An all-order Phonon approach to Thermal Diffuse Scattering

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Thermal Diffuse Scattering (TDS)

- X-ray-phonon scattering is the source of TDS, occurs in all materials involves all phonons[1]
- Often TDS is a nuisance as it is broad in reciprocal space, overlapping other features

Motivation

- Phonons: Crucial for understanding material properties, including superconductivity and elastic properties, relevant to fields like geology and in quantum phase transitions
- Detecting phonon anomalies is essential for understanding and explaining novel material properties
- Current software: TDS analysis relies on single phonon approximations and lacks computational efficiency, need for new solutions[2]

Simulation Approach

1. DFT → Dynamical Matrix
2. Dynamical Matrix → k, ω, ε
3. k, ω, ε → γ (via FTT) → Γ
4, Γ → Diffuse Scattering (via Yell[3])

Results

- Accurate reproduction of measured diffuse scattering intensities; calculations take seconds to minutes
- Slight inaccuracies in Bragg peaks due to incomplete application of multiplicities, to be addressed in an upcoming update

Outlook

- Other sources for the dynamical matrix: Universal potentials[4] or semi-empirical methods
- Apply to systems like Magnetite or Lanthanum Manganite, which exhibit interesting effects due to lattice dynamics but are overshadowed by thermal diffuse scattering

References

[1] Bosak, A. et al. J. Phys. D: Appl. Phys, **2015**, 48, 504003
[2] Wehinger, B. et al. Phys. Rev. Lett, **2017**, 118, 035502
[3] Simonov A. et al. Y, J Appl Crystallogr, **2014**, 47, 1146–1152
[4] Lee, H. & Xia, Y. Appl Phys, **2024**, 124, 102202
[5] Xu, R. & Chiang, T. C. Z. Kristallogr. Cryst. Mater, **2009**, 220, 1009–1016

