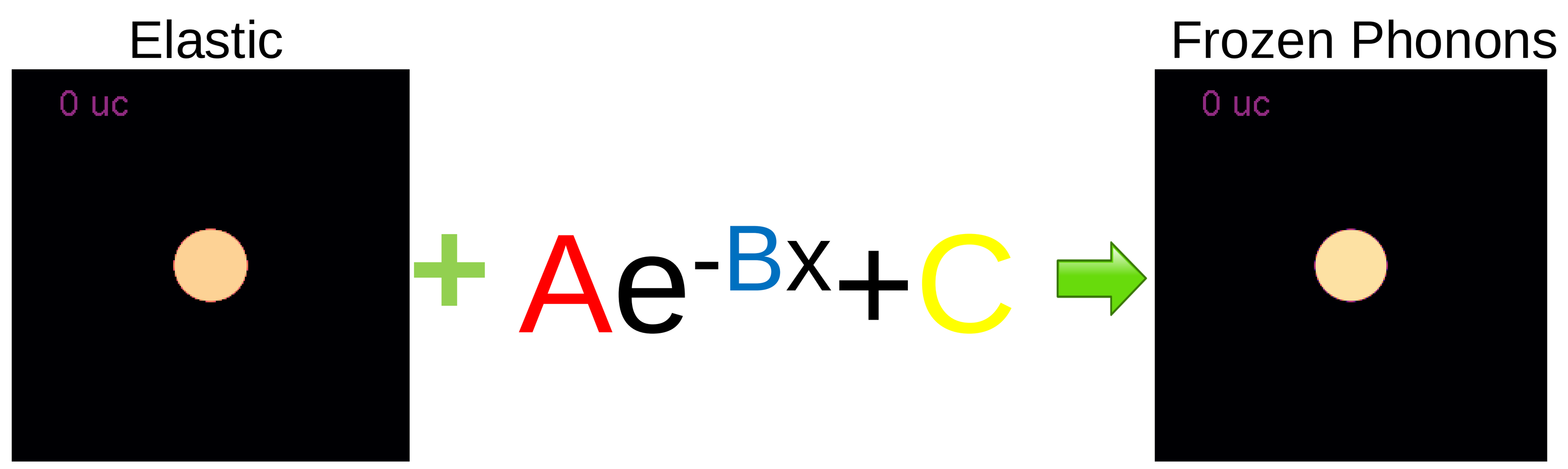
In a purely elastic model of electron diffraction, we show that the scattering in the dark field region is concentrated primarily in the higher order Laue zone (HOLZ) rings but gets redistributed across the dark field region if thermal vibrations are added into the model using the frozen phonon approximation. This high angle region in diffraction space carries information about the atomic number (Z) of the scattering species. Since the forward model in ptychography uses a purely elastic calculation for diffraction patterns ptychographic reconstructions have poor Z-sensitivity. Using a correction term, we fit the azimuthally averaged intensities in the dark field region with an exponentially decaying function, and show that the fit parameters have a correlation with Z. Using this correction term to minimize the difference between the modeled elastic pattern and experimental pattern might enable us to extract Z information.

Methods

- We performed multislice simulations of electron diffraction patterns of a $SrTiO_3$ crystal, with the probe focused on top of i) Sr column, ii) Ti-O column, and iii) O column and for thickness ranging from 0 – 200-unit cells. The simulations were done using the abTEM simulation package.
- We compared diffraction patterns simulated with a pure elastic model as well as with the frozen phonon model, the latter used to include the effects of thermal vibrations.



