Investigating coating material properties for future generations of gravitational wave detectors

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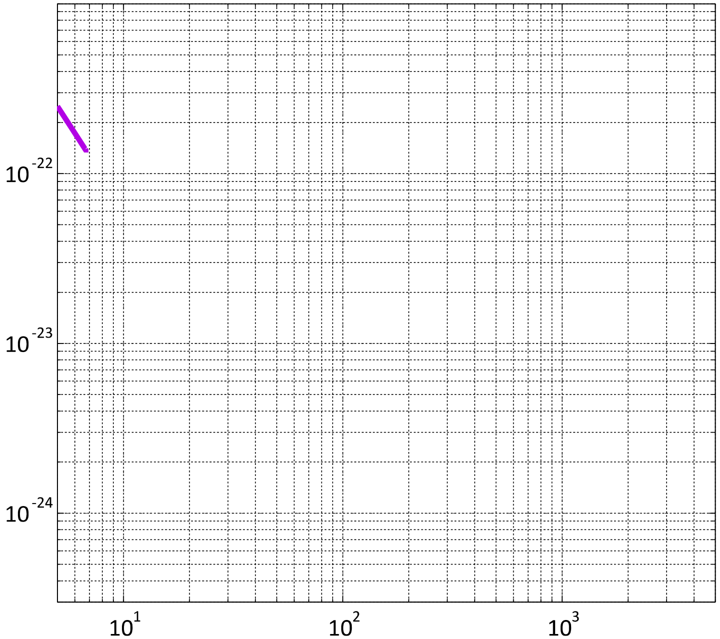
Overview

- Introduction
- Optical absorption measurements
  - Photothermal Common-path Interferometry (PCI) measurements
  - Preliminary temperature dependent results amorphous silicon coatings
- Atomic structure investigations
  - Atomic structure investigations using Transmission Electron Microscopy (TEM)
  - Nuclear Magnetic Resonance (NMR) measurements
- Single crystalline coatings
  - GaP/AlGaP Molecular Beam Epitaxial (MBE) coatings
- Summary of key experimental techniques
- Conclusions

Introduction

- Research into the materials used in the detector optics is vitally important to improve the sensitivity of future detectors
  - Advanced LIGO is pushing the limits for current coating materials
  - In order to improve upon this, new materials and technologies will need to be developed
- In order to investigate the coating material properties several experimental techniques have been developed
- Aim is to relate loss sources to changes in the atomic structure for amorphous coatings
- Investigate possible alternative to amorphous coatings such as single crystal GaP/ AlGaP coatings



GWINC Advanced LIGO noise budget

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Optical absorption measurements

PCI optical absorption measurements:

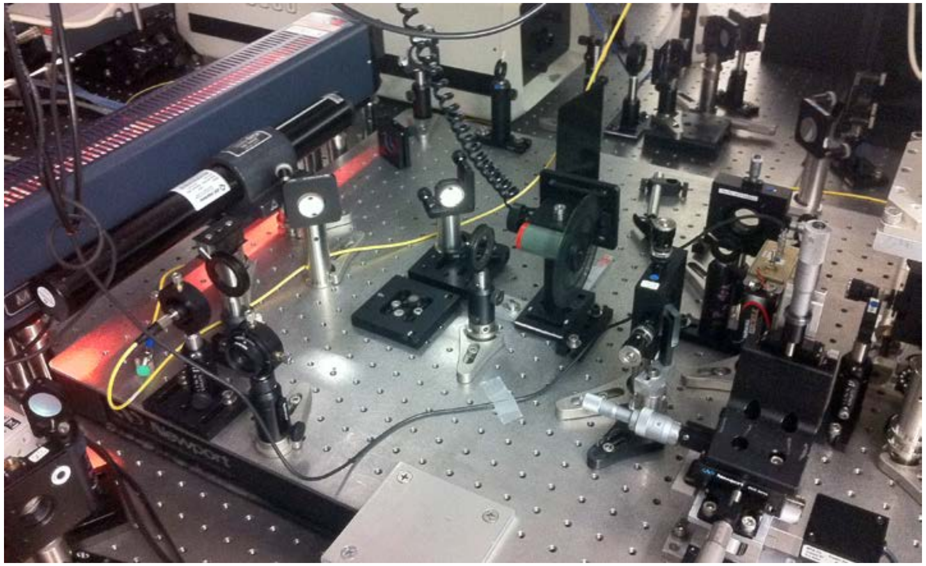
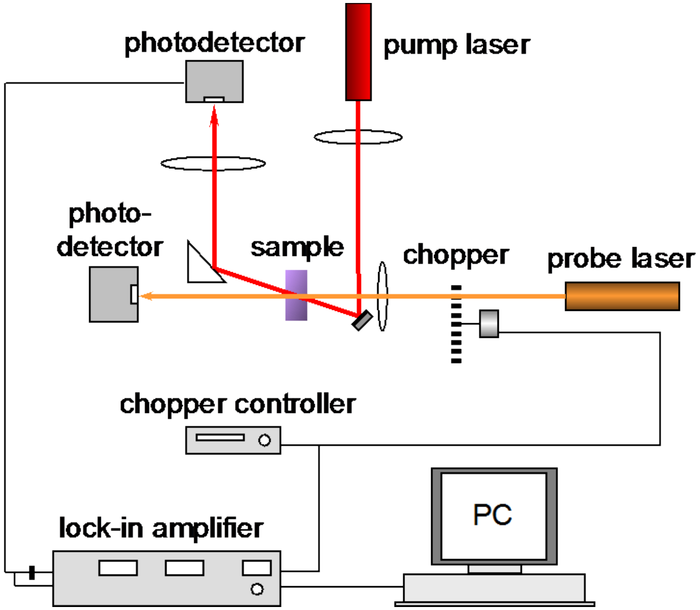