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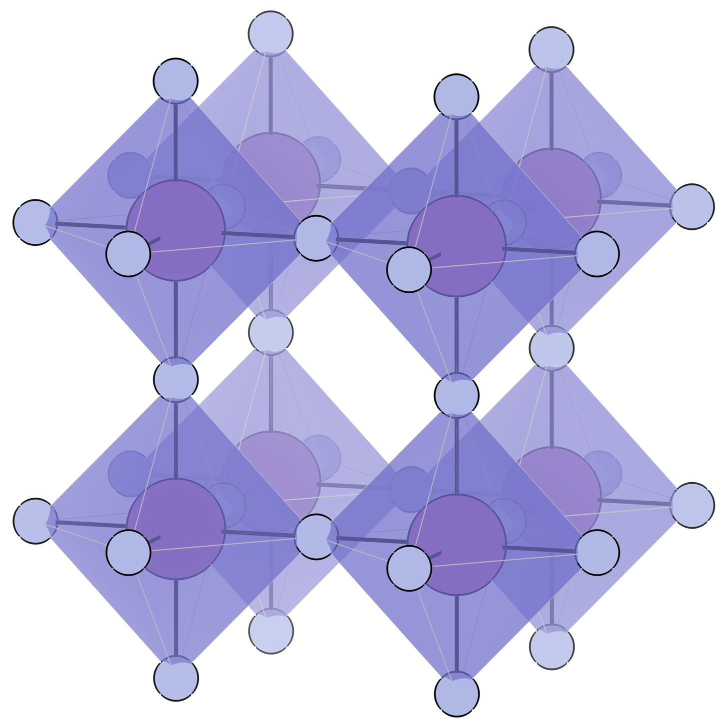
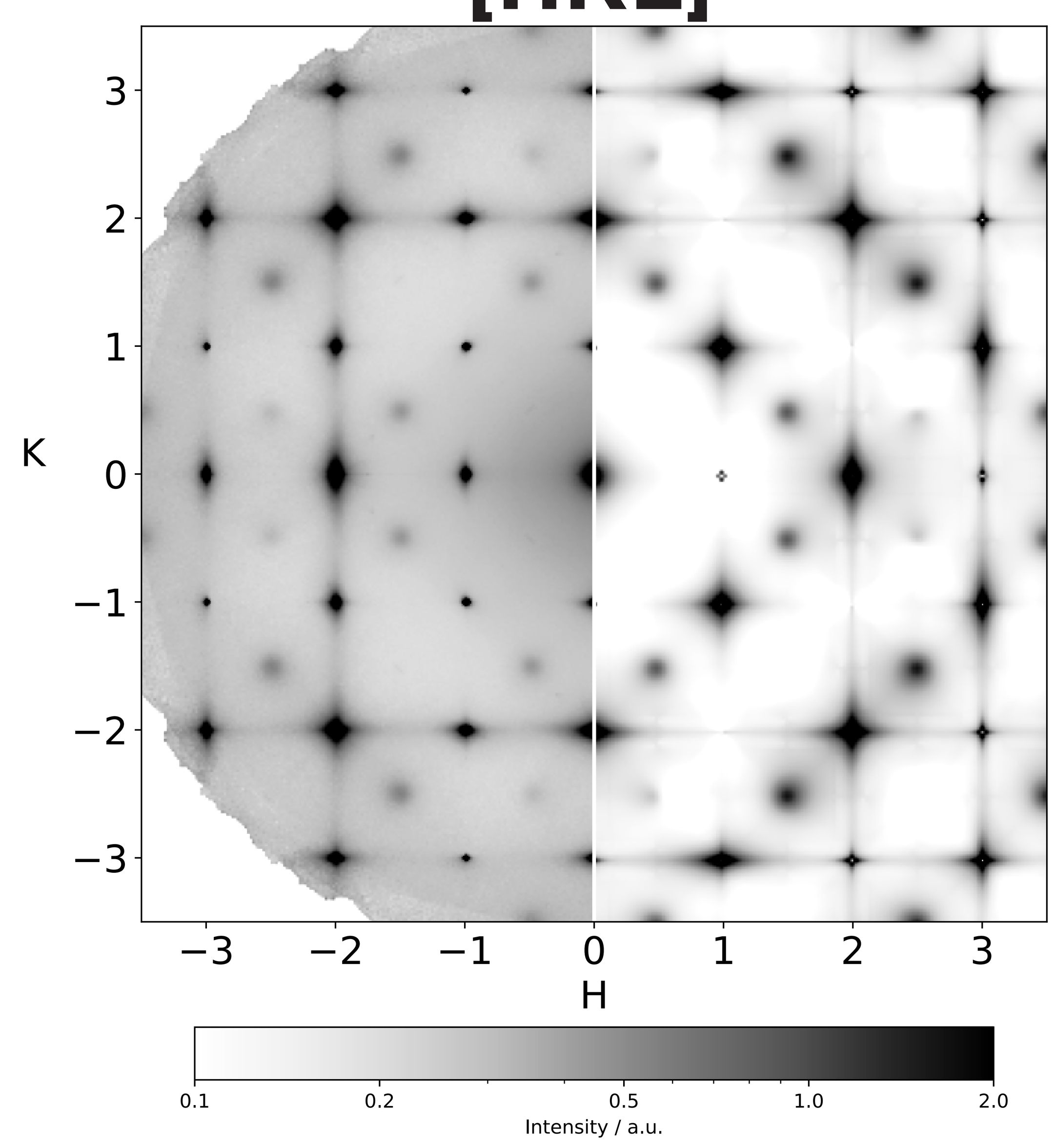
ScF_3 Crystal Structure: Pm-3m

