

DEPAUL UNIVERSITY

**Exploring Extended X-ray  
Absorption Spectroscopy and  
Pair-Distribution Function  
Methods in Amorphous  
Semiconductors**

by

Brett Freese

A thesis submitted in partial fulfillment for the  
degree of Physics

Dr. Gabriela Gonzalez  
Physics

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# Declaration of Authorship

I, Brett Freese, declare that this thesis titled, ‘Exploring Extended X-ray Absorption Spectroscopy and Pair-Distribution Function Methods in Amorphous Semiconductors’ and the work presented in it are my own. I confirm that:

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- Where I have consulted the published work of others, this is always clearly attributed.
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*“You don’t even reason with logic.”*

- Timothy Holmes

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# *Abstract*

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My thesis will be an exploration on the differences between two methods of x-ray spectroscopy in the analysis of amorphous semiconductors. Specifically, I will focus on the differences between the Extended X-Ray Absorption Fine Structure (EXAFS) and the Pair-Distribution Function (PDF) methods, the latter of which was the technique used for an experiment for which I performed data analysis. I will show the benefits and drawbacks of each method as well as explore how each technique works to provide an understanding of the atomic structure of a given material.

# *Acknowledgements*

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# Abbreviations

<b>EXAFS</b>	<b>Extended X-ray Absorption Fine Structure</b>
<b>IO</b>	<b>Indium Oxide</b>
<b>ND</b>	<b>Neutron Diffraction</b>
<b>PDF</b>	<b>Pair-Distribution Function</b>
<b>TCO</b>	<b>Transparent Conducting Oxide</b>
<b>XRD</b>	<b>X- Ray Diffraction</b>
<b>ZITO</b>	<b>Zinc-Indium-Tin Oxide</b>
<b>ITO</b>	<b>Indium-Tin Oxide</b>

# Quantities

$\mu$	Modulated absorption coefficient
$\mu_0$	Unmodulated absorption coefficient
$\chi$	EXAFS function
$\Psi$	Scattering amplitude
$\mathbf{b}$	Scattering power coefficient
$\mathbf{N}$	Number of atoms
$\mathbf{Q}$	Wavevector
$\mathbf{I}$	Intensity as a function of wavevector
$\mathbf{G}$	Intensity as a function of radial position

# Chapter 1

## Introduction

X-ray spectroscopy is a powerful tool in modern material physics whenever information about the atomic structure of materials is desired. The refractive properties of short-wavelength light allow the determination of the atomic structure of a compound. Understanding the correlation between structural parameters, such as bond length and coordination number, and desirable properties can help to improve a material. In this paper, I will focus on two specific methods applied to the study of amorphous semiconductors: pair-distribution function (PDF) [1] and extended x-ray absorption fine structure (EXAFS) [2]. These two methods have been used in recent studies of amorphous semiconductors with the goal of relating mechanical and electrical properties on the macroscopic scale to their local atomic structure.

I will introduce each method by explaining the theory behind them, how they work in an experimental setting, and what types of results they produce. Then, I will compare the two methods, exploring their respective benefits and drawbacks. This comparison is useful because both methods can be used to make similar measurements on similar materials. To do this, I will combine personal experience in data analysis of the PDF method, as well as employ the knowledge of experts in the field.

## 1.1 Amorphous Semiconductors

One of the many types of compounds utilized by materials scientists is amorphous semiconductors. Amorphous semiconductors generally share many of the electronic properties of crystalline semiconductors, allowing them to be used in many applications like switches, transistors, and diodes, among other exotic uses. However, unlike most semiconductors whose atomic structure is often characterized by a crystalline, lattice-like configuration, amorphous semiconductors are unique in that there is no long-range atomic ordering. In other words, the location of other atoms becomes more random as their distance increases.

### 1.1.1 Transparent Conducting Oxides

Transparent conducting oxides (TCOs) are semiconductors that are of interest to material physicists and engineers. This group of semiconductors has the unique property of being able to conduct electricity while simultaneously being transparent to the visible spectrum of light. Not surprisingly, this group of materials has no shortage of consumer applications, such as in solar-panel technology and in electronic displays.