Photo of PCI setup at Stanford University

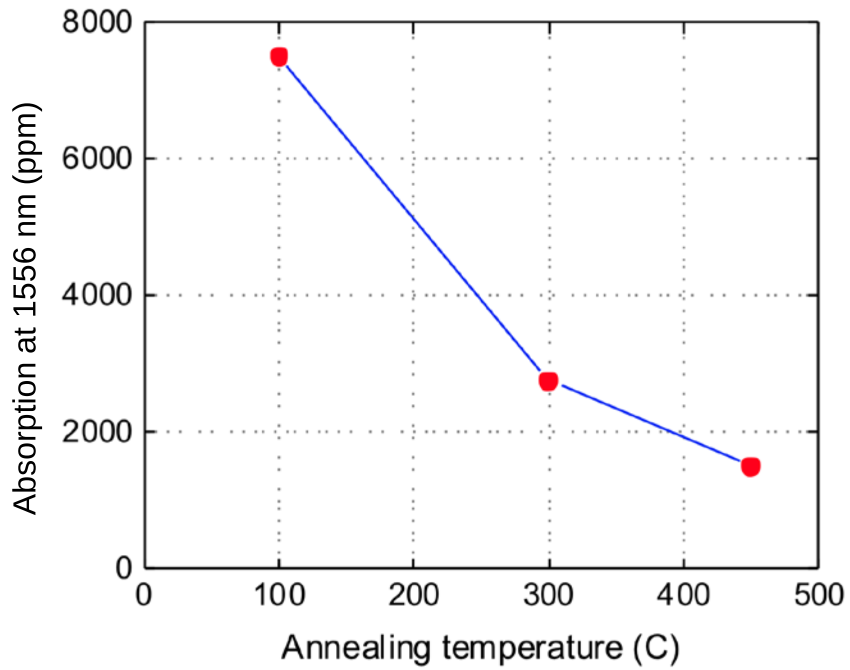


Schematic of PCI setup

- Photo-thermal Common-path Interferometry (PCI)
  - Allows measurement of bulk and coating optical absorptions
  - Capability for T-dependent measurements from 15 K from recent addition of cryostat
  - Measures thermal lensing of the pump beam caused by optical absorption
  - Maximum sensitivity at 9 W pump beam for coatings is 0.05 ppm and bulk is 0.2 ppm/cm

Optical absorption measurements

Preliminary α-Si coatings room temperature measurements



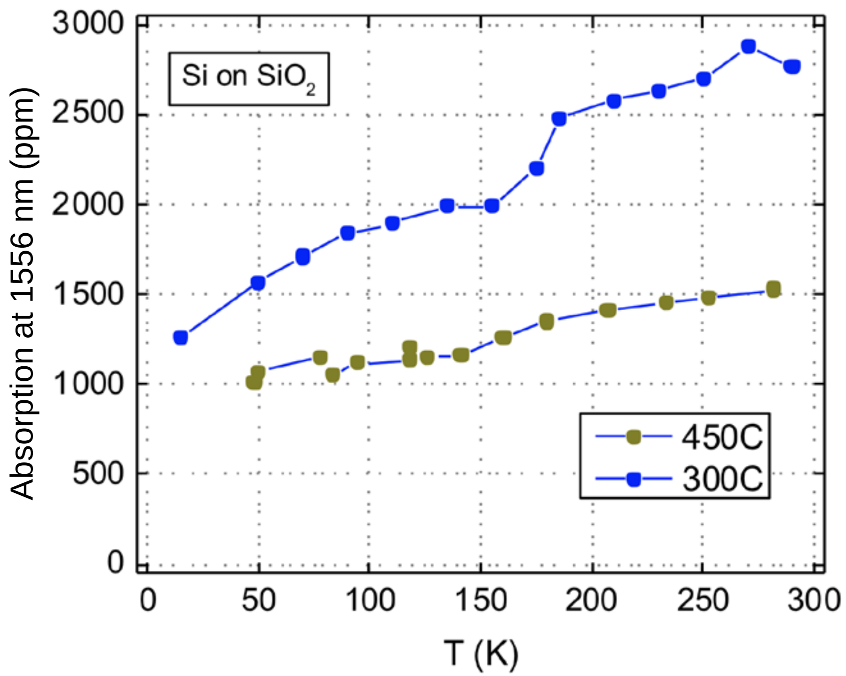
Optical absorption of α-Si coatings vs. annealing temperature
(in air at room temperature)

- Optical absorption of three amorphous (α) Si coatings
  - Measurements made at 1556 nm for as-deposited, 300ºC and 450ºC annealed
  - Shows ~70% drop in absorption between as-deposited and 450ºC annealed
  - Similar trend to silica/ tantala coatings
  - Further study is required in deposition techniques and post-deposition treatments which can reduce absorption

Optical absorption measurements

Preliminary α-Si coatings T-dependent measurements

- Recent integration of a flow cryostat to the PCI setup has given the capability for temperature dependent absorption measurements



Temperature variation of the optical absorption of two annealed amorphous Si coatings

- Preliminary temperature dependent optical absorption for the 300ºC and 450ºC annealed α-Si coatings
  - Results show decrease in optical absorption at 1556 nm as temperature is decreased

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Optical absorption measurements

