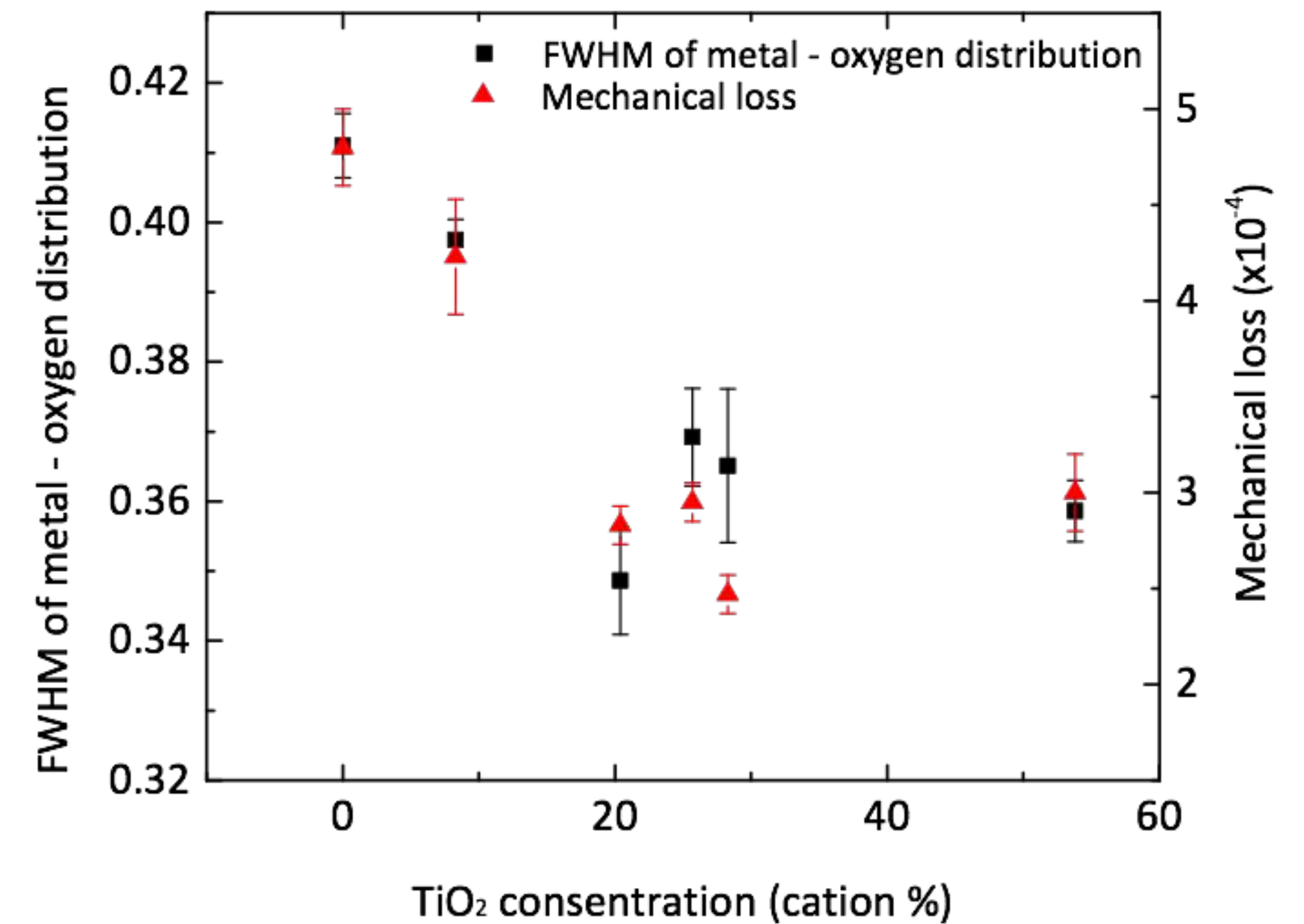# Atomic Structure

Riccardo Bassiri

Stanford University

G1702166

Introduction

- Changes in mechanical loss are the result of changes in atomic structure

Introduction

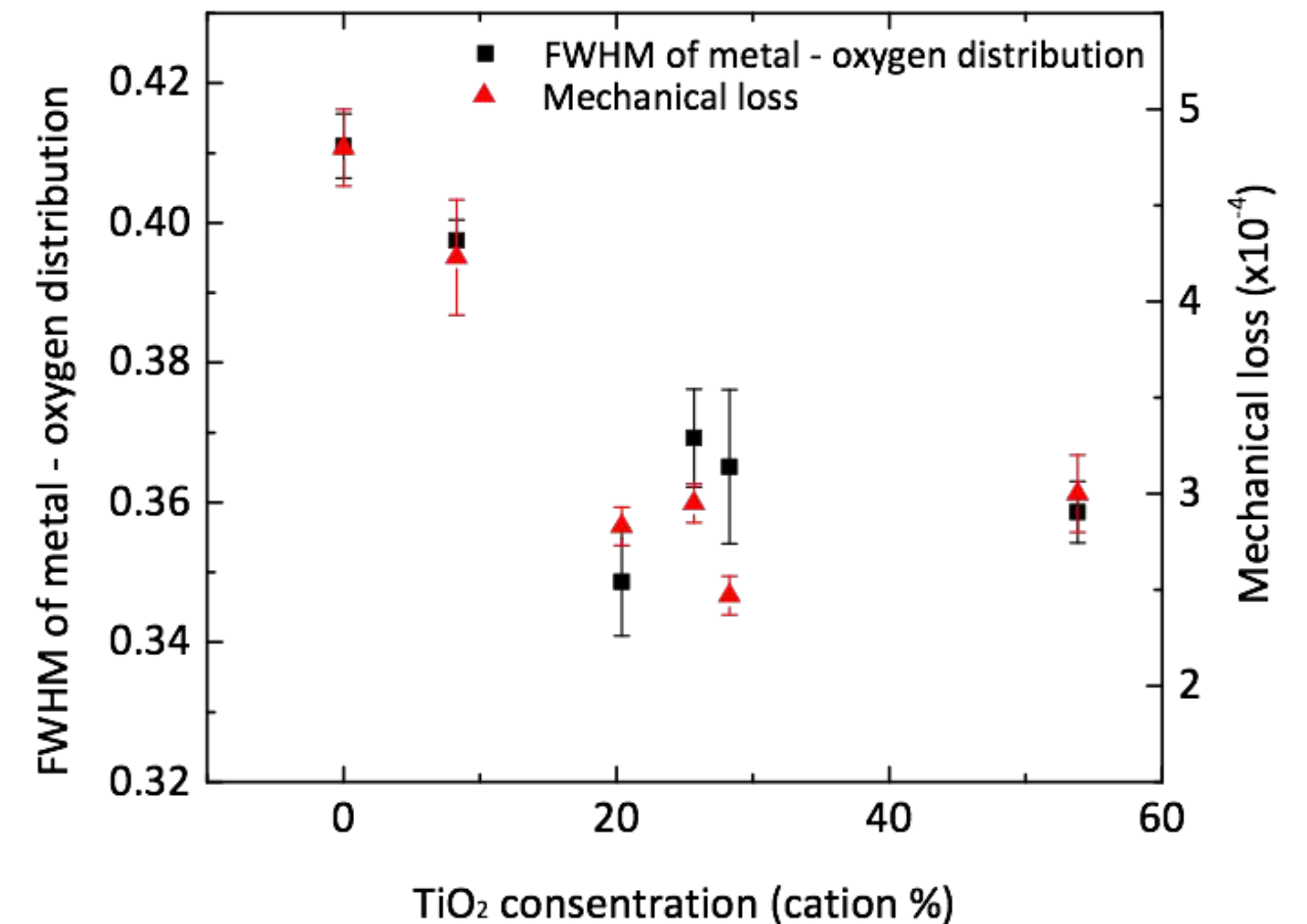- Changes in mechanical loss are the result of changes in atomic structure

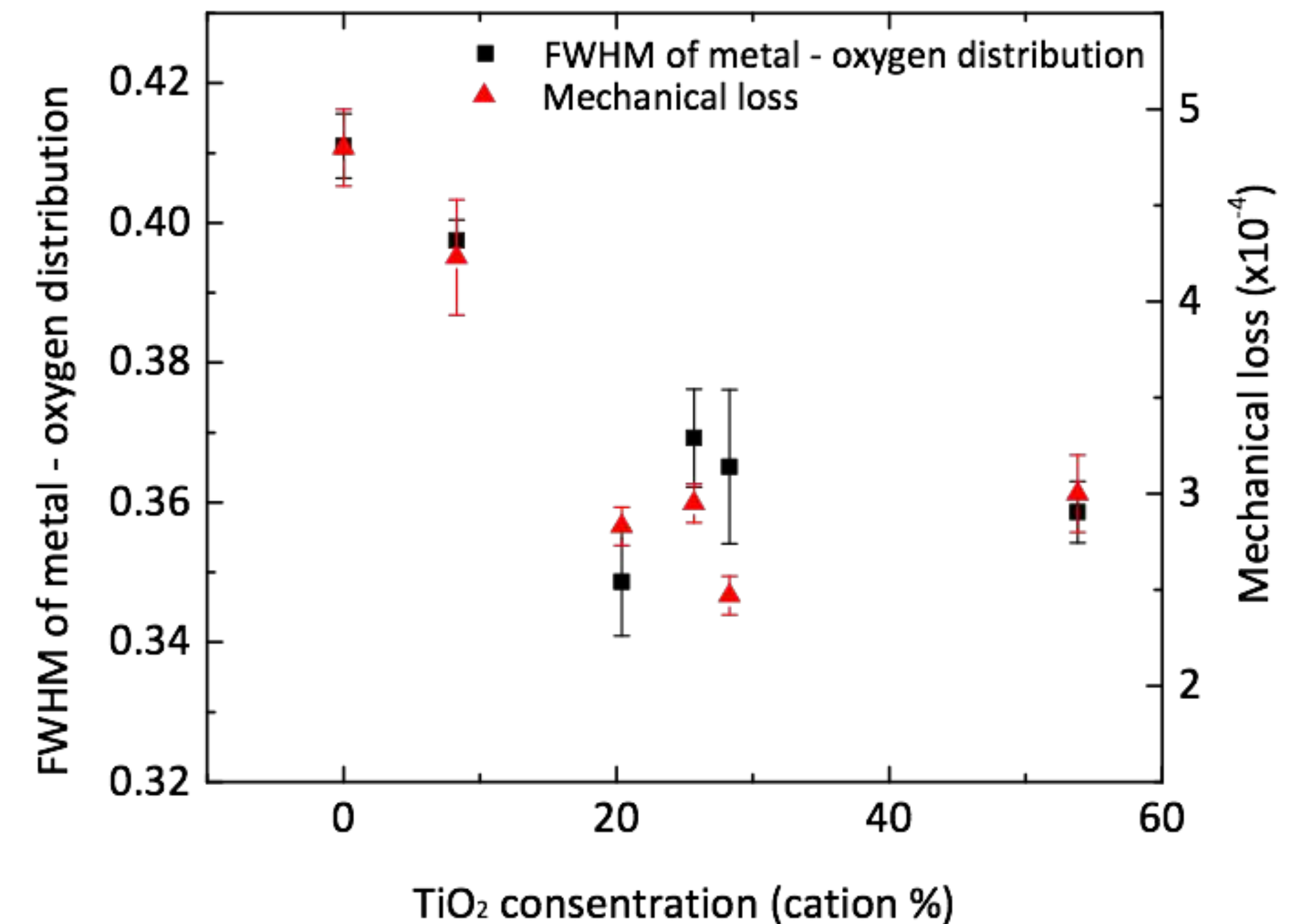[R Bassiri et al, Acta Mat., **61**, 1070-1077 (2013)]

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- Measure structure at the short (< 0.5 nm) and medium range (> 0.5 nm)

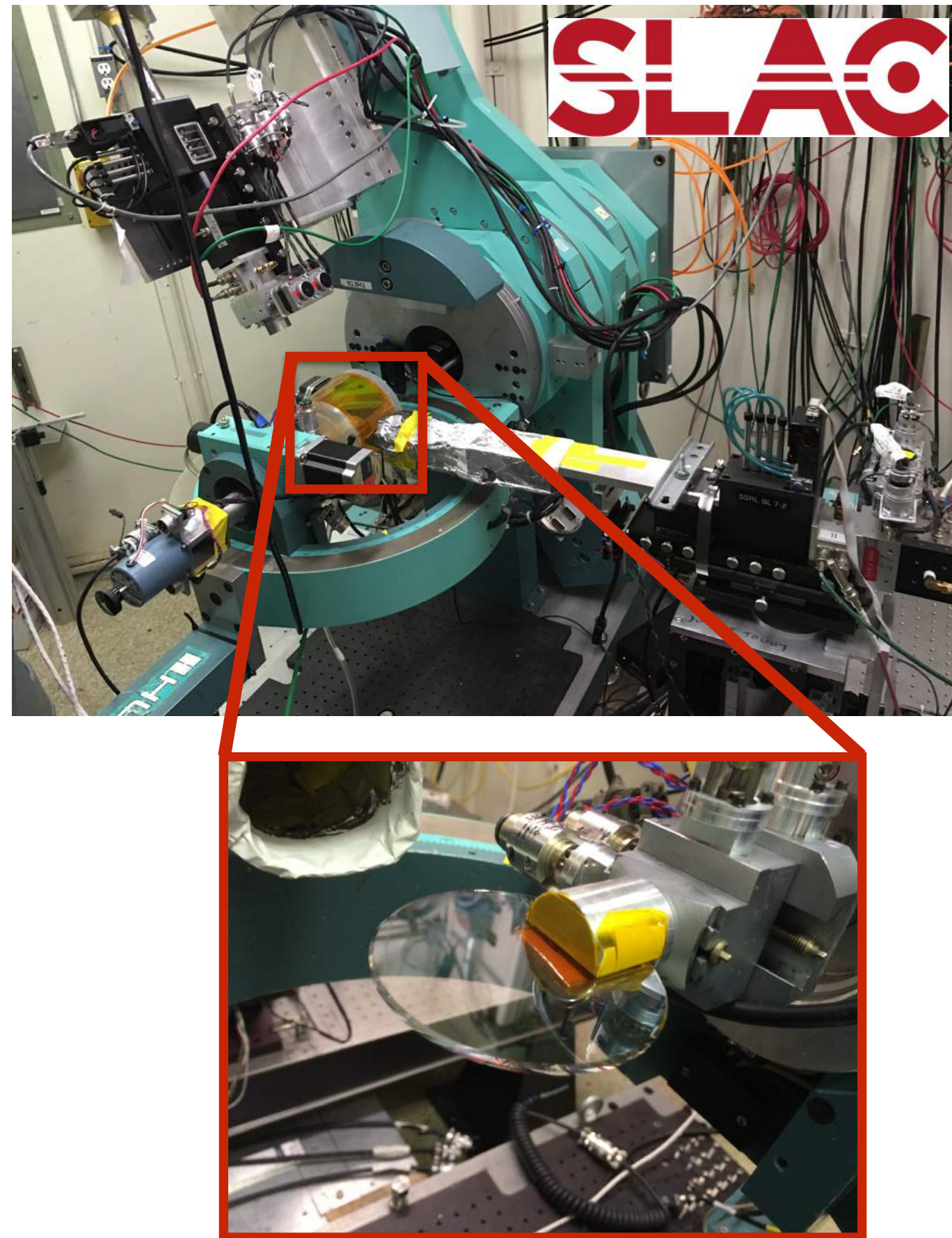[R Bassiri et al, Acta Mat., **61**, 1070-1077 (2013)]