It is well known that growing various TCOs at differing temperatures causes a drastic change in the resulting atomic structure [3]. In other words, a TCO can be created such that it is crystalline, exhibiting long-range atomic order, or amorphous, exhibiting only local atomic order. This difference in atomic structure of a given TCO not only affects the mechanical properties of the material, such as strength and flexibility, but more importantly, its electrical properties. Chiefly among these is carrier mobility, which is a proxy for the efficiency of the material to conduct electricity. For example, in indium-oxide based TCOs, the carrier mobility of a sample seems to peak when the sample is synthesized at a specific temperature in the amorphous region, but then decreases when the sample is grown

at a hotter or cooler temperature. The cause of this phenomenon is still unknown and is a driving force in the study of amorphous TCOs. Optimizing the carrier mobility and other electronic and mechanical properties of the component in a smart window or curved television screen can significantly affect the performance of the component positively, meaning that the study of TCOs could have a large impact on the industrial applications of semiconductors.

I worked with a TCO called ZITO, or zinc-indium-tin oxide. This compound was created by doping indium oxide with both zinc and tin oxides. It was one of a series of oxides studied in order to better understand how the atomic structure of amorphous TCOs changes the electrical properties, such as why certain deposition temperatures can maximize the electrical conductivity.

## 1.2 Research Considerations

For crystalline TCOs, larger grains in the structure produce higher carrier mobility and electrical conductivity. When a sample is created at a higher temperature, there is more energy for the atoms to arrange themselves in an ordered fashion, which causes grains to grow more at a higher deposition temperature. Larger grains allow for a larger unimpeded path of electrons, which is why the mobility increases as the size of the grains increases [4].

Commercial TCOs are doped semiconductors, meaning that desirable dopants are added to the atomic structure to alter the density of electrons, increasing electrical conductivity. These dopant atoms introduce atomic-scale defects into the material. In order to produce a model with predictive capability that accurately describes how atomic-scale defects change the desirable properties of the material, the effects of the structure need to be understood. One hypothesis is that there is some relationship between the coordination number (how many neighboring atoms within a unit radius) or the bond length (distance between certain atomic bonds)

and the conductivity. Once these relationships are known, it may be possible to describe a substance with an optimal set of atomic properties, and thereby create a material that has an even greater carrier mobility, or create a material that is even more flexible or corrosion resistant. This procedure is dependent upon a method that could deliver useful information about the atomic structure for both the crystalline and amorphous samples. Figure 1 illustrates how a crystalline and an amorphous atomic structure might differ from each other, and how the local atomic order is preserved even in an amorphous sample.

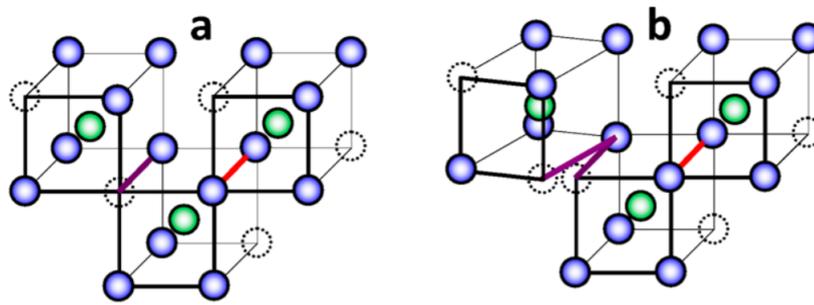


Figure 1. Arrangements of atoms in (a) a crystalline structure and (b) a possible amorphous structure of indium oxide. [4]

Each green sphere, which represents an indium atom surrounded by oxygen atoms, will have similar first coordination shell environments in both the crystalline and amorphous cases. In other words, the distance of those oxygen atoms will not vary that much in this short-range scale. However, for the amorphous samples, the structure of these cubes can be, instead of bound at a face of the cube, be bound by an edge or even a corner only. These small variations in orientation add up and are magnified, which causes the randomness of an amorphous material to be very high far away from the initial atom.

## Chapter 2

# Extended X-ray Absorption Fine Structure

The first method I will introduce that is applicable within the study of TCOs is Extended X-ray Absorption Fine Structure (EXAFS). In this chapter I will go over how EXAFS works, the experimental setting of EXAFS measurements, and the results that EXAFS can produce.