Ongoing and future work

- Continue to develop T-dependent measurement capabilities
- Aim to measure absorption of bulk single crystal silicon
  - Currently obtaining high quality **float-zone silicon** for measurements
  - T-dependent measurements planned

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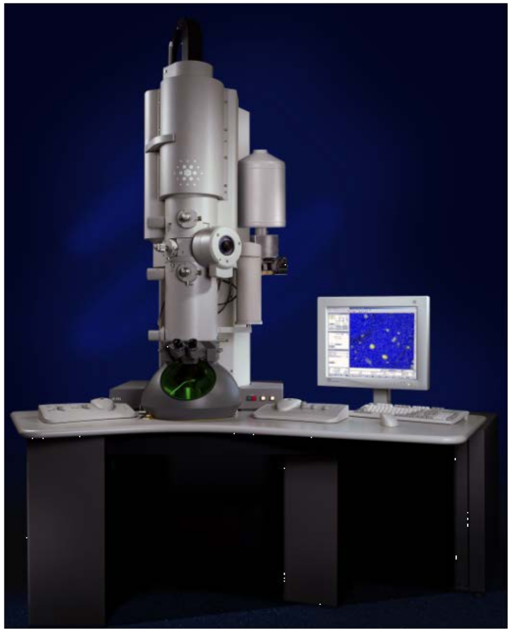
Atomic structure investigations: RDF investigations



Tecnai F20 TEM

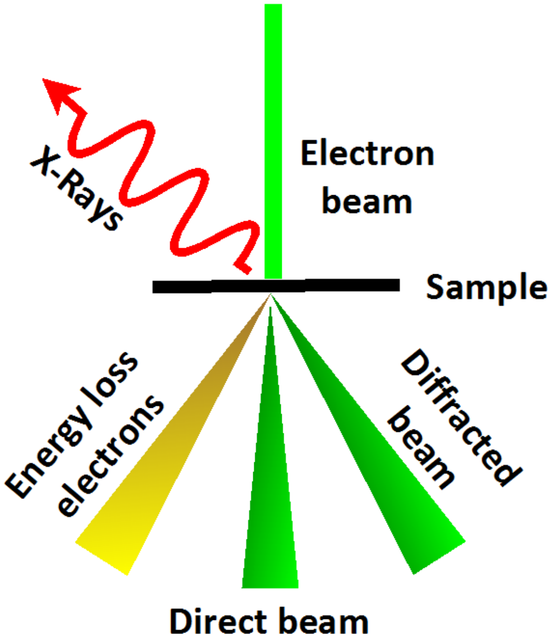
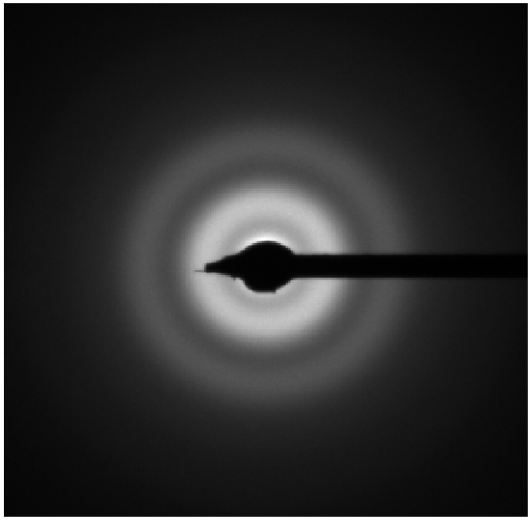


Diagram showing electron beam interactions

- Transmission Electron Microscopy (TEM)
  - Ideal tool for studying the atomic structure and chemistry of the coatings
  - Major tools are imaging, diffraction and spectroscopy
  - Extensive capabilities at both Stanford and Glasgow
  - Major tool for amorphous materials is the Reduced Density Function (RDF)

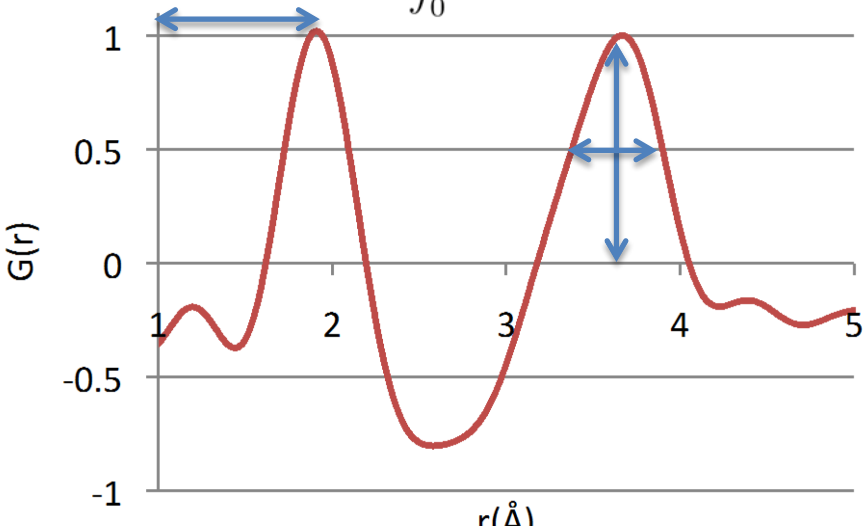
Atomic structure investigations: RDF investigations

- RDFs provide a statistical representation of where nearest neighbor atoms sit with regards to a central atom:



TEM diffraction pattern of a typical amorphous Ta_2O_5 coating

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

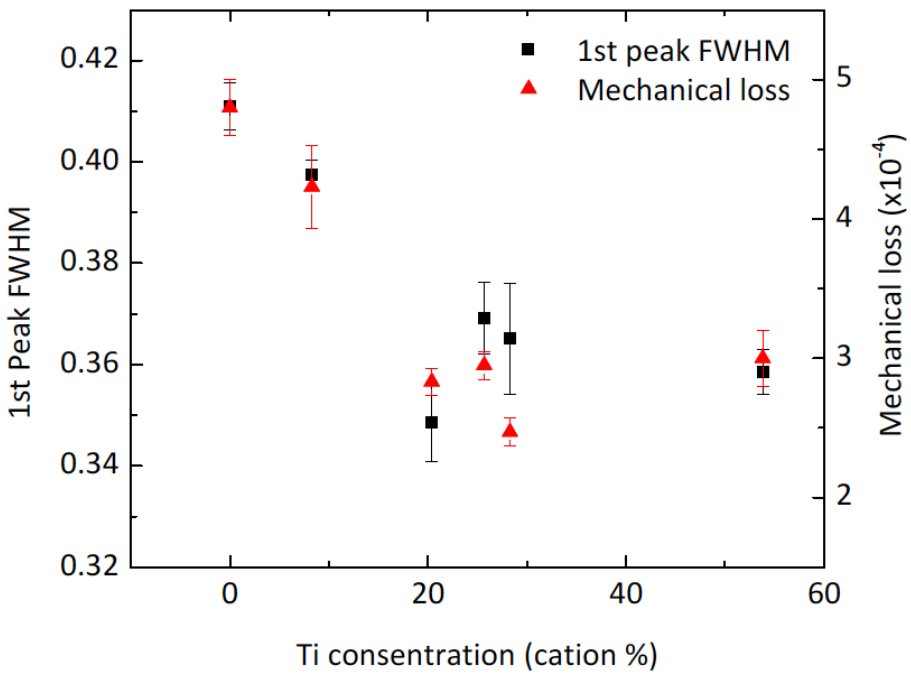


RDF of Ta_2O_5 coating

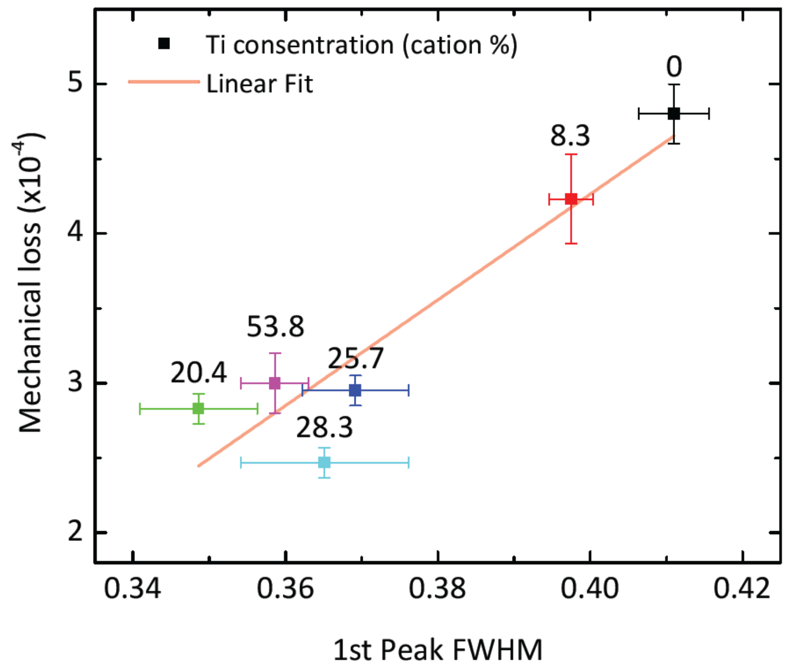
- RDF analysis:
  - 1st peak relates mostly to metal – oxygen bonds
  - 2nd peak relates mostly to metal – metal distances
  - Peak positions indicate most likely place for atomic neighbors to sit
  - Peak height indicate and peak width indicates level of homogeneity or 'local order' in structure