Introduction

- **Changes in mechanical loss are the result of changes in atomic structure**

- Measure structure at the short (< 0.5 nm) and medium range (> 0.5 nm)

- Two main measurement techniques:
  - GI-PDFs
  - FEM

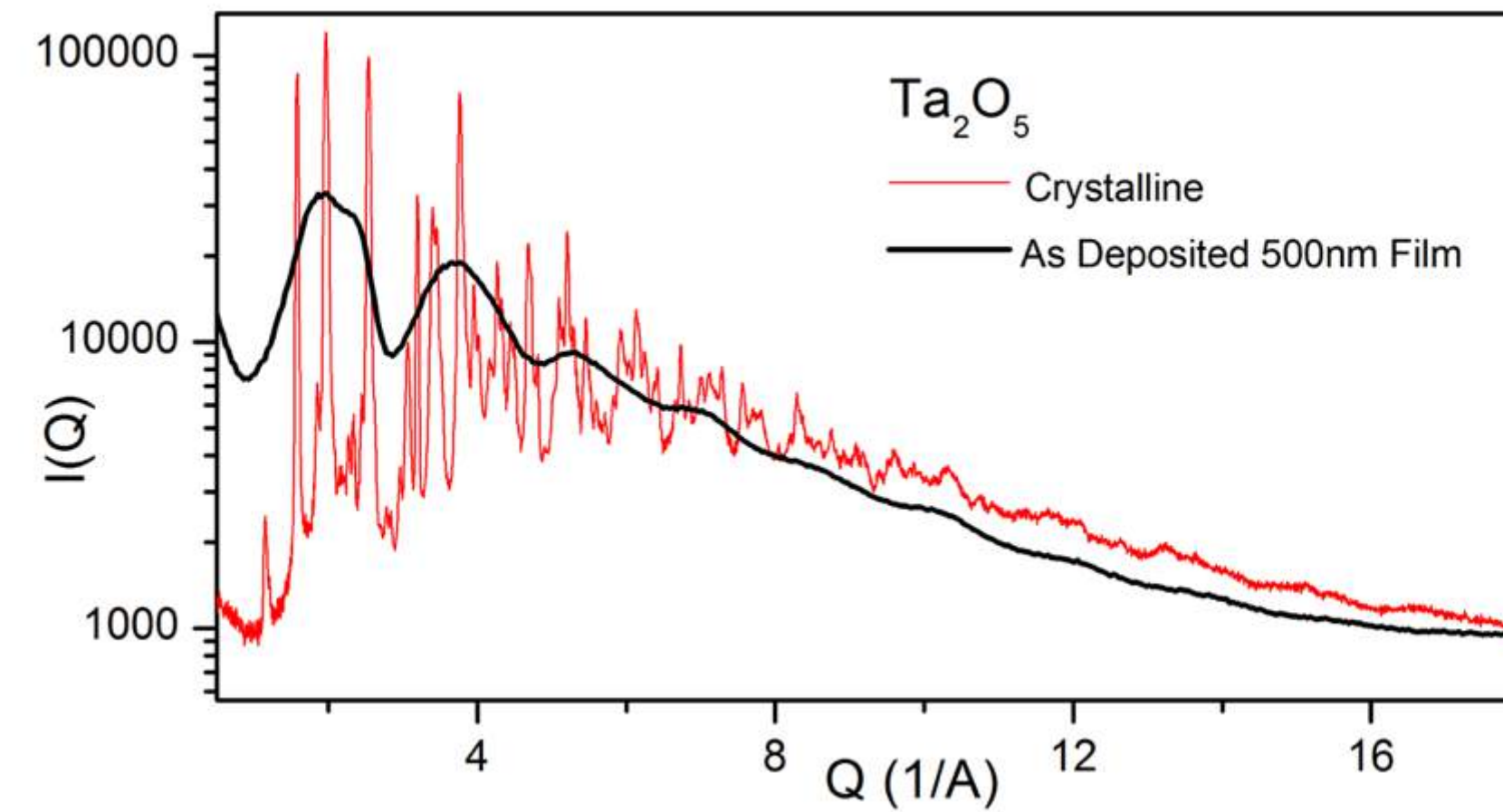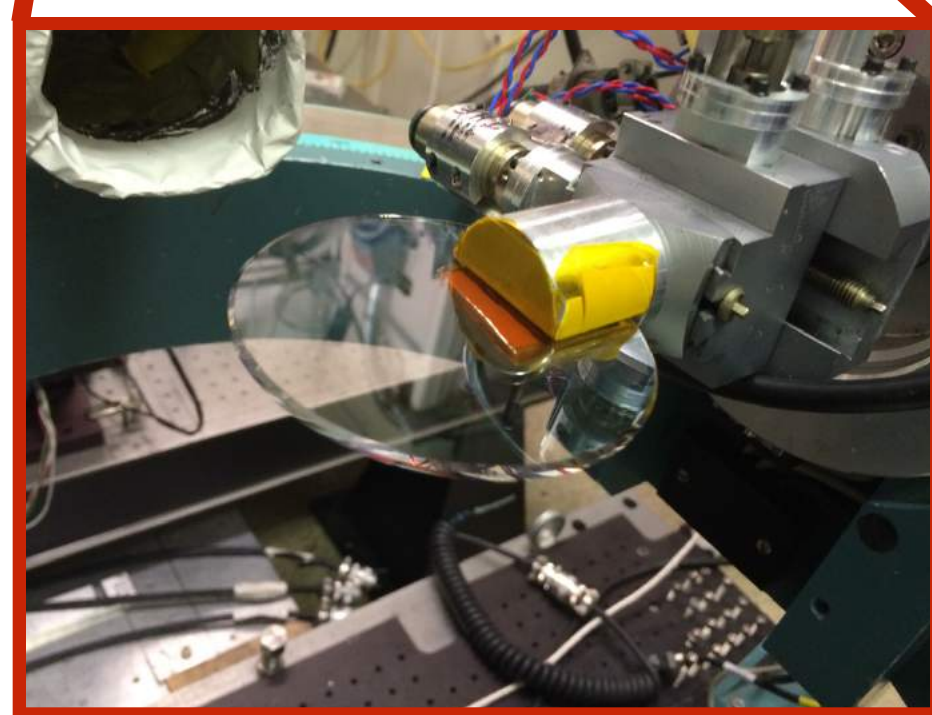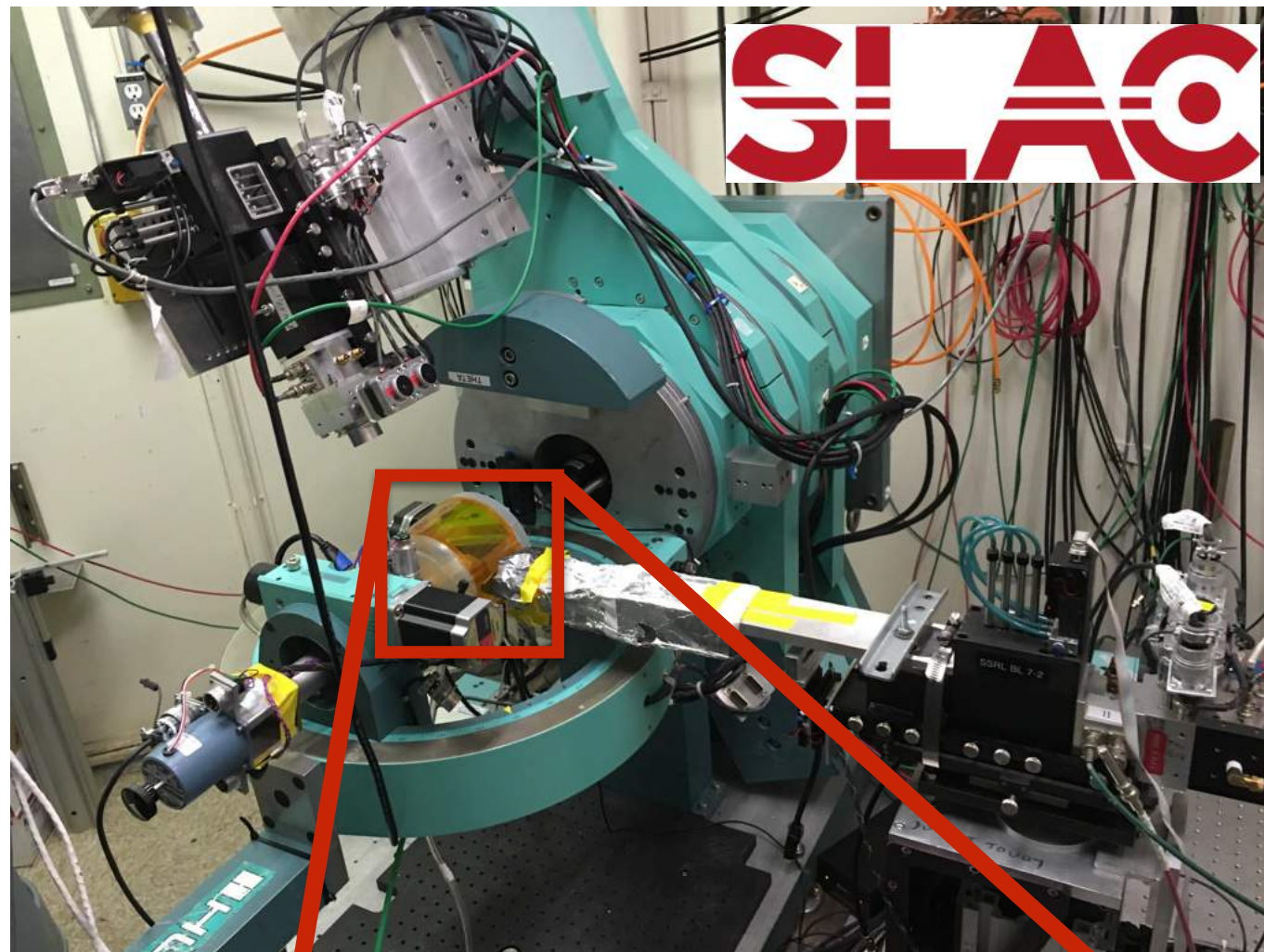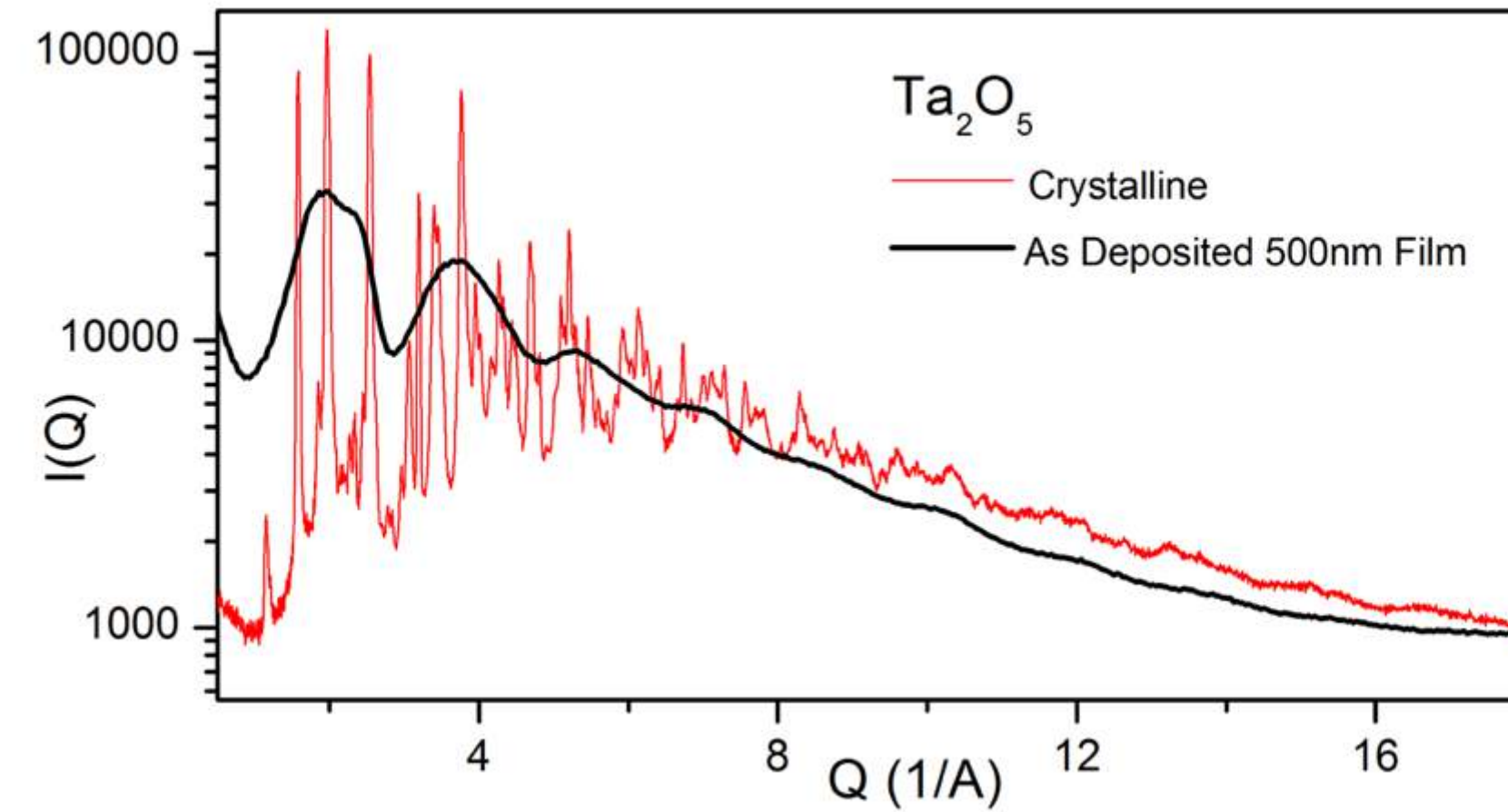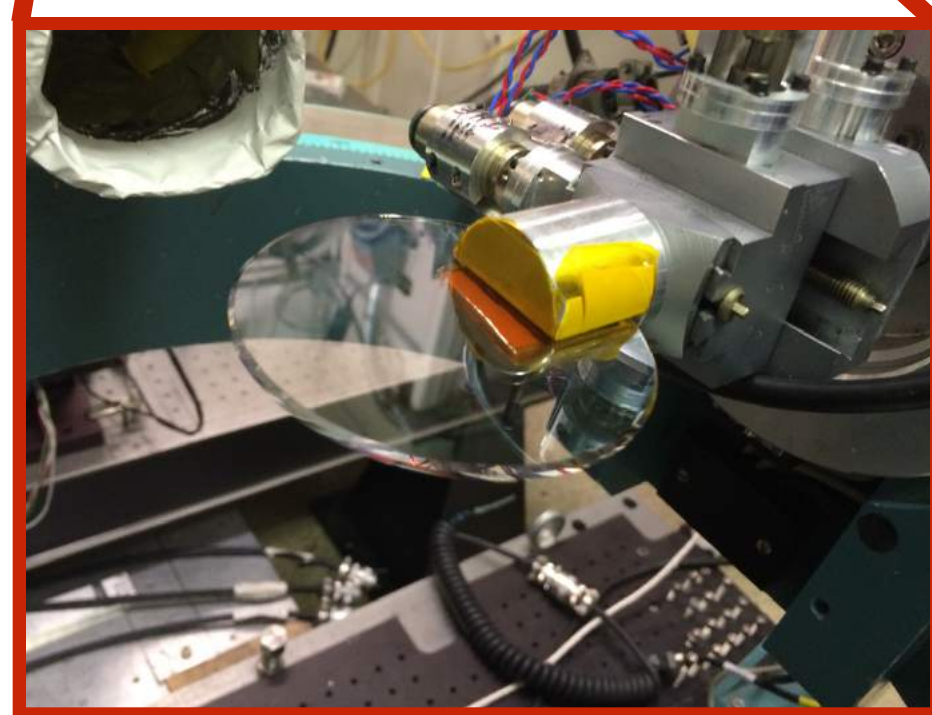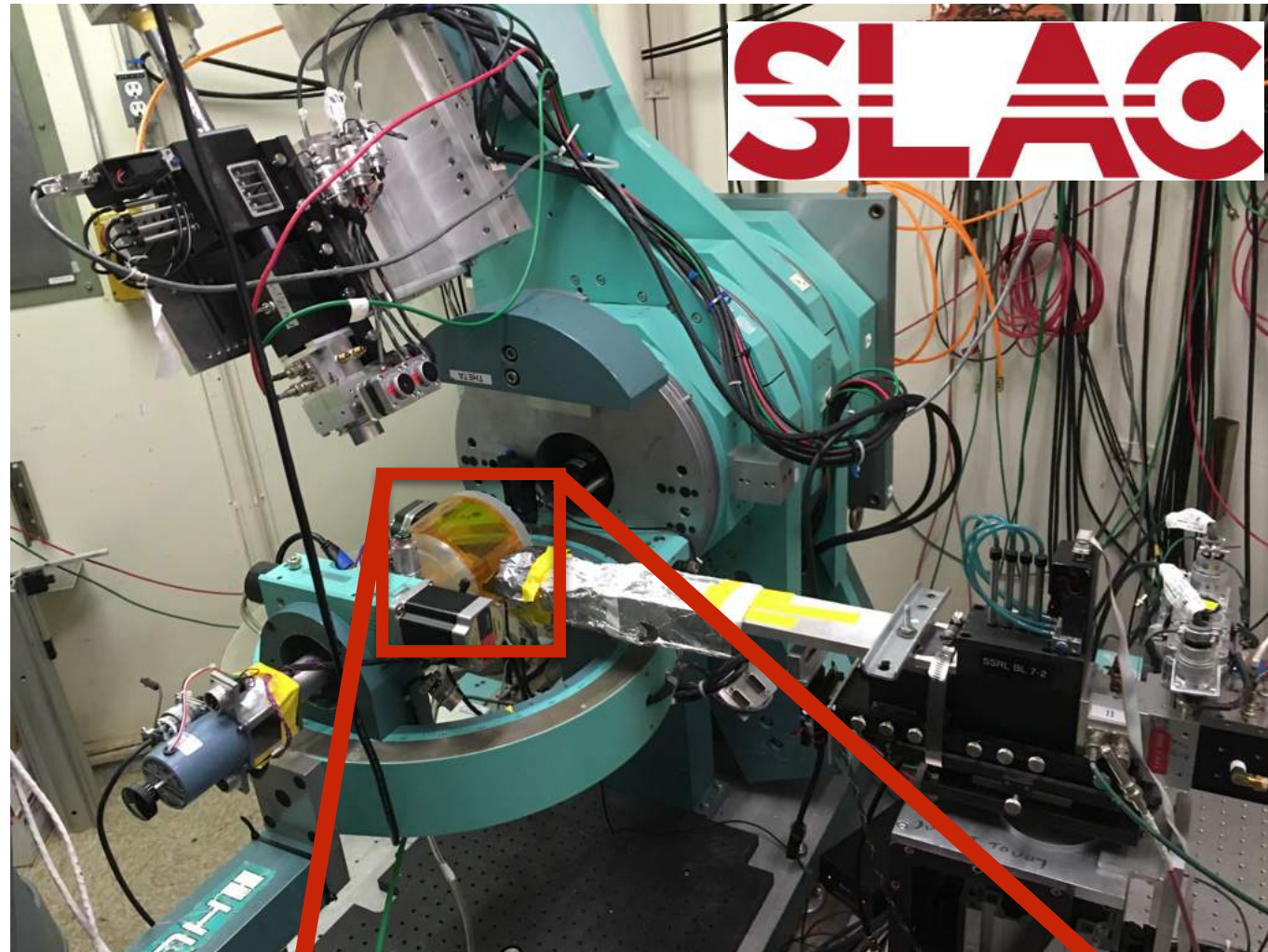[R Bassiri et al, Acta Mat., **61**, 1070-1077 (2013)]