### 2.1 How Does EXAFS Work?

EXAFS is one experimental technique used to obtain valuable information about crystalline and amorphous TCOs in the local region. In EXAFS, an x-ray beam is directed into a sample (such as tin-oxide, indium-oxide (IO), or zinc-indium-tin-oxide (ZITO)). Depending on the thickness of this sample, the energy of the x-ray, and the atomic composition of the sample, a certain amount of the initial x-rays are either absorbed or transmitted through. The absorption coefficient of the sample can be determined from the ratio of the logarithm of the transmitted and incident beams per unit thickness of the sample. Knowing the absorption

coefficient  $\mu$  of a given sample is integral to EXAFS. The absorption coefficient is given as:

$$\mu = -\ln(I_t/I_0)/x \quad (2.1)$$

where  $I_t$  is the intensity of the transmitted x-ray, and  $I_0$  is the intensity of the initial beam. Because the electrons surrounding a given atom are bound to it in an orbit by a certain amount of energy, energetic photons can be used to excite these electrons. If the incident photons possess that same energy, then the electrons could be excited to a higher energy state, emitting a photoelectron on its way back down. As the incident energy approaches an absorption edge of an atom within the material, the sample begins to absorb a much greater percentage of the incoming x-rays than before, causing the transmitted portion of the initial x-rays to decrease in turn. This is known as a modulation of the absorption coefficient  $\mu$ . The EXAFS function is expressed as a fraction of the modulated absorption coefficient ( $\mu(k)$ ) to the unmodulated one ( $\mu_0(k)$ ), and is a function of the non-radial wavevector  $k$ , as shown in Eq. 2.2 below.

$$\chi(k) = \frac{\mu(k)}{\mu_0(k)} - 1 \quad (2.2)$$

Taking the Fourier transform of  $\chi(k)$  yields intensity as a function of radial position that contains real structural information about the sample's absorbing atom and its nearest neighbors. The EXAFS method utilizes an x-ray beam energy that is sufficient to cause the ejection of the innermost electrons of an atom. This energy increases as the elements become heavier since the electron configurations become more complex. Because some of the x-ray is scattered off an atom and some is absorbed, there will be an interference produced by the emitted photoelectrons and the scattered x-ray. When this interference between the absorbing atom and its neighbors occurs, the Fourier transform of  $\chi(k)$  results in a radial distribution

in real space. When it is in the EXAFS region, we can deduce certain properties of the absorbing atom's neighbors and its local atomic structure. Below is a diagram that explains how the photoemission by the absorbing atom is scattered and modulates the absorption strength during the scanning of photon energy [5].

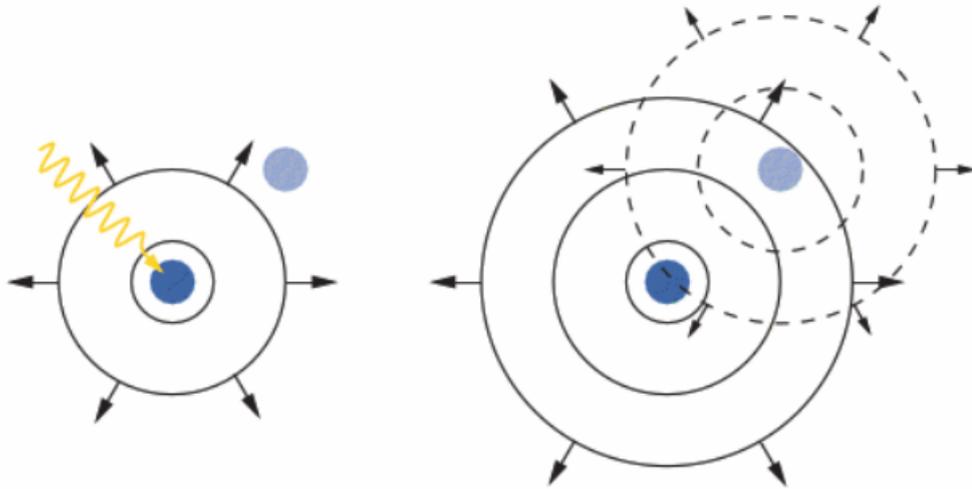


Fig. 2. The origin of EXAFS. An x-ray photon is absorbed by an atom, resulting in promotion of a core-level electron to an unoccupied continuum state. As the electron wave propagates out from the excited atom (solid circles), it can be scattered by neighboring atoms. The scattered waves (dashed circles) interfere with the outgoing waves, thereby modulating the absorption cross-section as a function of photon energy. [5]