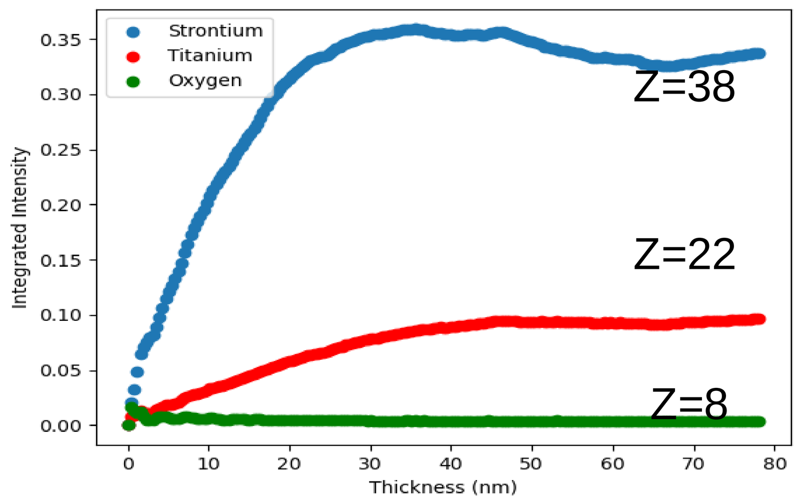




Results/Findings

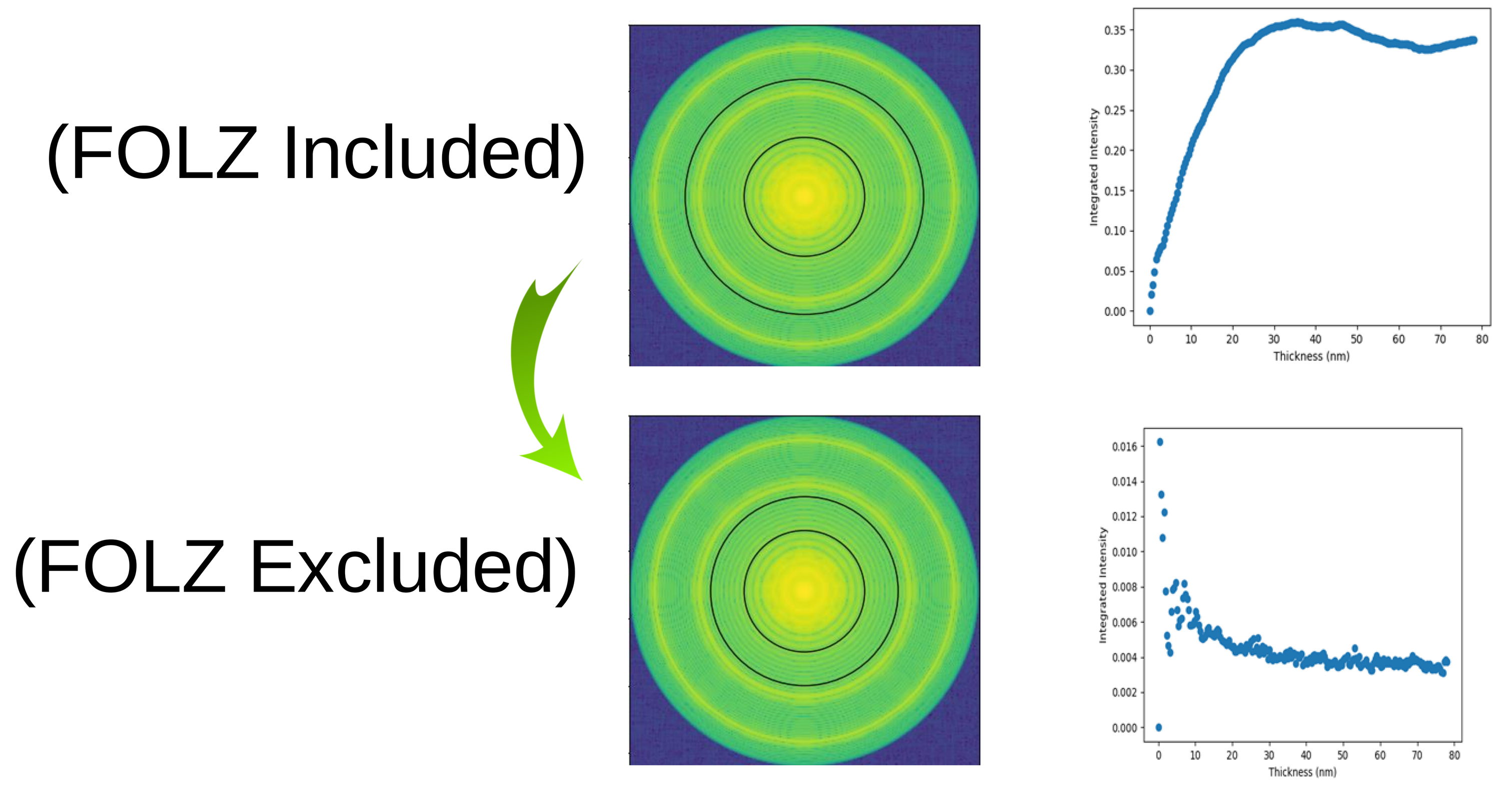
(I) Graphing Intensities

- We concluded that there is a direct relationship between the scattered dark field intensities and the atomic number, where a high atomic number yields higher intensity and vice versa with lower atomic numbers.