Measurement techniques:

GI-PDF: Grazing Incidence Pair Distribution Functions

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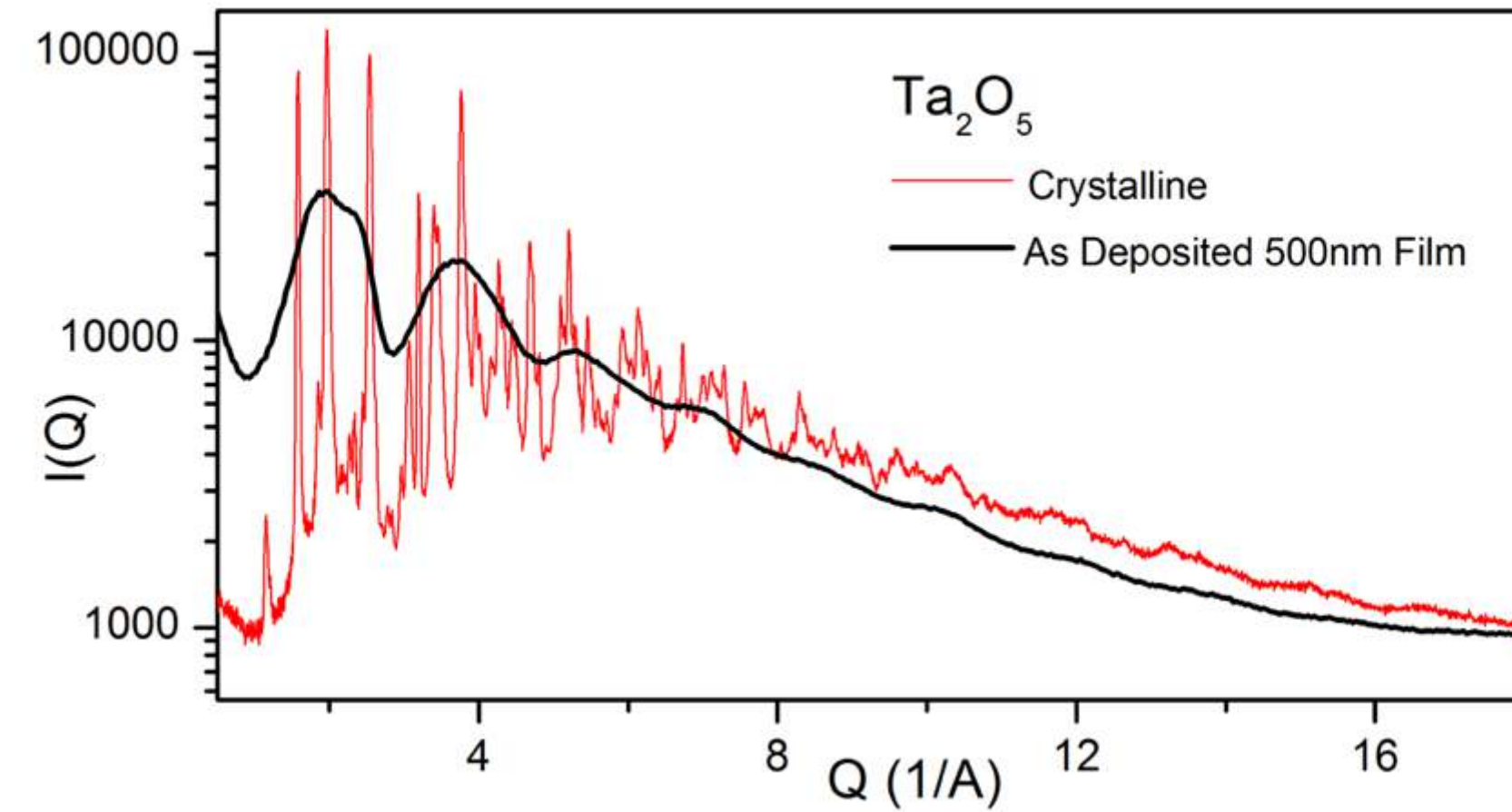## *GI-PDF: Grazing Incidence Pair Distribution Functions*