## 2.2 Experimental Context of EXAFS

EXAFS can be used in conjunction with traditional x-ray diffraction (XRD) or neutron diffraction (ND) methods when trying to understand the total atomic structure and model the atomic defects and their impact on electrical and mechanical properties of a crystalline TCO. For most energies, the x-ray scattering intensity is dictated by the number of electrons of a given atom. Because of this,

it is hard to differentiate the scattering effects between atoms with similar numbers of electrons (elements that are close to each other on the periodic table). Because the absorption coefficient spikes at energies that would excite an electron, very small differences in these energies, and therefore scattering intensities, are magnified greatly near the EXAFS region. However, because these interactions between photoemission and x-ray scattering only occur locally between the absorbing atoms and their nearest neighbors, EXAFS cannot be used to determine physical properties beyond the local structure.

TCOs such as indium-tin oxide (ITO) or ZITO have elements that are close to each other on the periodic table, such as indium and tin, which have 49 and 50 electrons respectively. Therefore, a method such as EXAFS is beneficial in determining atomic properties of these materials. An experiment involving an EXAFS measurement requires a synchrotron as opposed to a conventional laboratory x-ray beam. This is so that the x-ray energy can be carefully scanned during the experiment. The x-ray beam starts out just below the absorption edge of an element, and then the detectors record the scattered intensity as the x-ray energy slowly increases to the absorption edge and then slightly past it. This measurement of the scattered intensity is Fourier transformed and results in a graph in real space of intensity vs radial position, such as in Fig. 3 below.

## 2.3 Results of EXAFS

Because an EXAFS experiment works in determining the local structure of a certain sample, information about an absorbing atom's neighboring atoms is obtainable. This includes information like the bond length, coordination number, and the Debye-Waller factor (DWF).

The coordination number of an atom is the number of neighboring atoms. If at a radius  $r$  from an absorbing atom there were 6 oxygen atoms, then the coordination

number would be 6. The first coordination shell is the radius around the atom where the nearest atomic neighbors lie. The second coordination shell would be the radius at which the next set of atomic neighbors are positioned, and so on.

The bond length is the distance from the absorbing atom to a neighboring atom. Because the interaction between an absorbing and reflecting atom corresponds a different intensity of the scattered wave, a shell's position directly refers to the separation between the atoms. Figure 2 shows the results of the radial distribution obtained from an EXAFS experiment conducted on amorphous indium-oxide (a-IO). The value on the x-axis of the first peak is the bond length for the first In-O shell.

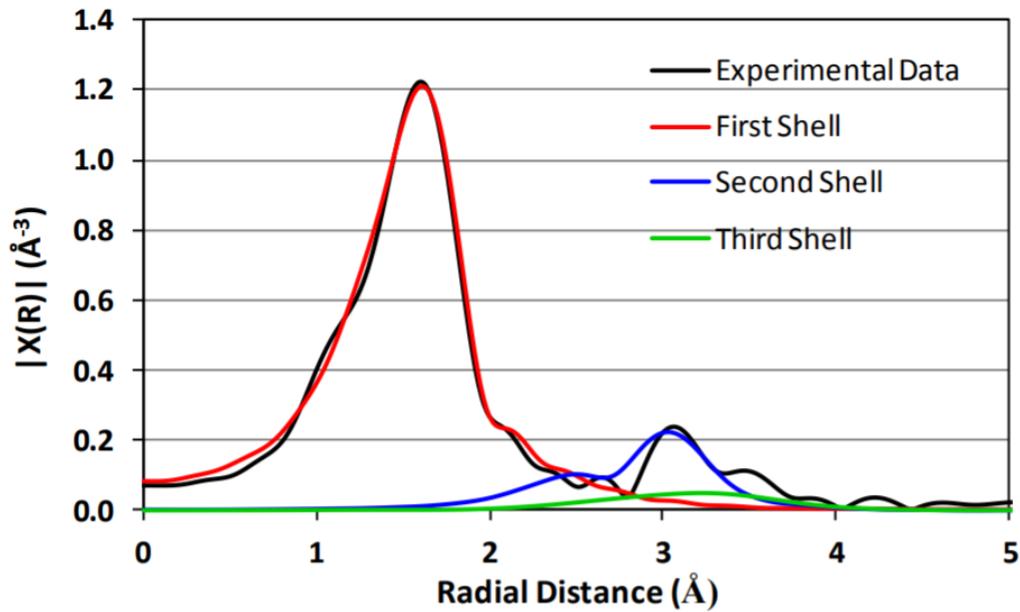


Fig. 3. Experiment radial distribution for a-IO (black), contribution of first shell (red) contribution of second shell (blue) and contribution of third shell (green). [4]