Atomic structure investigations

Atomic structure investigations: TiO_2 doped Ta_2O_5



RDFs 1st peak FWHM and mechanical loss Vs. Ti concentration

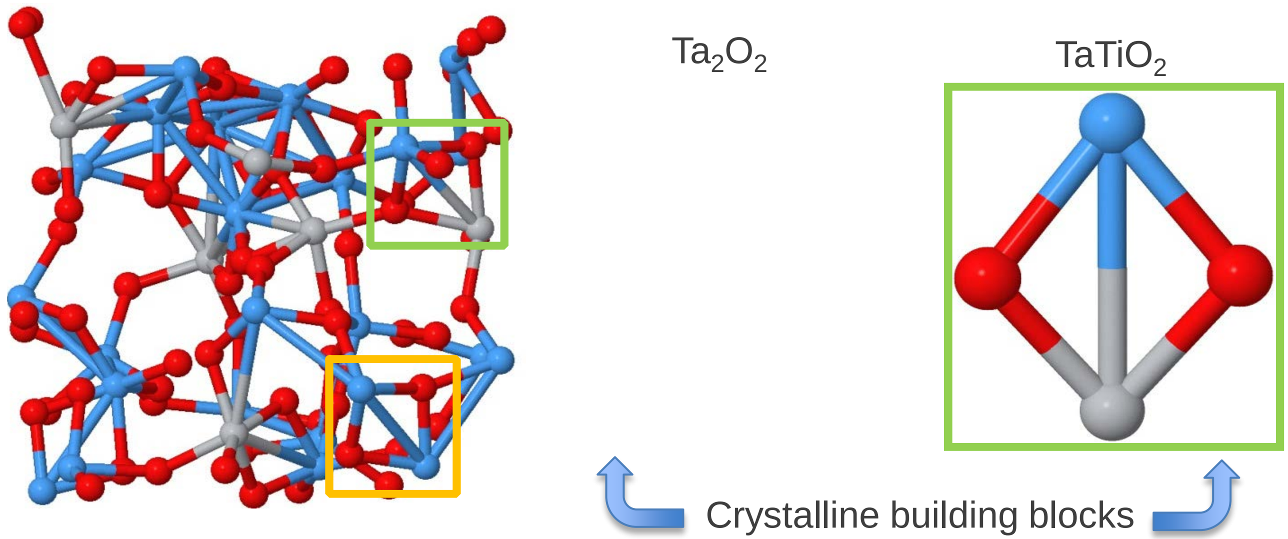


Correlation between Mechanical loss and 1st peak FWHM

- Relationship to mechanical loss
  - Strong relationship from changing properties in the experimental RDFs
  - Strong correlation between mechanical loss and changing atomic structure properties
  - Pearson correlation coefficient, r = 0.93

Atomic structure investigations

Atomic structure investigations: TiO_2 doped Ta_2O_5

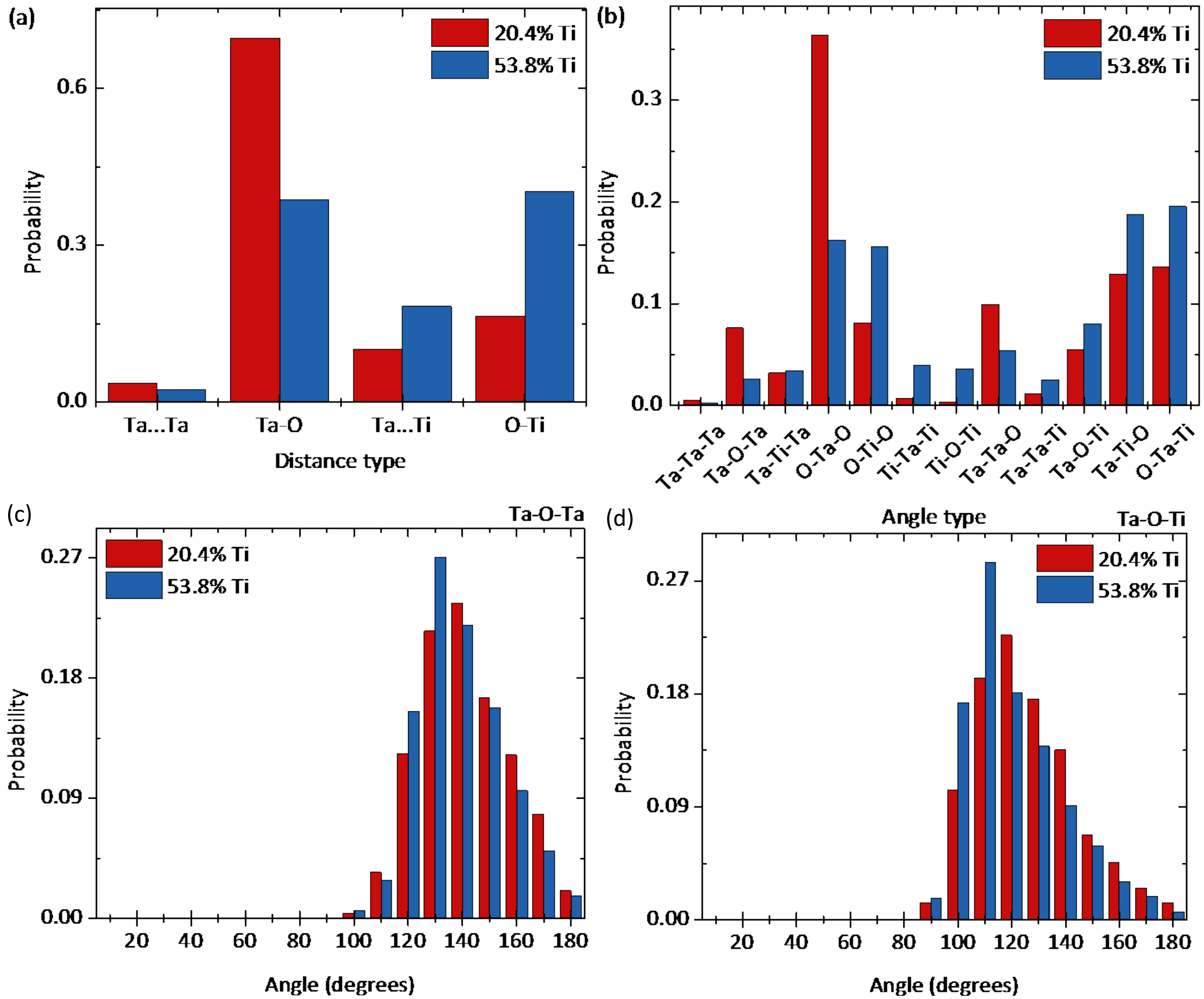


Atomic model of the 20.4% TiO_2 doped Ta_2O_5 coating, highlighting the Ta_2O_2 and $TaTiO_2$ crystalline building blocks