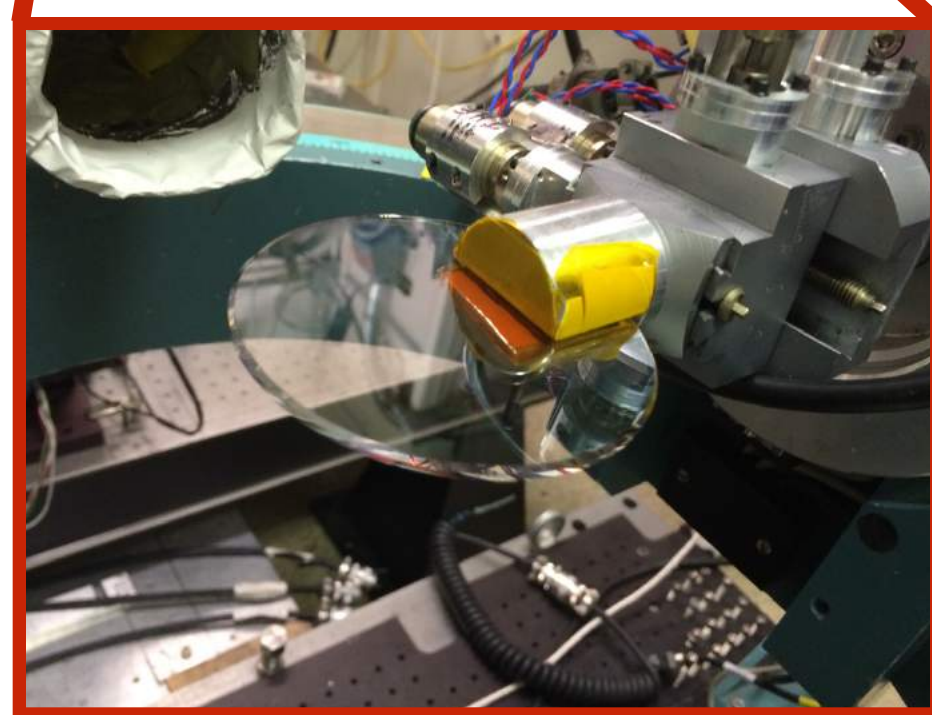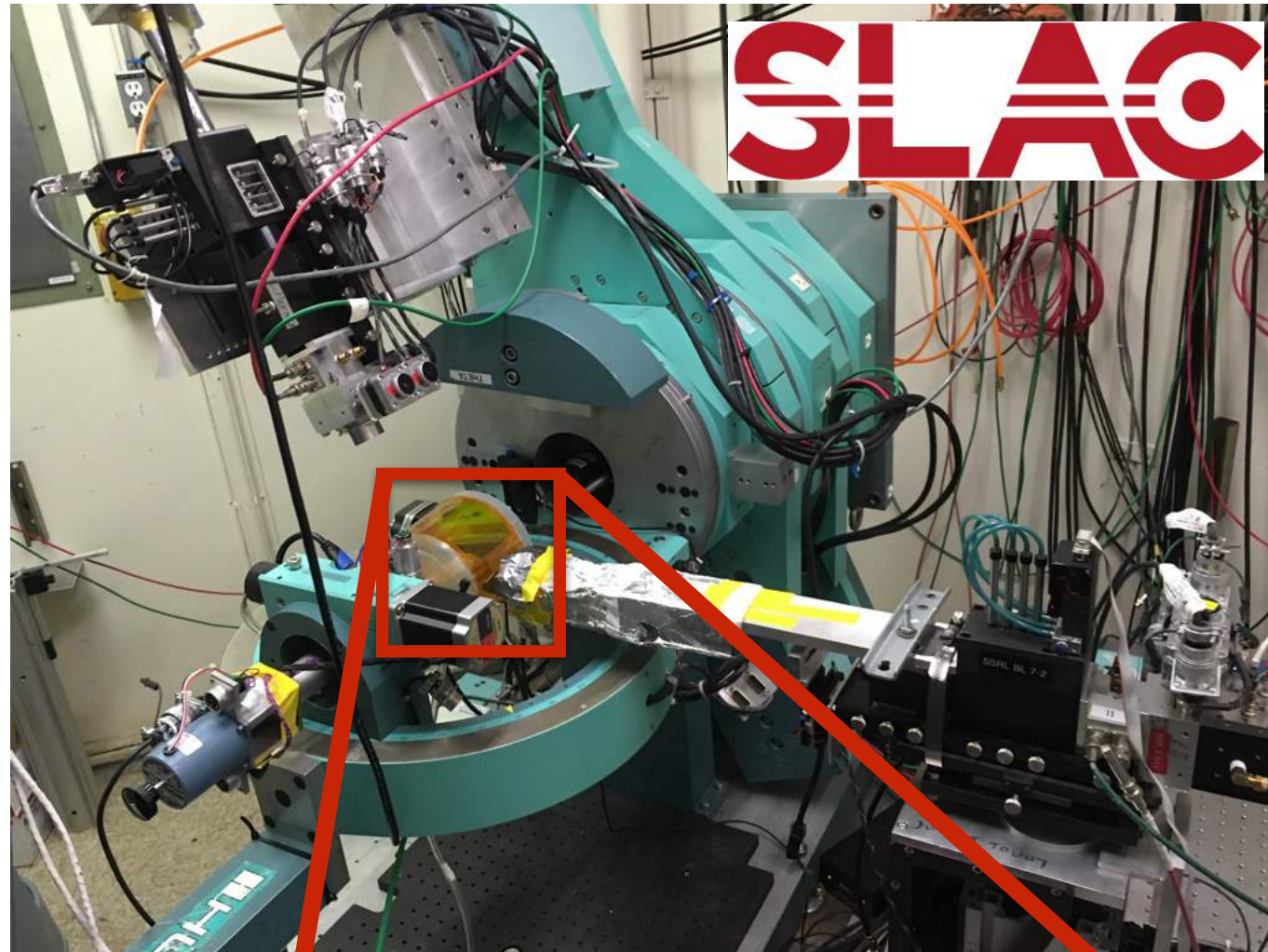$$G(r) = 4 \int_0^\infty \varphi(q) sin(qr) dq$$
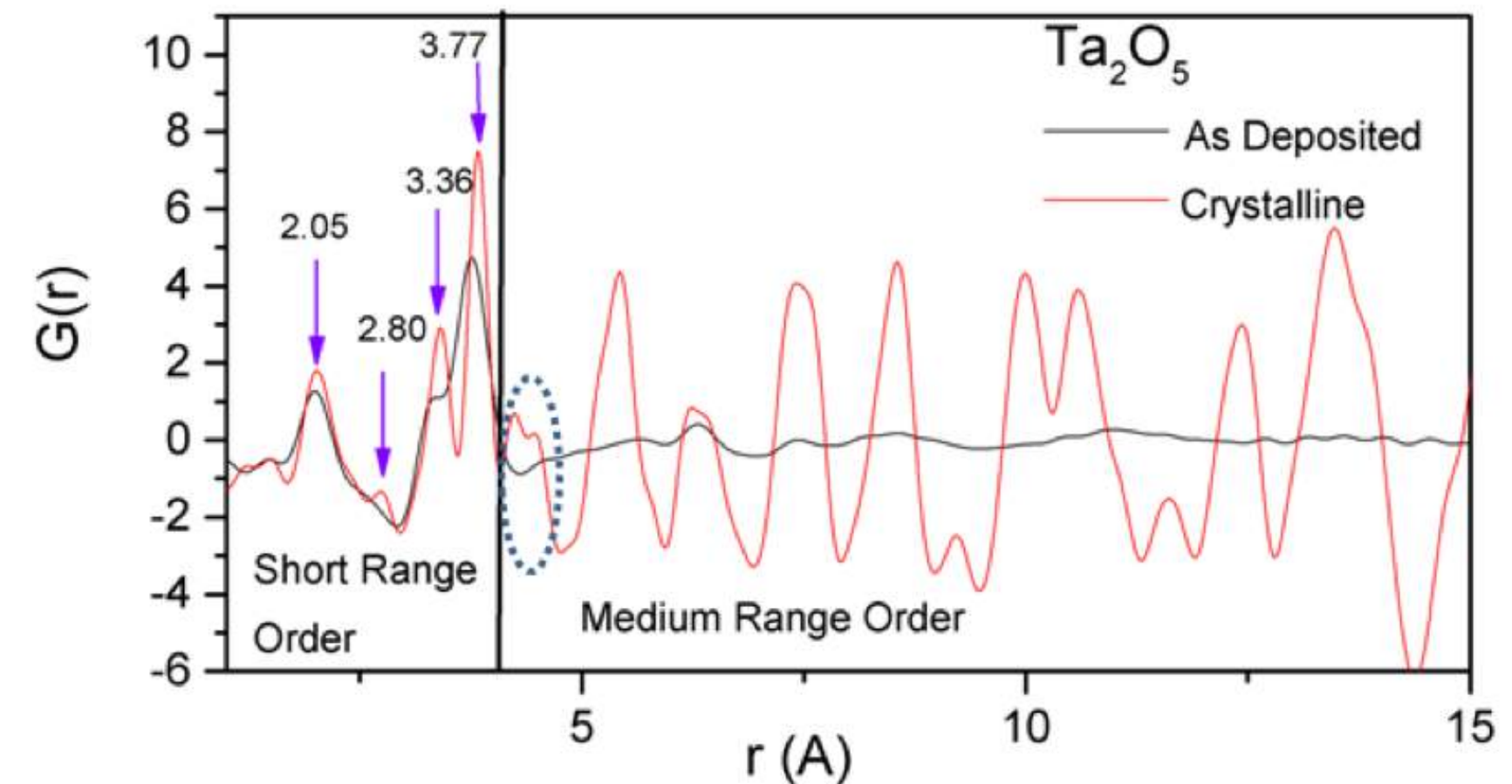
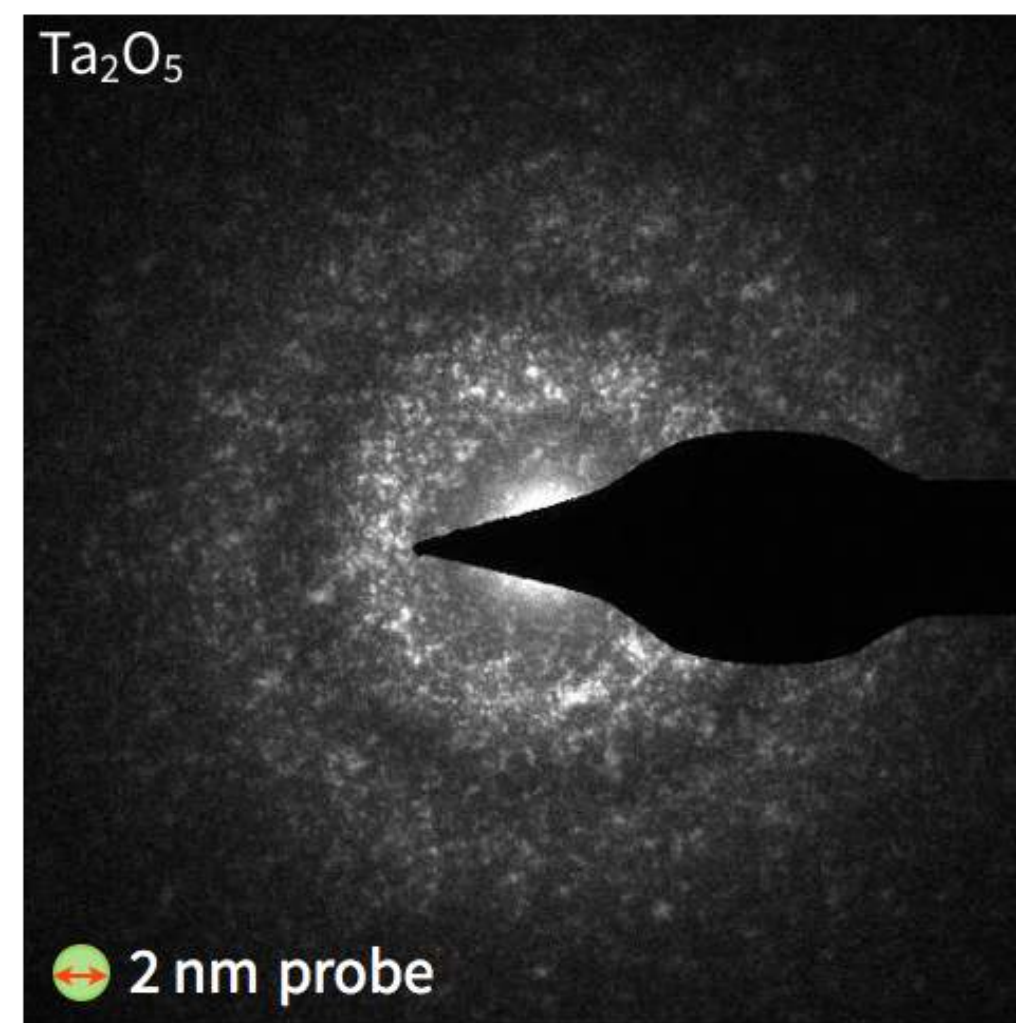# Measurement techniques:

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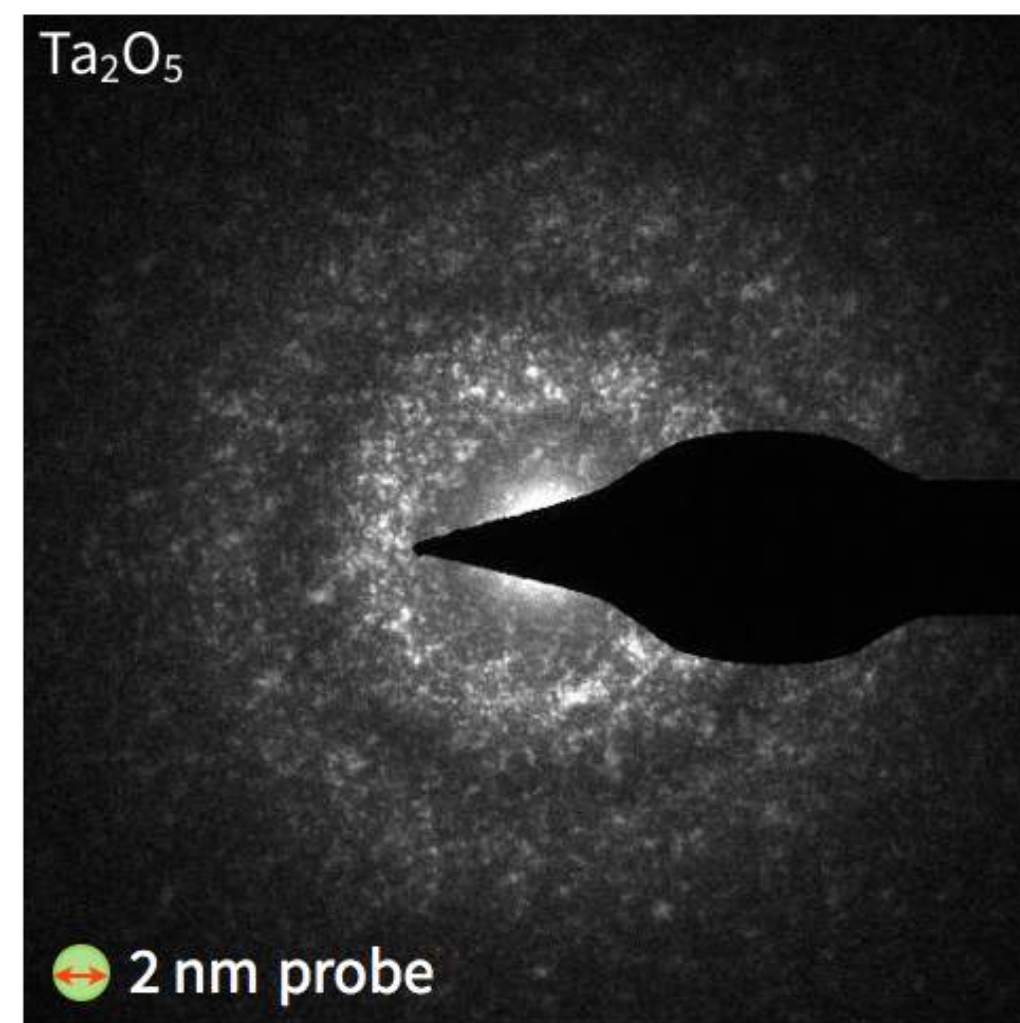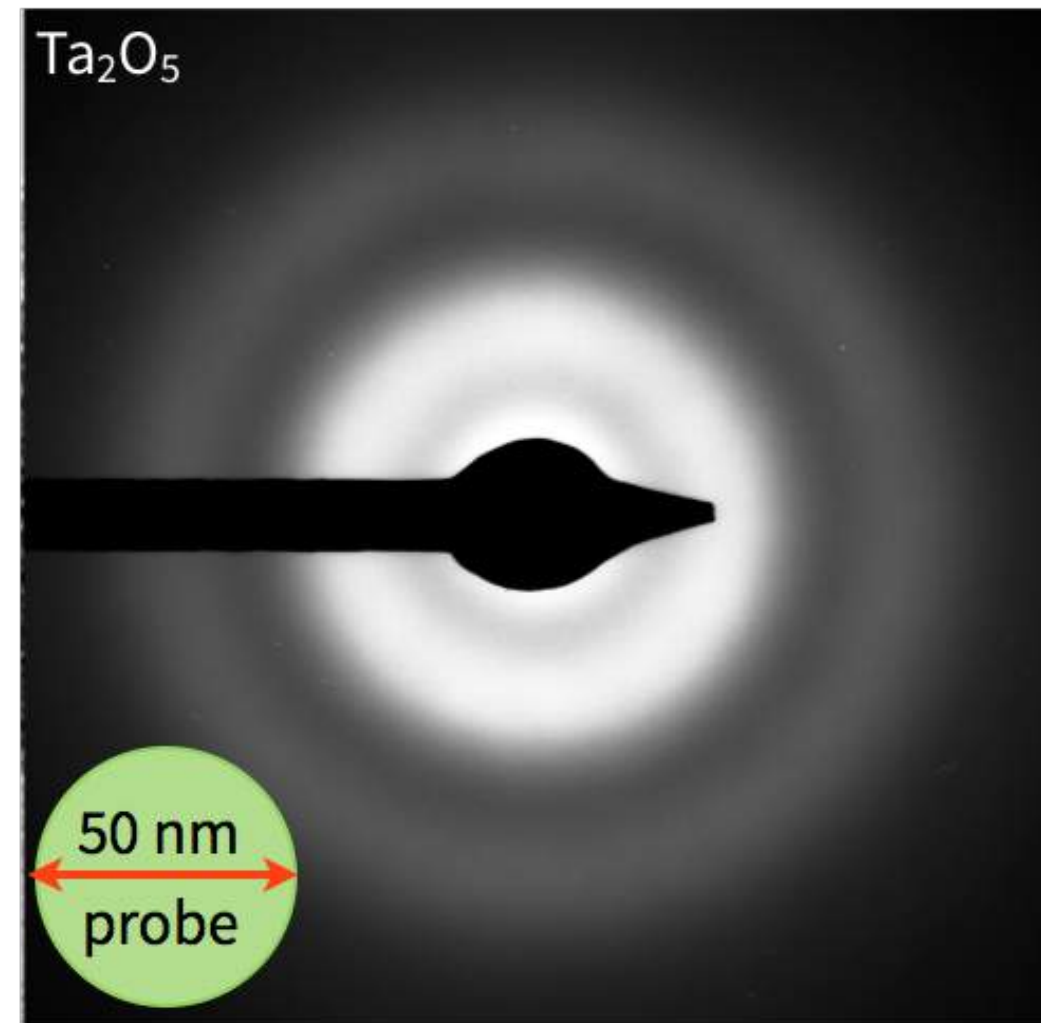
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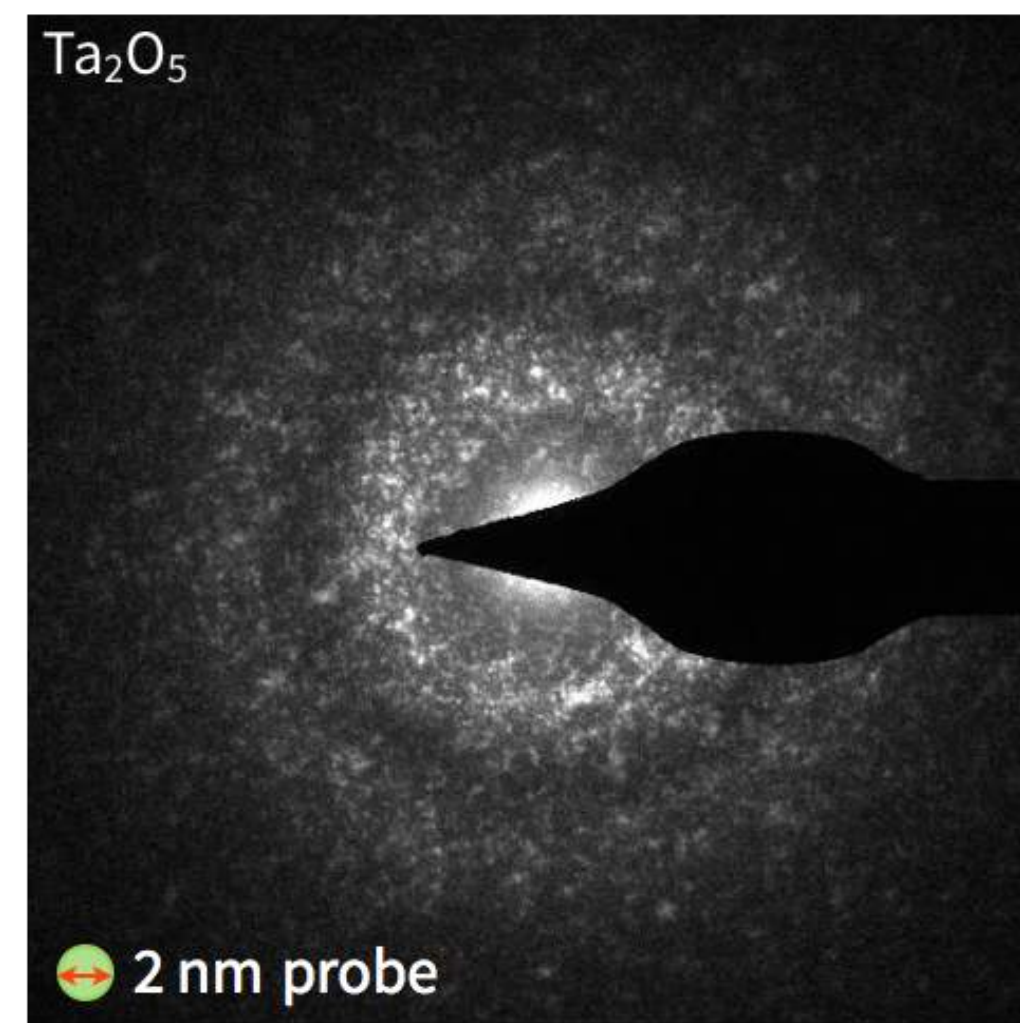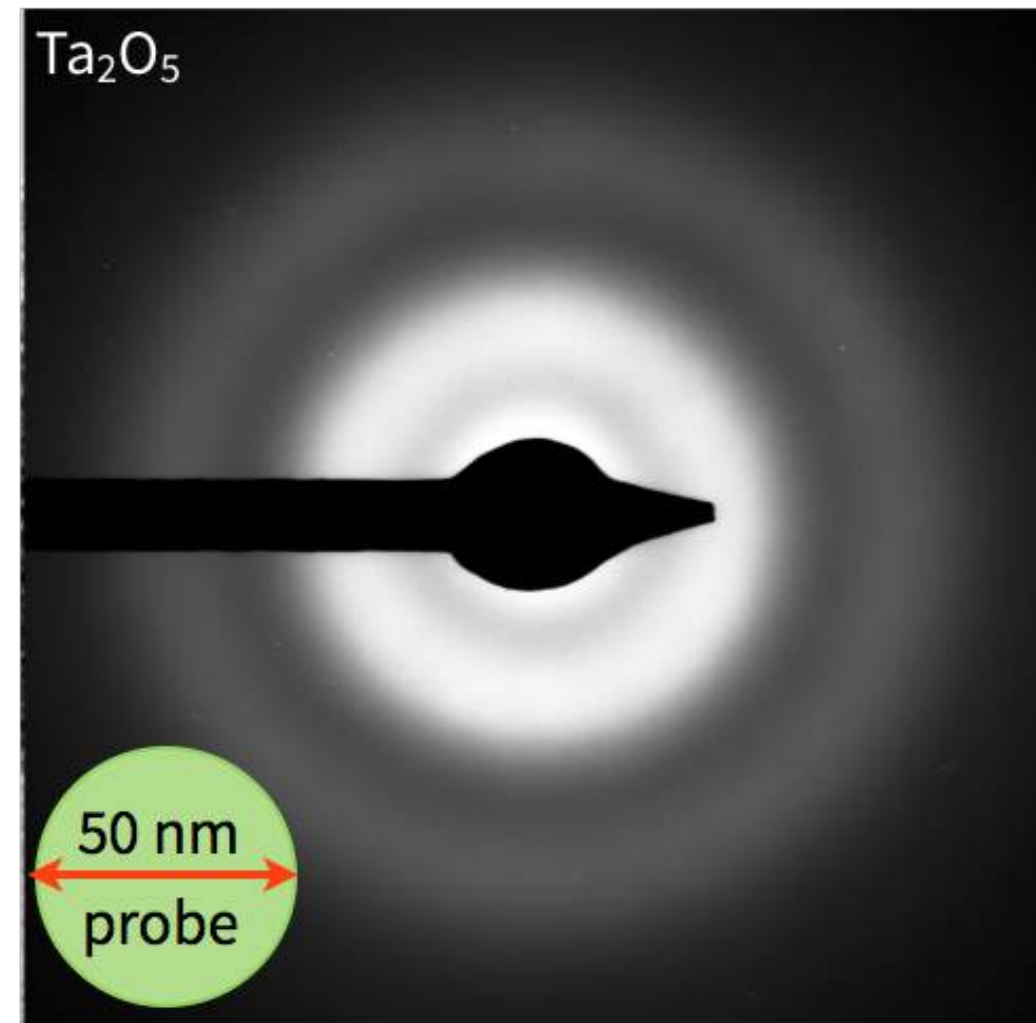
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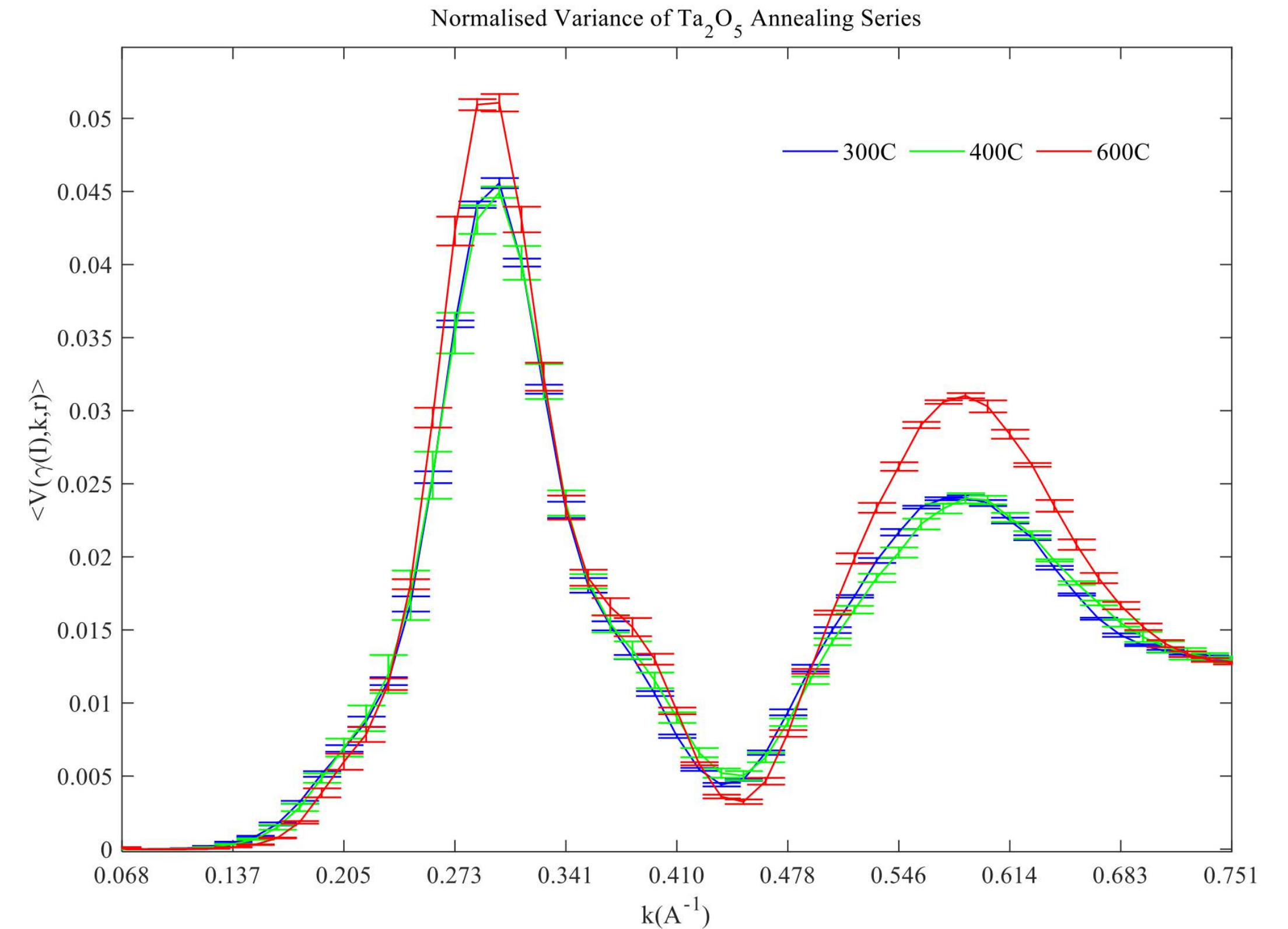
[M. Hart et. al., J. Non-Cryst. Solids, **438** 10 - 17 (2016)]