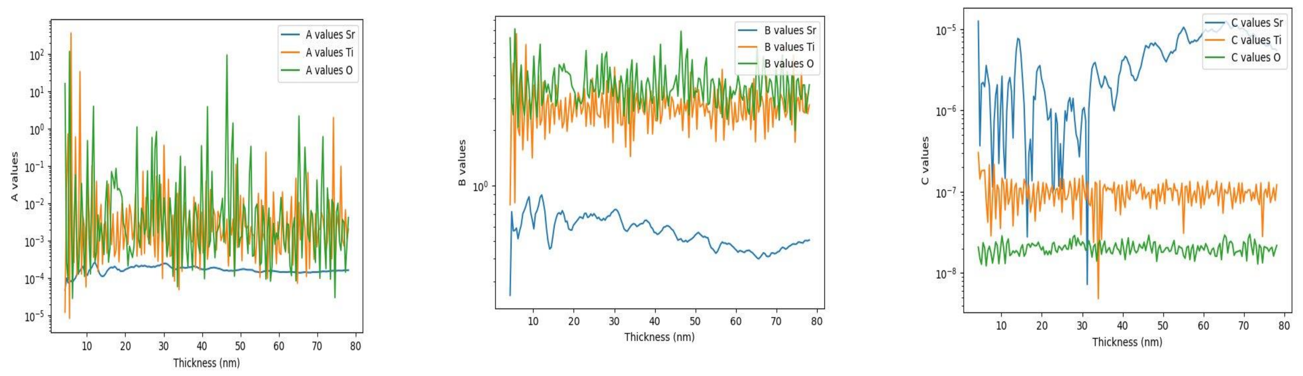
(II) Excluding FOLZ

- After we excluded the FOLZ, we saw from the graphs that the intensity percentage decreased greatly, which helped us conclude that most of the scattered intensity is concentrated in the First Order Laue Zone (FOLZ).

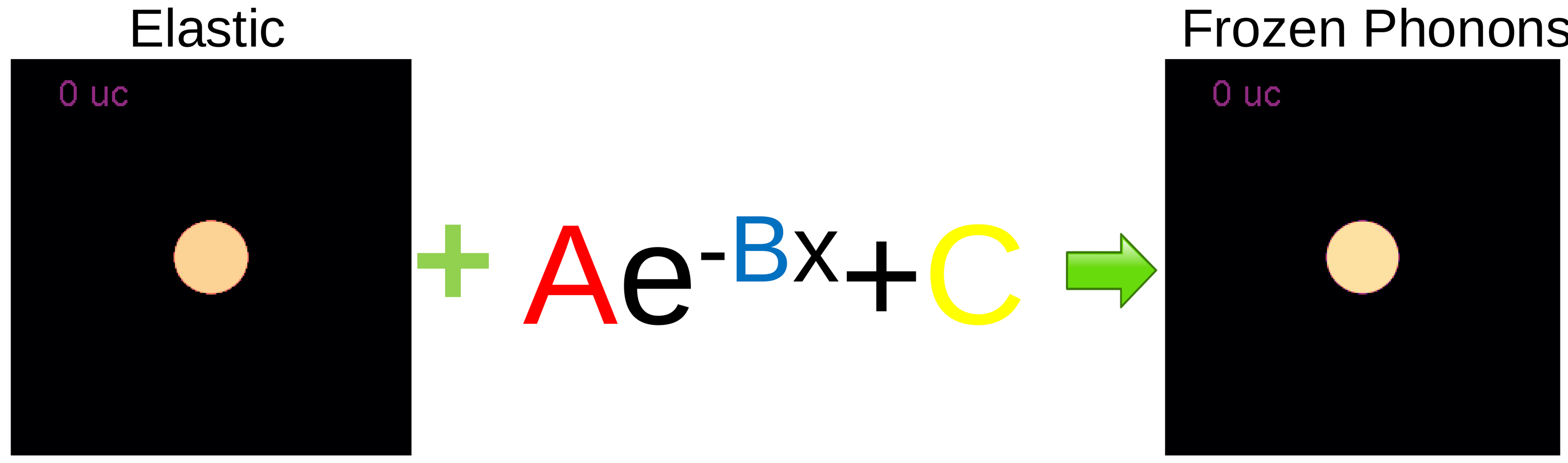


(II) Using Correction Term

- When we used the correction term on all of the diffraction patterns to try and mimic the frozen phonons model, we were looking for a correlation with thickness and atomic number. Although we did not see a trend with the thickness, we noticed a trend with atomic number. The trend we saw was in the "B" and "C" parameters, where a high atomic number yields a low "B" value, and a high atomic number yields a high "C" value.



Future Work



- Since we saw a qualitative trend with the "B" and "C" fit parameters, in future experiments, we can use different diffraction patterns, and we will get different "A," "B," and "C" values, we can still expect a trend with the "B" and "C" values in the future as well.

Summary/Conclusions

- In conclusion, we concluded that there is a direct relationship between the scattered dark field intensities and the atomic number, where a high atomic number yields higher intensity and vice versa with lower atomic numbers.
- We also found that most of the scattered intensity in a pure elastic calculation is concentrated in the FOLZ ring because we saw the key difference between the intensity percentages when the FOLZ ring was excluded.
- A simple exponential fit to model the dark field region in a frozen phonon calculation shows Z-dependence on some parameters, which could be useful in extracting Z information from ptychographic data.

References/Acknowledgements

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