- Models are generated from experimental diffraction data using Reverse Mote Carlo (RMC) and Molecular Dynamics (MD) simulations
- Crystalline ring building blocks seen in all models
- Atomic models provide many different possibilities for understanding the material properties
- Studying these building blocks, and larger structures, may provide an insight into the mechanisms responsible for mechanical loss (as in the case for silica)

Atomic structure investigations: TiO_2 doped Ta_2O_5

- Bond and distance analysis provides detailed understanding of the local structure environments
- Distance type and angle type distributions show clear differences between the 20.4% Ti and 53.8% Ti doped models
- In contrast angle type distributions show only subtle changes
- Ta-O-Ta, Ta-O-Ti shows reduced peak position by 10° as Ti doping is increased



Bond and distance distributions for TiO_2 doped Ta_2O_5 coatings

Atomic structure investigations

NMR measurements

- Nuclear Magnetic Resonance (NMR) spectroscopy
  - NMR uses splitting of nuclear spin energy level of specific nucleus in a magnetic field
- Capable of quantifying the distributions of and connections among structural units
- Sensitive to the local structure
  - Nuclear specific, e.g. ^{17}O NMR

Varian NMR with Oxford Magnet

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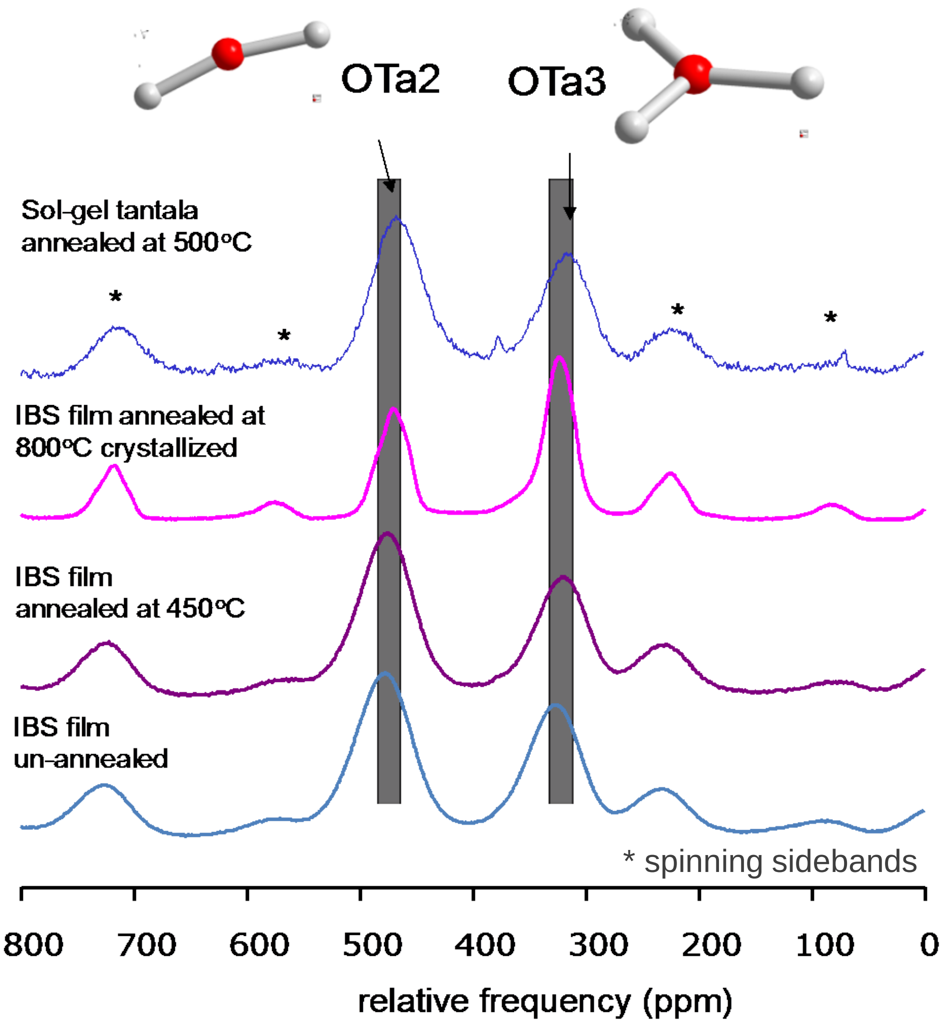
Atomic structure investigations

NMR measurements: ^{17}O NMR of sol-gel and IBS Ta_2O_5



- Two peaks were assigned based on the known crystalline structure $^{[3]}O$:$^{[2]}O$ ~ 3:2
- The difference in relative intensities between amorphous and crystalline Ta_2O_5 suggests a difference in OTa_2/OTa_3 ratio in amorphous Ta_2O_5
- Amorphous Ta_2O_5 from different preparation methods do not show any significant difference
- Subtle differences can be observed (linewidths, peak positions, etc.) and is currently under investigation