Tantala: GIPDF

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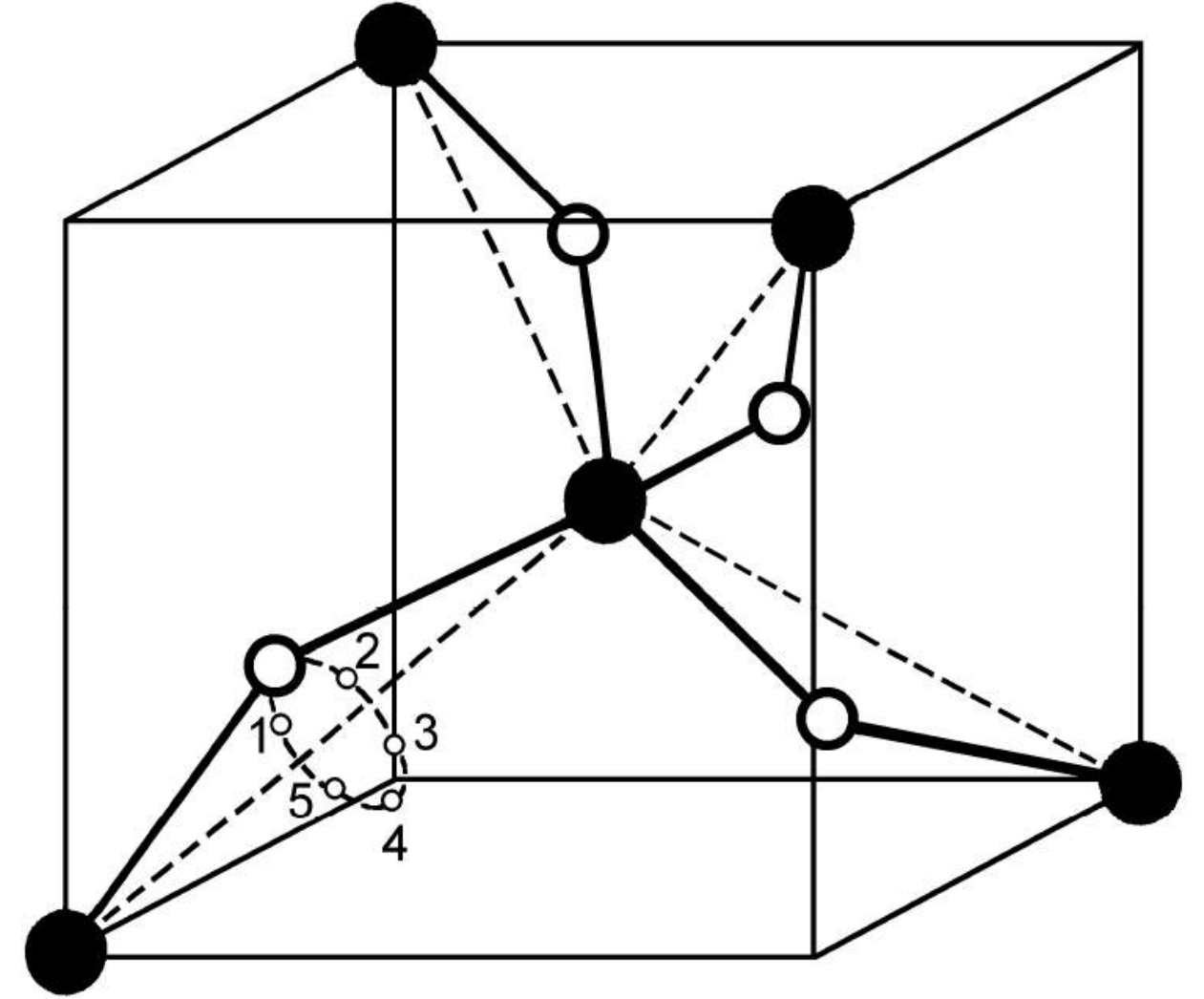
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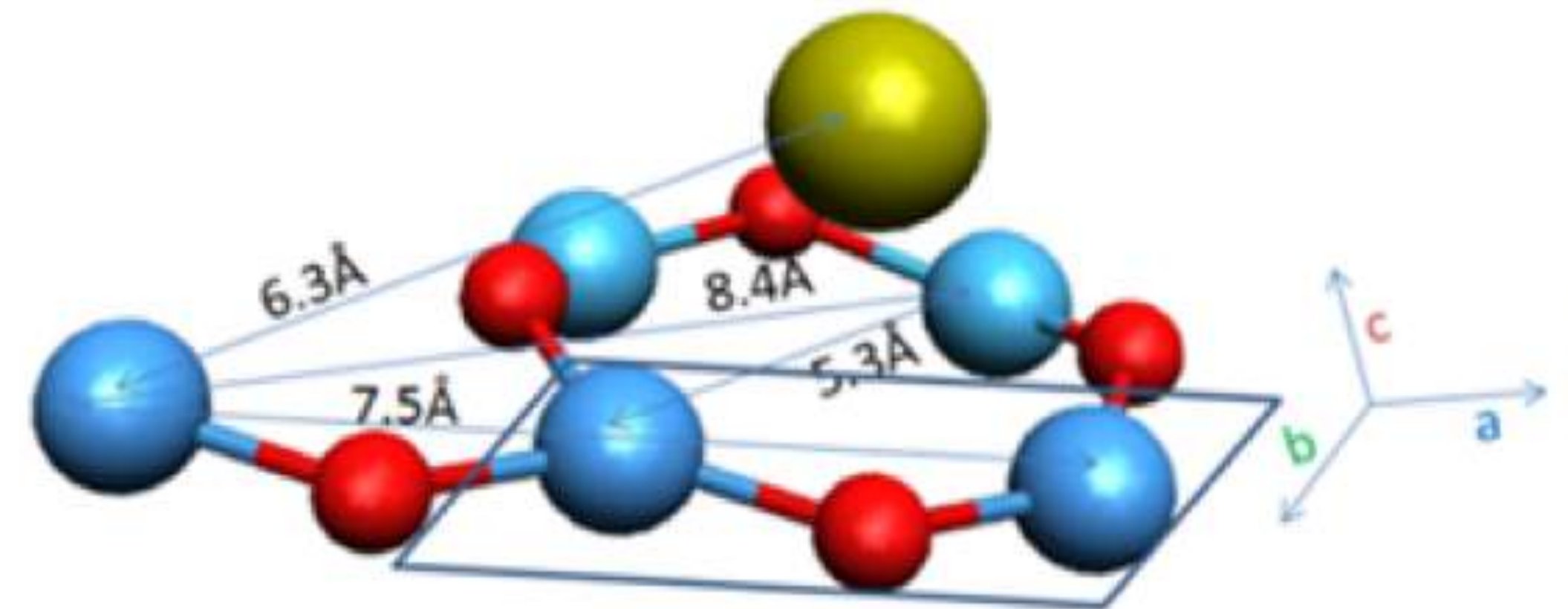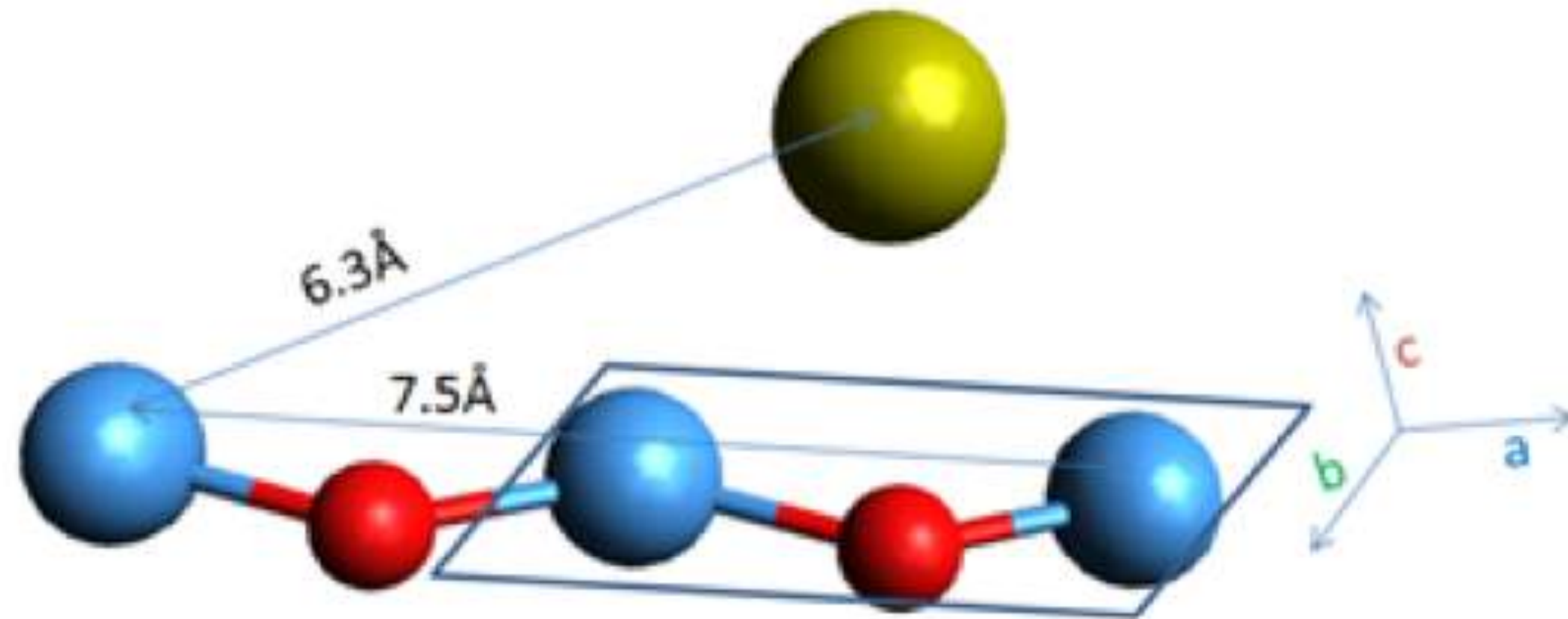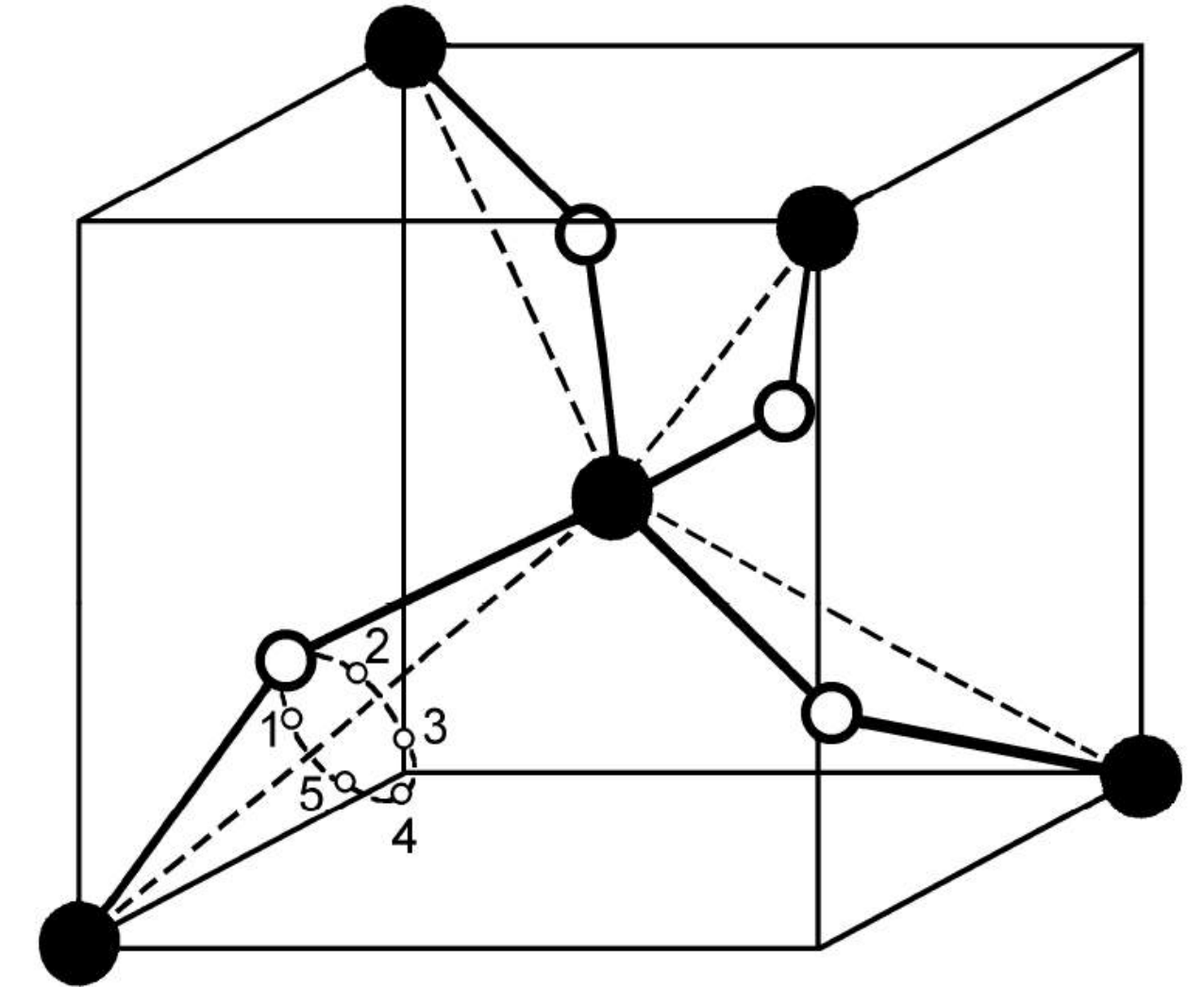
[B Shyam et al, Sci. Reports **6** 32170 (2016)]