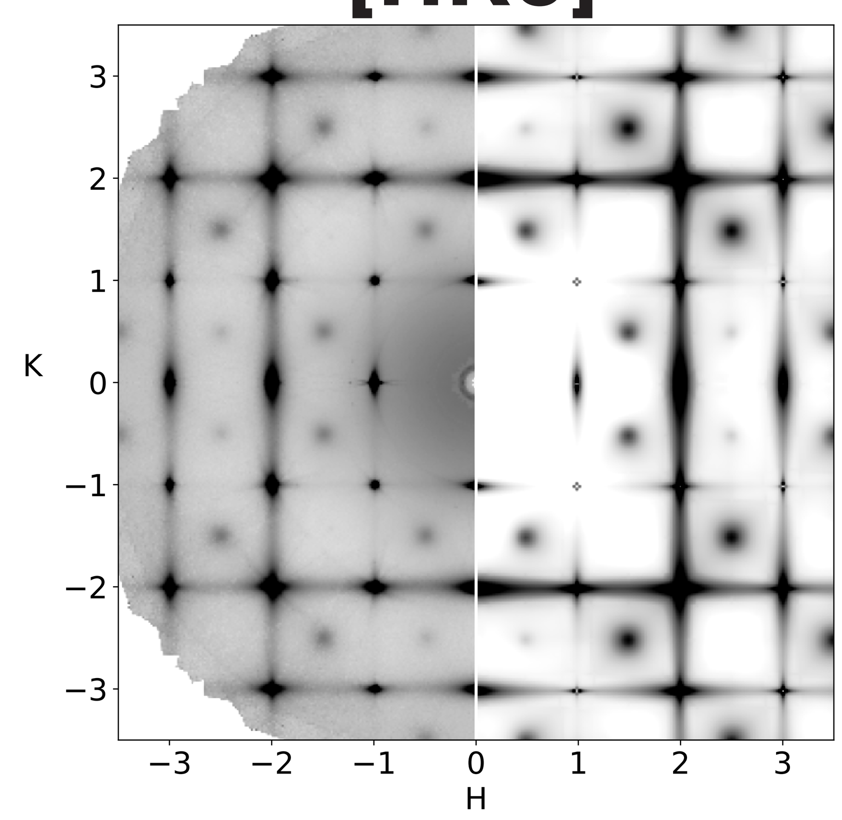


Measured | Simulated

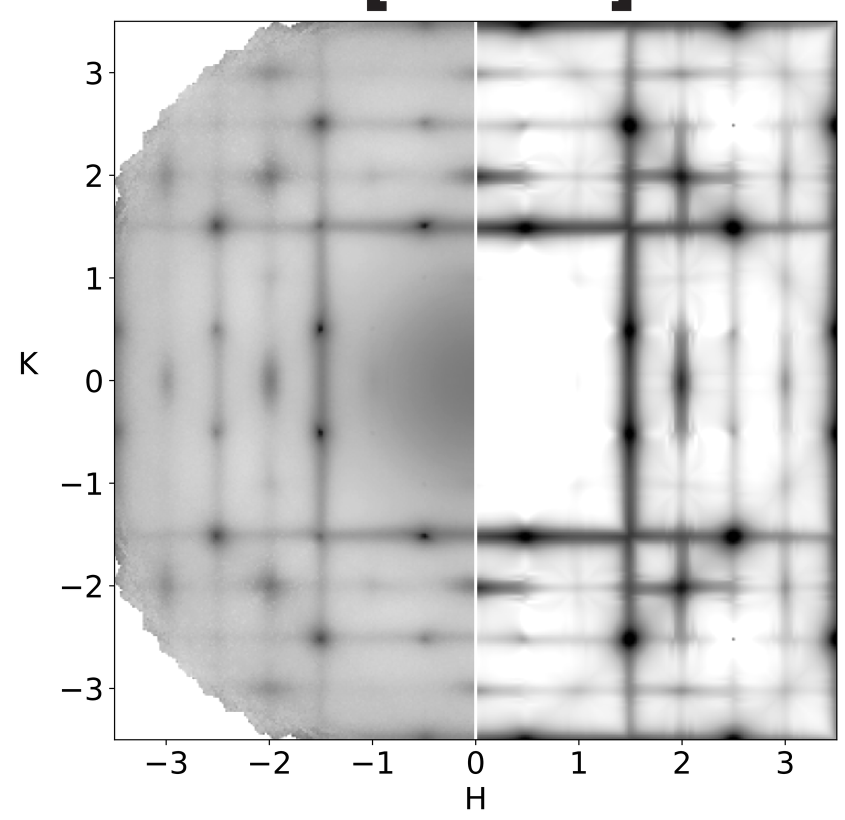
[HK1]



[HK0]



[HK½]



Reciprocal Space: correlated-ADPs:[5]

$$\gamma_{s,s'}(\mathbf{k}) = \frac{\hbar}{2\sqrt{\mu_s \mu_s}} \sum_j \frac{1}{\omega_{\mathbf{k},j}} \coth\left(\frac{\hbar\omega_{\mathbf{k},j}}{2k_B T}\right)\left(\mathbf{e}^*_{\mathbf{k},j,s} \otimes \mathbf{e}_{\mathbf{k},j,s'}\right)$$