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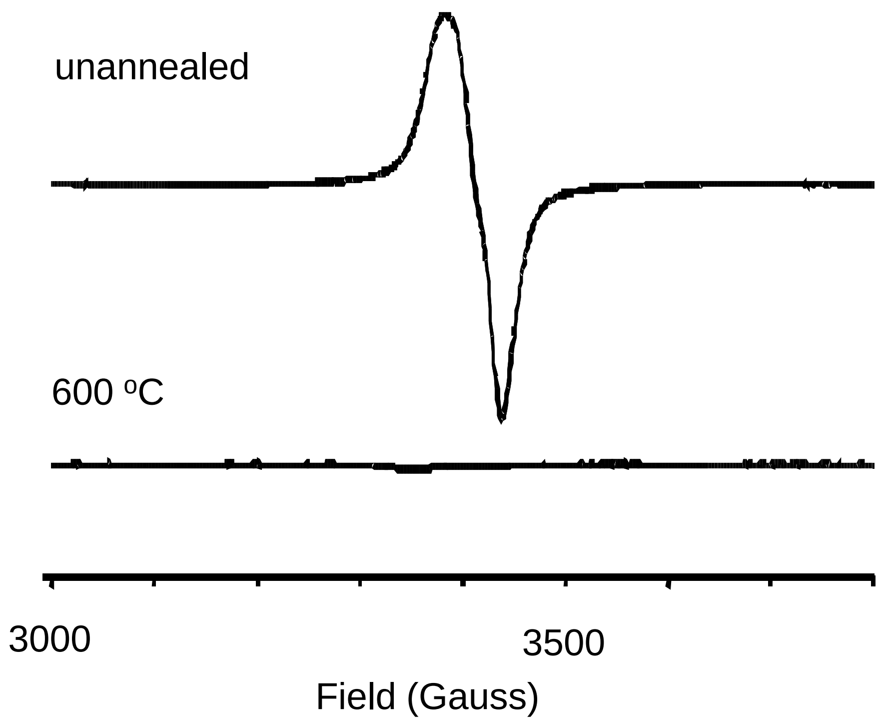
Electron Paramagnetic Resonance (EPR) Spectroscopy measurements: heat-treated Ta_2O_5 coatings



EPR Spectra of tantala with varying annealing temperatures (collaboration with Prof. Ed Solomon, Stanford, Chemistry)

- EPR detects unpaired electrons in the sample
- Only the unannealed amorphous tantala shows an unpaired electron
- EPR signal is most likely due to oxygen deficiency in un-annealed sample, estimated ~ 0.2%
- Oxygen deficiency may play an important role in improvement of optical and mechanical properties upon annealing

Atomic structure investigations

Ongoing and future work

- Experimental techniques which are important for accurate atomic structure investigations:
  - Density (X-ray Reflectometry)
  - Stoichiometry (Electron Energy Loss Spectroscopy)
  - Atomic nearest neighbor distributions (RDFs)
  - Other constraints (Crystal structures, NMR)

- X-ray absorption spectroscopy
  - Complimentary measurements to RDF studies
  - Direct measurement of local structure around Ta and Ti atoms in TiO_2 doped Ta_2O_5 coatings

- Further investigations are planned
  - TiO_2 doped Ta_2O_5 – NMR/TEM comparison to optical absorption and mechanical loss
  - Understanding changes in performance of coated silica vs. bulk silica
  - Medium range atomic structure of α-Si coatings

- Continuing development into linking coating loss to atomic structure measurements

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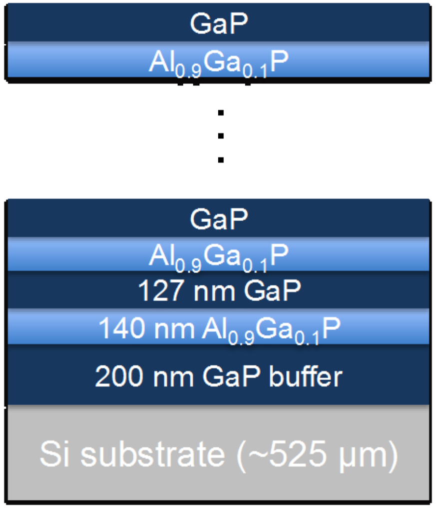
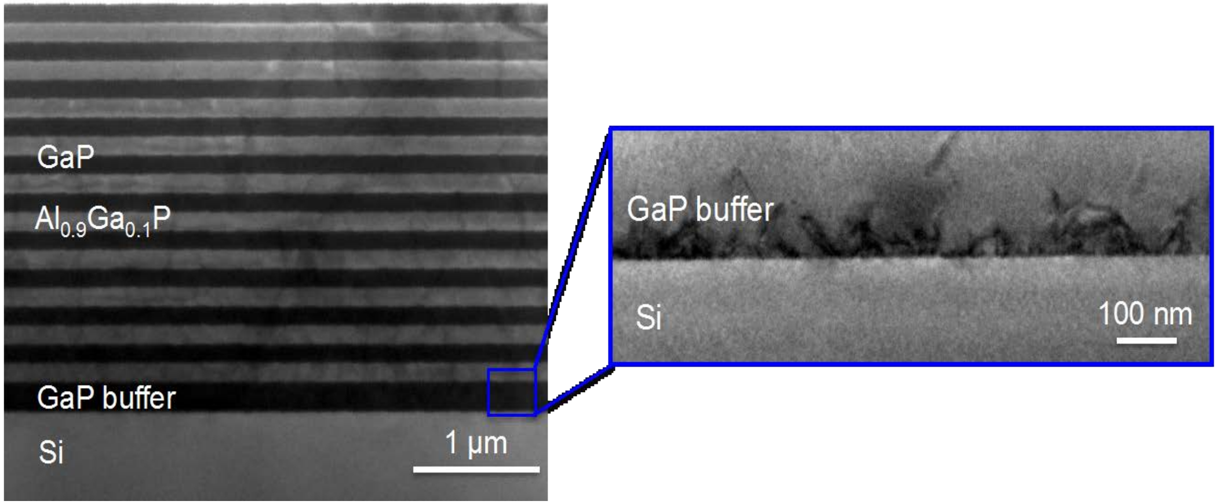
Single crystalline coatings