Tantala: FEM
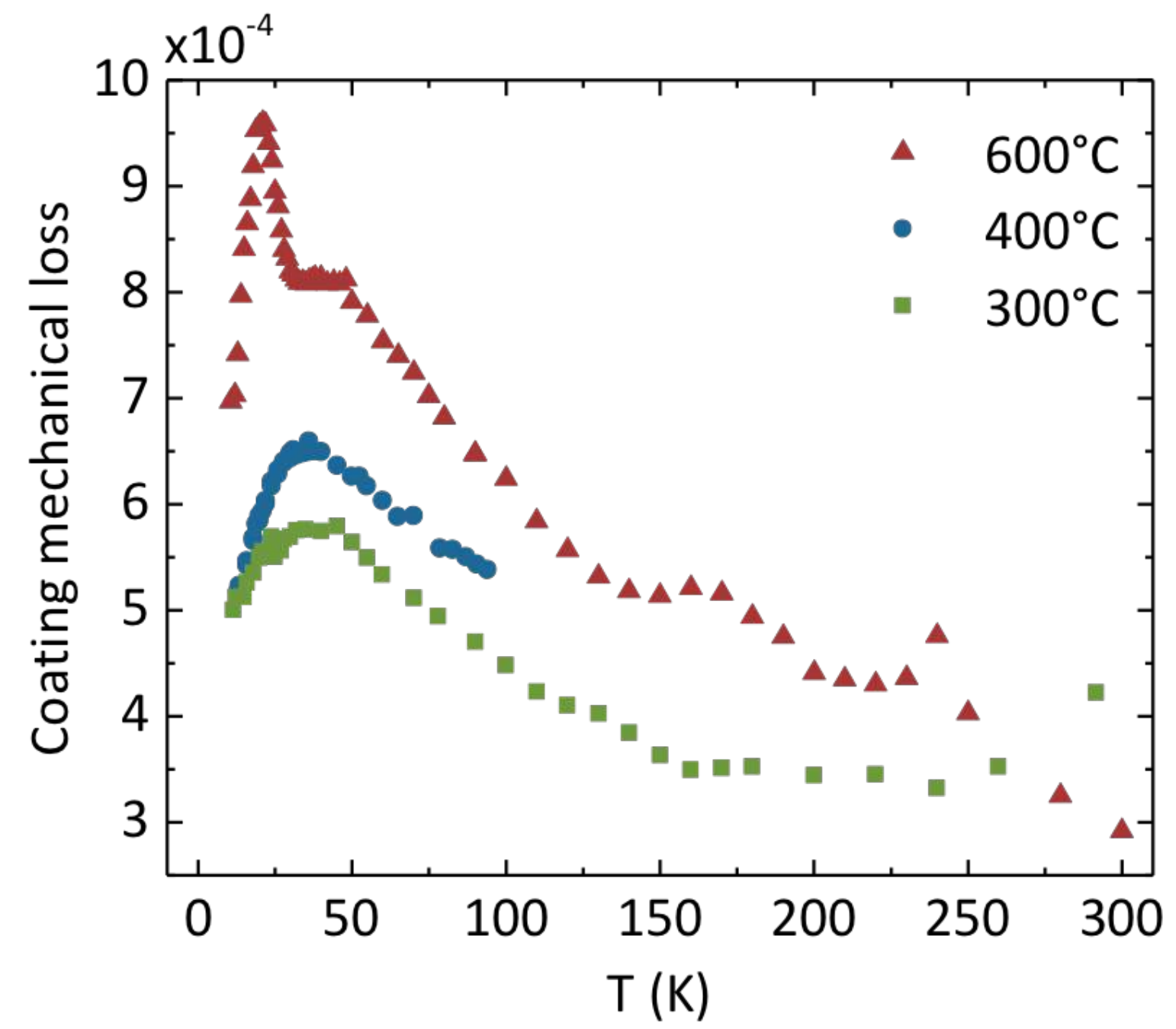
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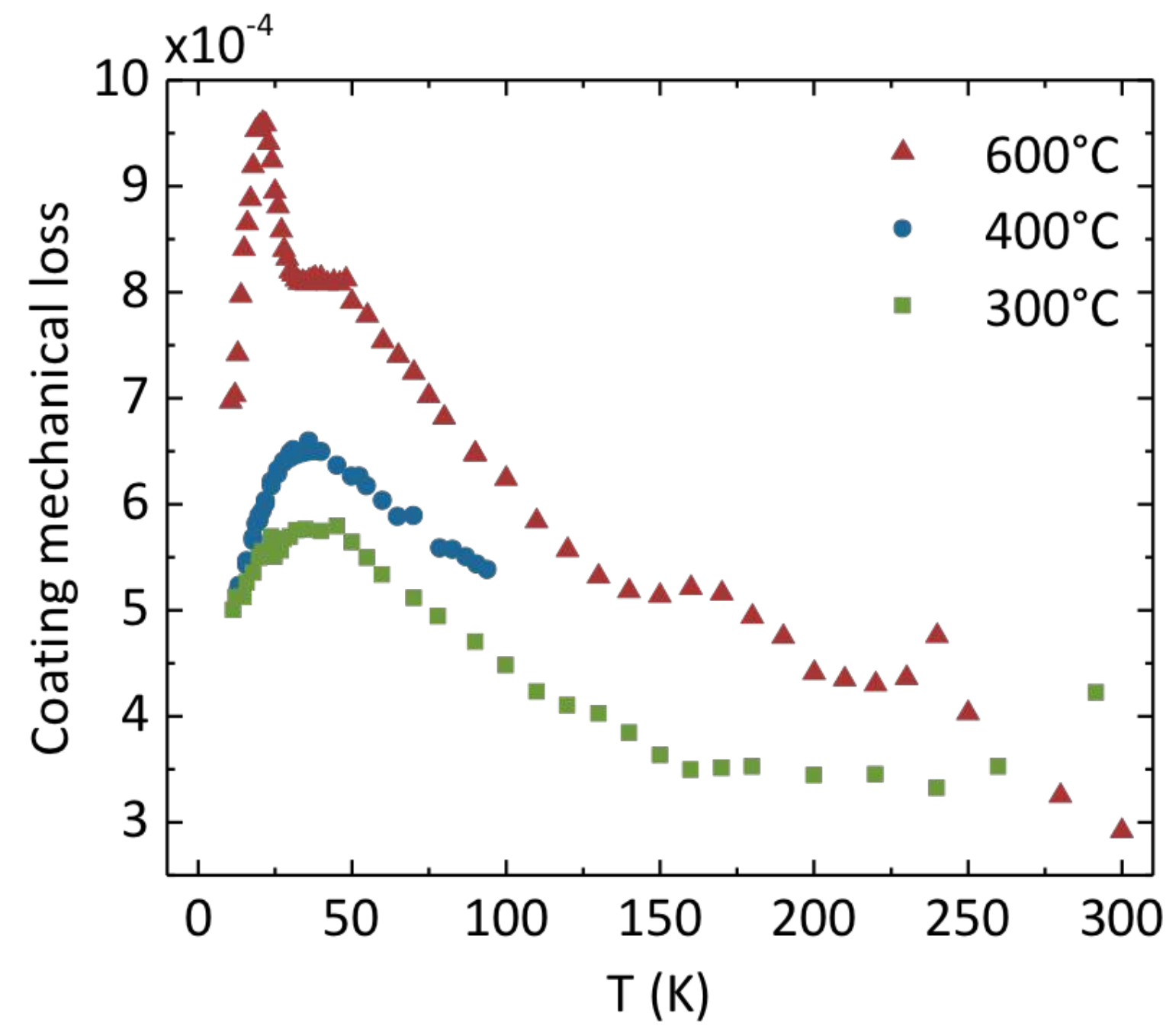
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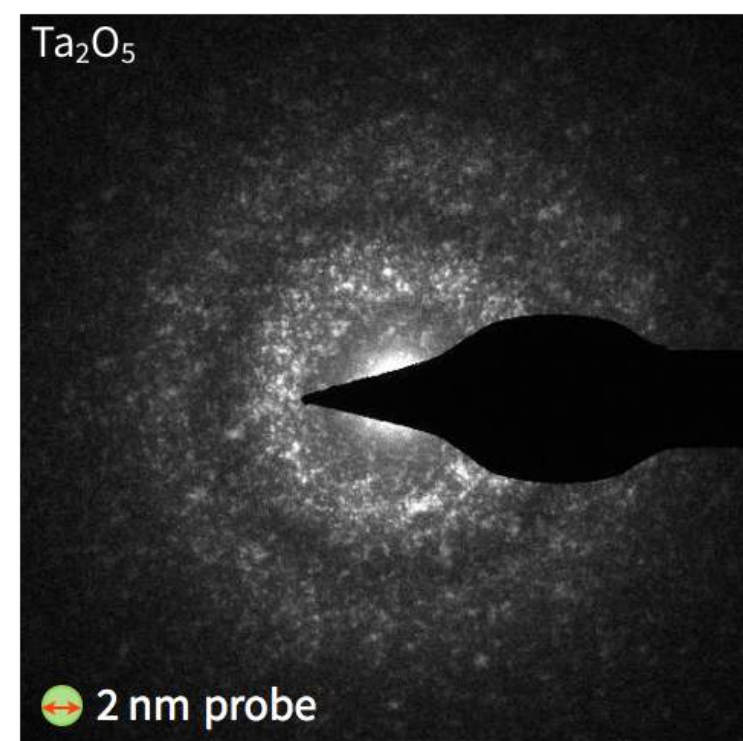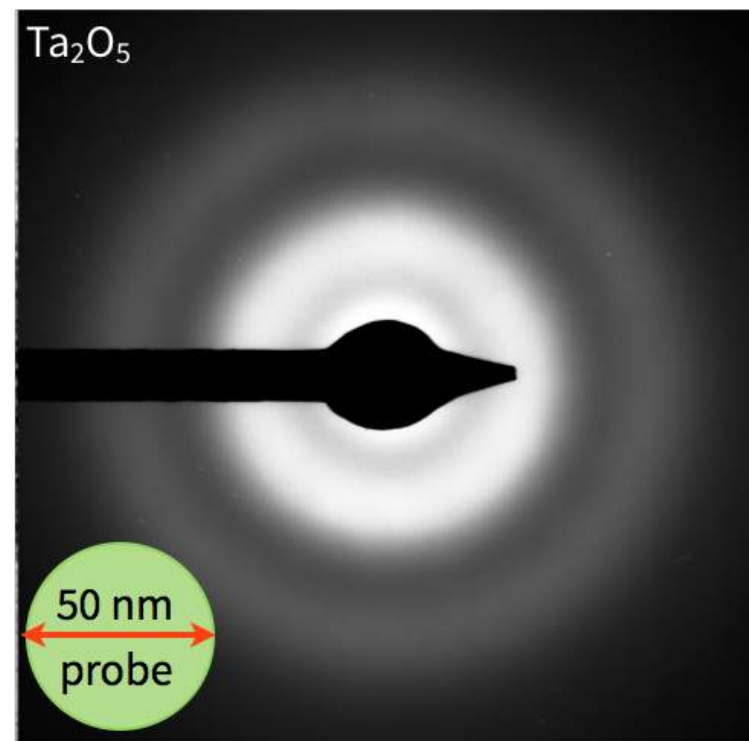
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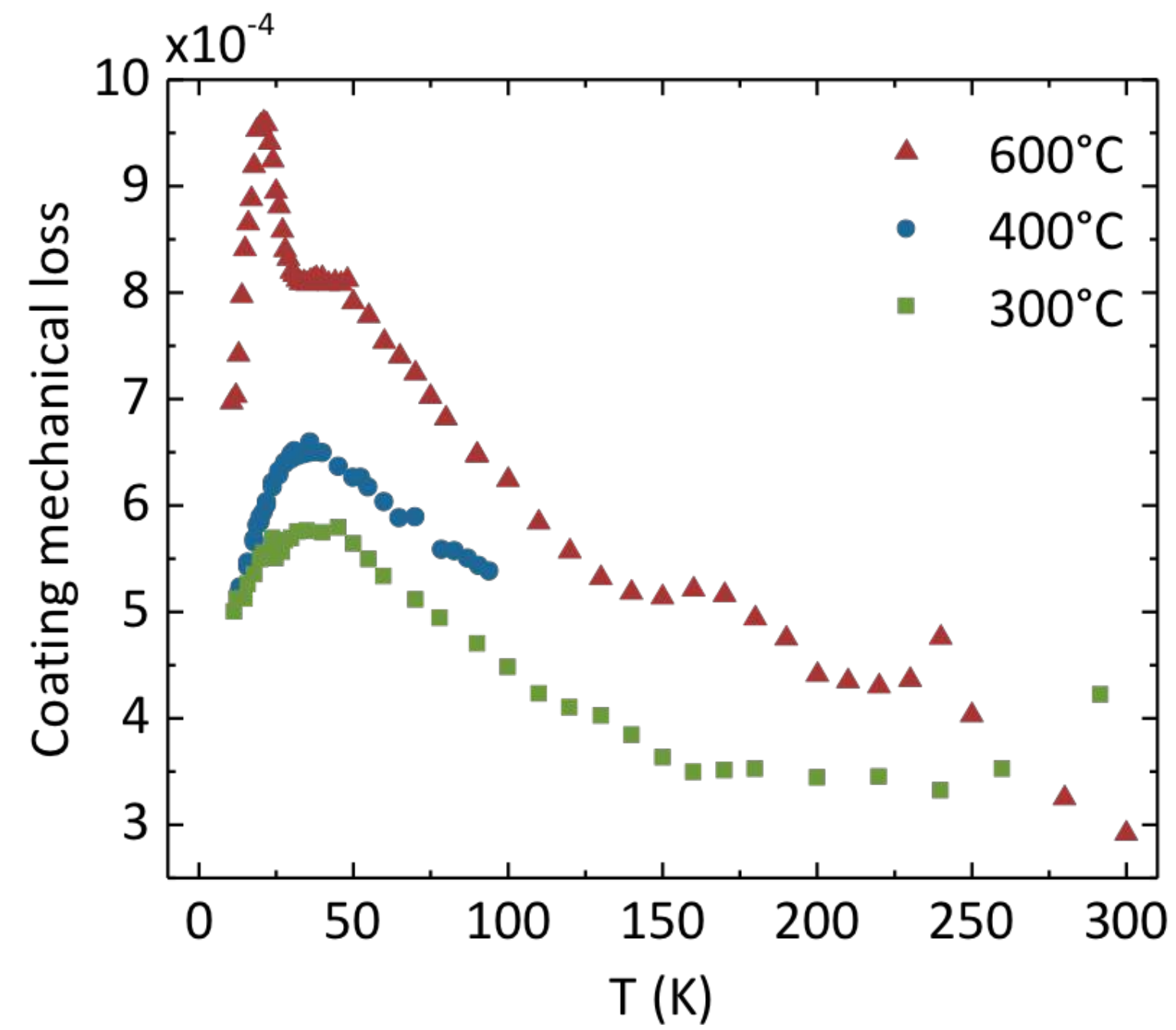
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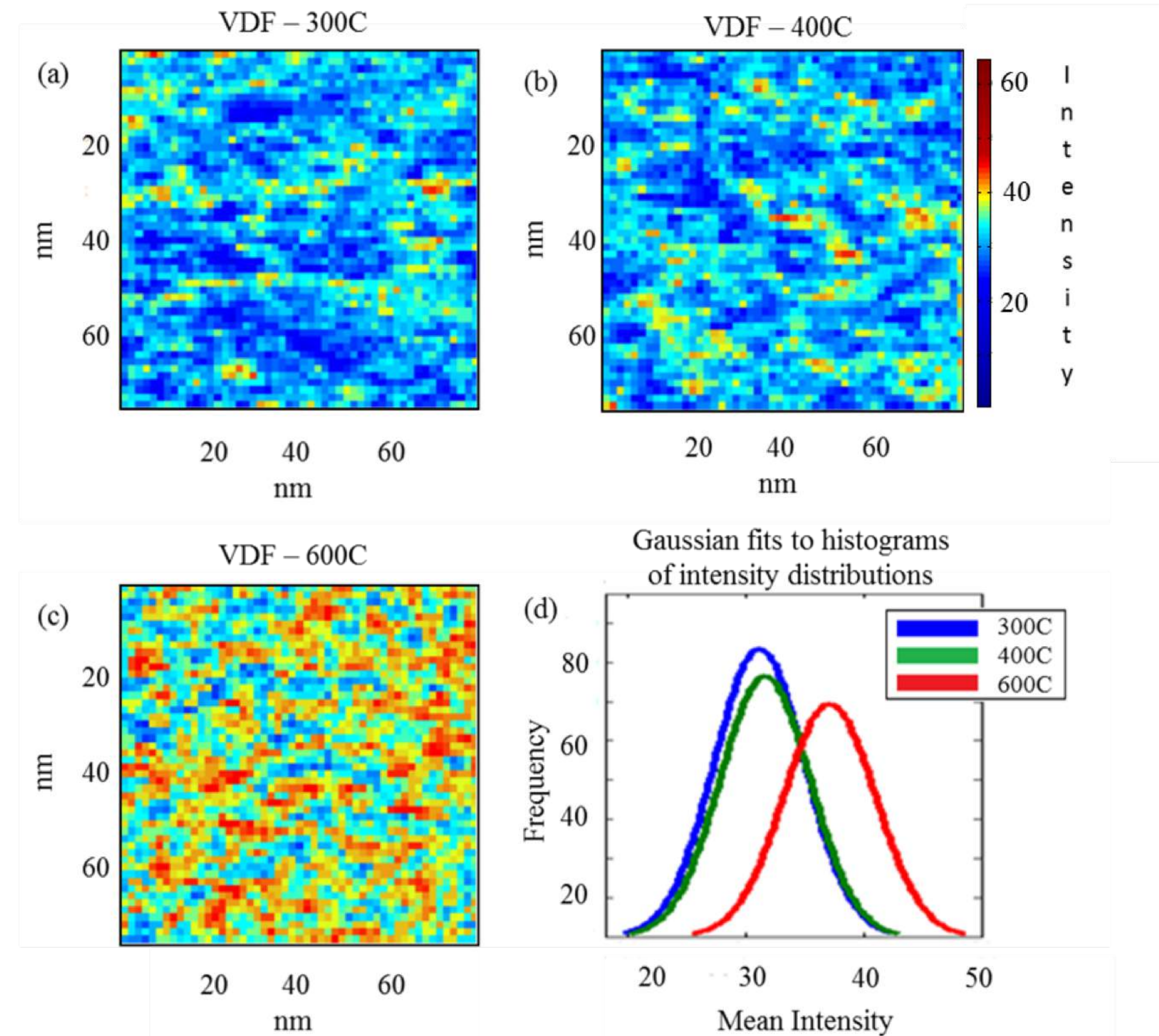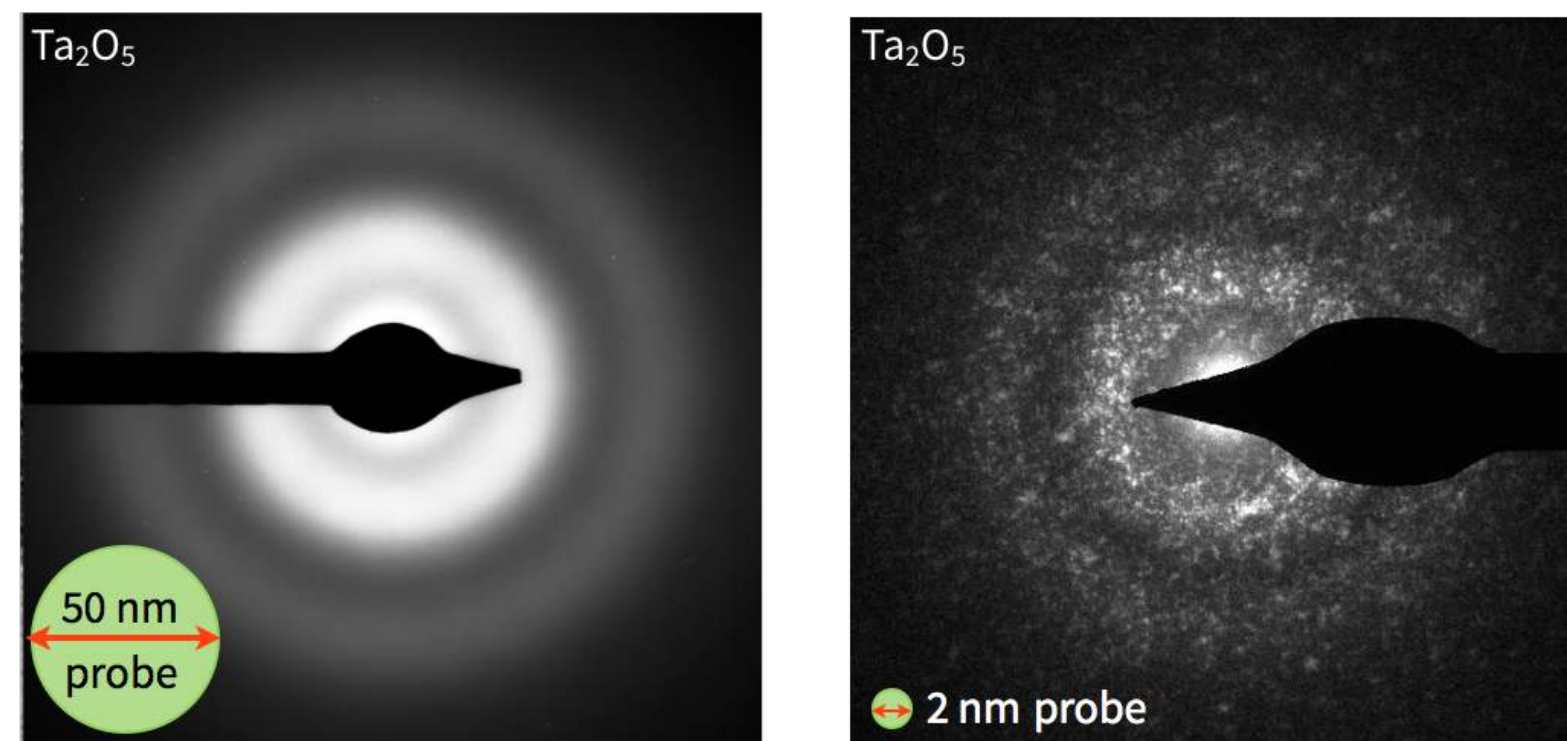
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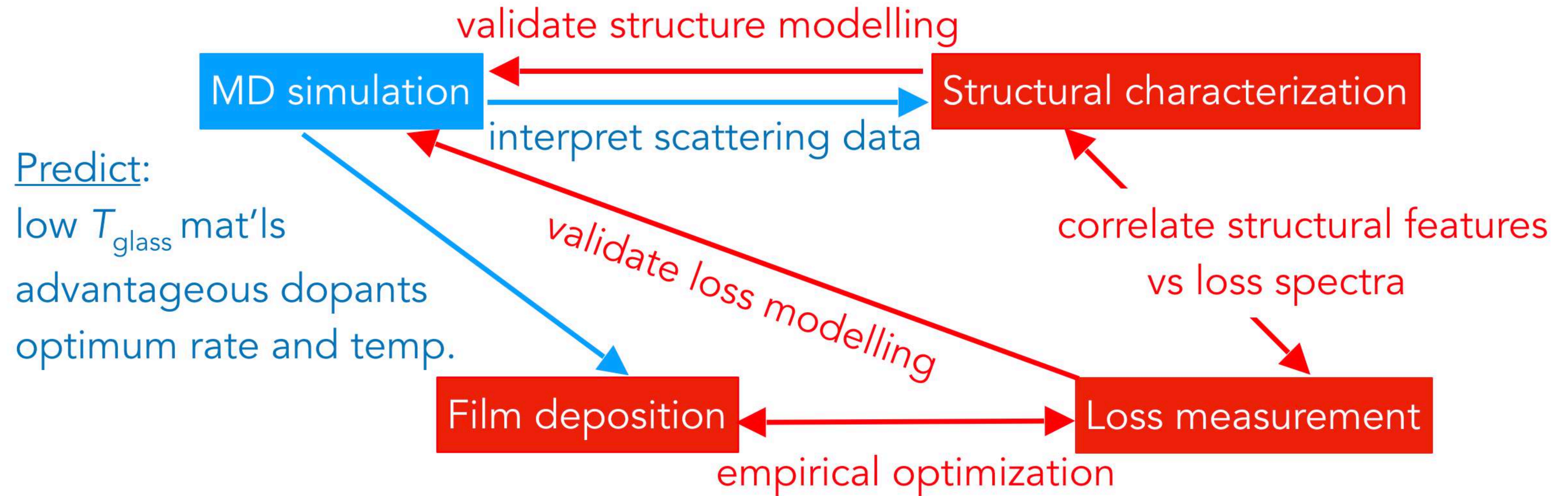
Integrated research approach