The intensity peaks created from the EXAFS scattering are only reliable in the local region for amorphous materials, and as the radius of observation increases, the intensities of the peaks decrease, and their widths increase. Therefore for

this specific experiment, only the first coordination shell has reliable information. When the wave is scattered and is measured by the detectors, there are higher intensities of certain wavevectors, corresponding to peaks due to the coordination shells once the data is Fourier transformed.

The Debye-Waller Factor (DWF) is a quantity that is related to the width of a peak in the radial distribution function. Information about the experimental resolution and disorder in the structure are related to the width of the peaks. A very narrow peak indicates that many atoms have very similar distances, while a peak that is very wide means that the atoms have a larger variance in their distances.

# Chapter 3

## Pair-Distribution Function

The second method I will introduce that is applicable within the study of TCOs is the Pair-Distribution Function (PDF). In this chapter I will go over how PDF works, the experimental procedure of the PDF method including some commentary on the data analysis process in which I have participated, and the results that the PDF method can produce.

### 3.1 What Is a Pair-Distribution Function?

An atomic pair-distribution function (PDF) gives information about all the different pairs of atoms in the structure, and doesn't necessarily convey information in relation to one single atom that has absorbed a photon's energy and emitted a photoelectron in response. The interaction of scattered waves between different types of atoms can be collected in such a way that, upon being processed by data analysis software, shows a superposition of different intensity peaks as a function of distance between pairs of atoms  $r$ .

The x-ray energy in a PDF measurement is much higher than the energy of an EXAFS measurement, which is normally tuned to be below, at, or just above

an absorption edge of a particular element. The resulting PDF scattering has contributions of every atomic pair. This strategy allows the experimenter to collect a very large range of data in reciprocal space, resulting in a higher resolution function in real space.

A PDF experiment measures x-ray or neutron scattered intensity, which theoretically can be thought of as  $|\Psi|^2$ , or  $\Psi^*\Psi$ , the complex conjugate of the wave function (of the scattered wave) times the wave function.  $\Psi$  is a function of  $Q$ , the wavevector. The wavevector proxies the reflected angle of the scattered x-rays, so a high  $Q$  value is indicative of a very large angle of scattering. The total amplitude of  $\Psi$  is the sum of each individual atom's contribution to the scattering, and that can be represented by its scattering power times an overall phase angle. The wave function is then divided by a weighted average of the scattering power of all the atoms to normalize it, and we are left with Eq. 3.1, the scattering amplitude.

$$\Psi(Q) = \frac{1}{\langle b \rangle} \sum_j b_j e^{iQR_j} \quad (3.1)$$

where  $\langle b \rangle$ , the expectation value of  $b$ , given by

$$\langle b \rangle = \frac{1}{N} \sum_j b_j \quad (3.2)$$

In the above equation,  $N$  is the total number of atoms, and  $b_j$  is the  $j^{th}$  scatter power coefficient. Eq. 3.2 becomes a weighted average of the scattering power of the atoms in a given sample. The scattering amplitude is an average of the  $j^{th}$  atom's scattering power at a given scattering angle. Because a PDF experiment measures the scattered intensity of pairs of atoms, the measured intensity can be related to the scattering amplitude and interpreted as:

$$I(Q) = \frac{1}{N} \sum_{j,l} b_j b_l e^{iQ(R_j - R_l)} \quad (3.3)$$

Eq. 3.3 above shows how the separation of each pair of atoms ( $R_j - R_l$ ) affects the overall phase of that pair's scattering intensity, amplified by the product of their scattering powers and normalized by the number of atoms. Taking the Fourier transform of the data in reciprocal space yields the reduced pair-distribution function in real space,

$$G(r) = \int_{Q_{min}}^{Q_{max}} Q \left( \frac{I(Q)}{\langle b \rangle^2} - 1 \right) \sin(Qr) dQ \quad (3.4)$$

Eq. 3.4 yields the radial-distribution function which is integrated with code from MatLab [6] to obtain information about the coordination number and bond length of particular pairs of atoms.