GaP/ AlGaP epitaxial coatings



Schematic of GaP/ AlGaP coatings



TEM image of GaP/ AlGaP coatings highlighting defects being annihilated in the GaP buffer layer

- Effort to develop an alternative to amorphous IBS coatings
- For use in cryogenic third generation detectors working at around 1550 nm
- The advantages of these coatings:
  - Can be grown on single crystal Si
    - Low bulk mechanical loss in Si (and crystalline films) at cryogenic temperatures
  - Large-area substrates (commercially-available 12” Si)
- Continued development to understand and minimize defects

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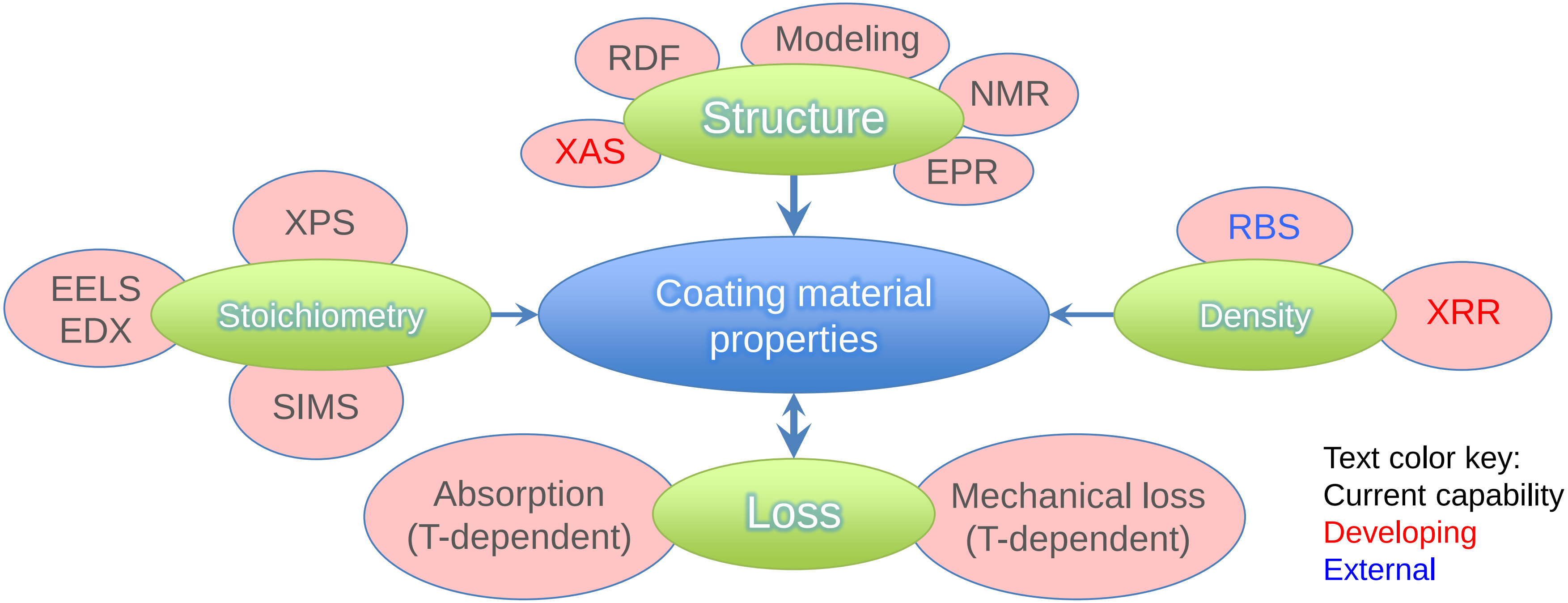
Summary of key experimental techniques

Atomic structure investigations (in collaboration with Glasgow)

- Experimental techniques that aim to link macroscopic material properties to the coating atomic structures:



Text color key:
Current capability
Developing
External

- RDF – Reduced Density Function
- NMR – Nuclear Magnetic Resonance
- XAS – X-ray Absorption Spectroscopy
- XPS – X-ray Photoelectron Spectroscopy
- EPR – Electron Paramagnetic Resonance
- RBS – Rutherford Backscattering Spectrometry
- EELS – Electron Energy Loss Spectroscopy
- EDX – Energy Dispersive X-ray (Spectroscopy)
- XRR – X-ray Reflectometry
- SIMS – Secondary Ion Mass Spectrometry

Conclusions

- Optical absorption measurements
  - PCI optical absorption measurements to probe both bulk and coating absorption at 1064 nm and 1556 nm
  - Preliminary measurements on amorphous silicon coatings show:
    - As increased post-deposition annealing (450°C current max) increases optical absorption decreases
    - T-dependent absorption decreases for 300°C and 450°C coatings as temperature decreases
  - Continued development into T-dependent measurement, with emphasis on bulk Si measurements
- Atomic structure investigations
  - TiO_2 doped Ta_2O5 show strong correlation between atomic structure properties and mechanical loss
  - NMR and EPR spectroscopy probe local co-ordination of Ta_2O_5 coatings which show signs of oxygen deficiency when coating is un-annealed
  - Continued development and use of a number of experimental techniques to accurately investigate the atomic structure and relate to sources of loss
- Single crystalline coatings
  - GaP/ AlGaP single crystal coatings provide an alternative to IBS coatings
  - Can be directly deposited onto silicon substrates
  - Continued development to understand and minimize defects

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