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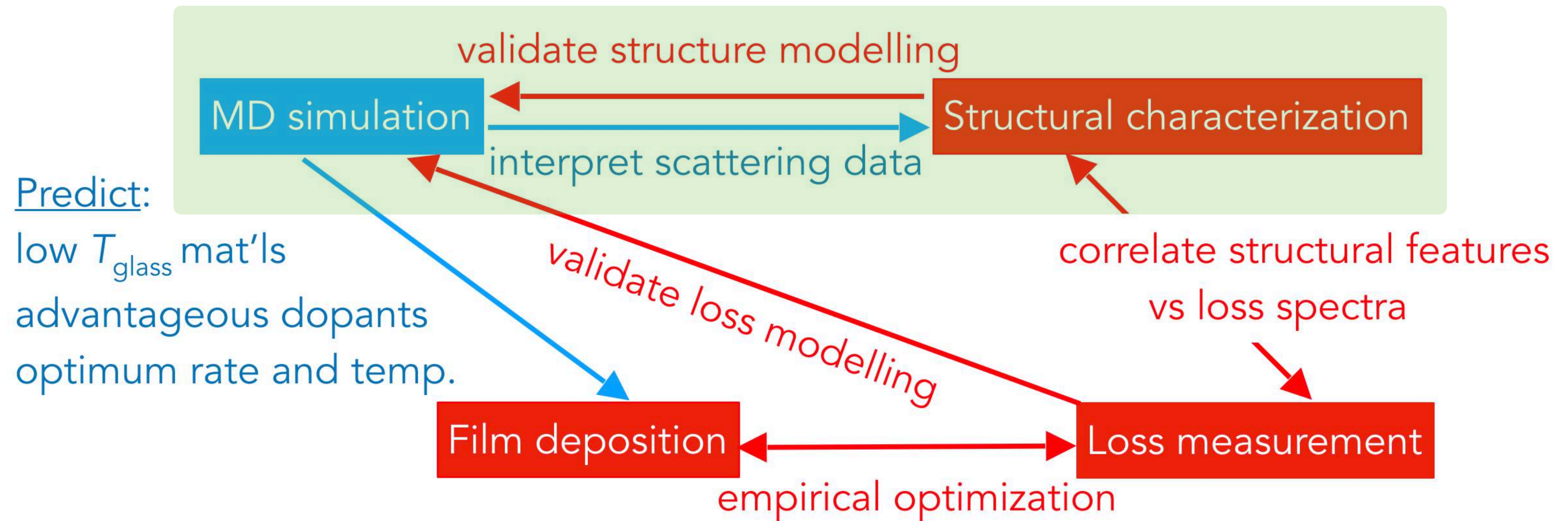
MD simulation

validate structure modelling

interpret scattering data

Structural characterization

Predict:

low T_{glass} mat'ls

advantageous dopants

optimum rate and temp.

correlate structural features vs loss spectra

validate loss modelling

Film deposition

empirical optimization

Loss measurement

Integrated research approach

Immediate plans

- MRO and mechanical loss in elevated temperature deposited tantala

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Outlook:
- Deposition modeling: develop a predictive tool for lower thermal noise coatings