The data analysis process results in a graph of intensity vs. distance with many different peaks centered at varying  $r$  values. Each of these peaks corresponds to a coordination shell, or in other words, an atomic pair. In the sample ZITO for example, a scattering intensity peak at an  $r$  value of approximately 2 angstroms would correspond to an indium-oxygen atomic pair. A peak around  $r = 3$  angstroms corresponds to an indium-indium pair, and there would be one for oxygen-oxygen, zinc-indium, and so on.

## 3.2 Experimental Context of PDF

In the summer of 2017, I was given the opportunity to participate in a PDF experiment on amorphous and crystalline ZITO samples as a research assistant and data analyst [7]. While completing this work, I got a chance to see in great

detail the experimental procedure as well as the process that goes into analyzing the raw data that were collected at Argonne National Laboratory.

The Advanced Photon Source (APS) at Argonne produces a beam of very high energy x-rays incident to a sample, and records the scattered signal onto a 2-dimensional detectors. Fig. 4 below shows what the experimental setup used for ZITO looked like.

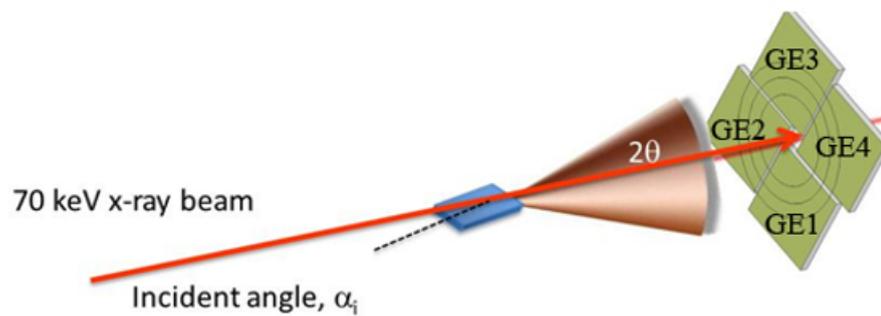


Fig. 4. The red line indicates the path of the x-rays, which hit the blue square representing the sample. These waves scatter and are captured by the 2-dimensional detectors. [8]

The recorded data are processed in software called GSAS-II [9], which takes the actual image file of the detector and radially integrates the intensity in reciprocal space. Fig. 5 shows the raw image of the scattered intensity before it is processed in GSAS-II.

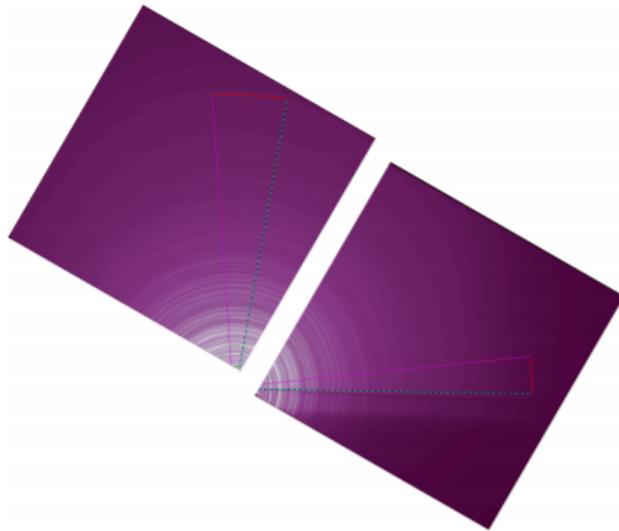


Fig. 5. Image of a PDF measurement of scattered intensity collected by two square-shaped detectors. [8]

Each 2D image is calibrated and integrated radially in GSAS-II. Another program called pdfgetx3 [10] is used to eliminate the signal that comes from the substrate and air scattering, account for truncation errors, and convert the reciprocal-space data to real space. In this process, the graphs are scaled so that the first peak, which corresponds to the first coordination shell, is normalized to have the same intensity. That way, any further differences in position of coordination shells or intensity are due to differences in the atomic structure of the samples. Fig. 6 shows a graph of the data in reciprocal space on top, and the same data in real space on the bottom.

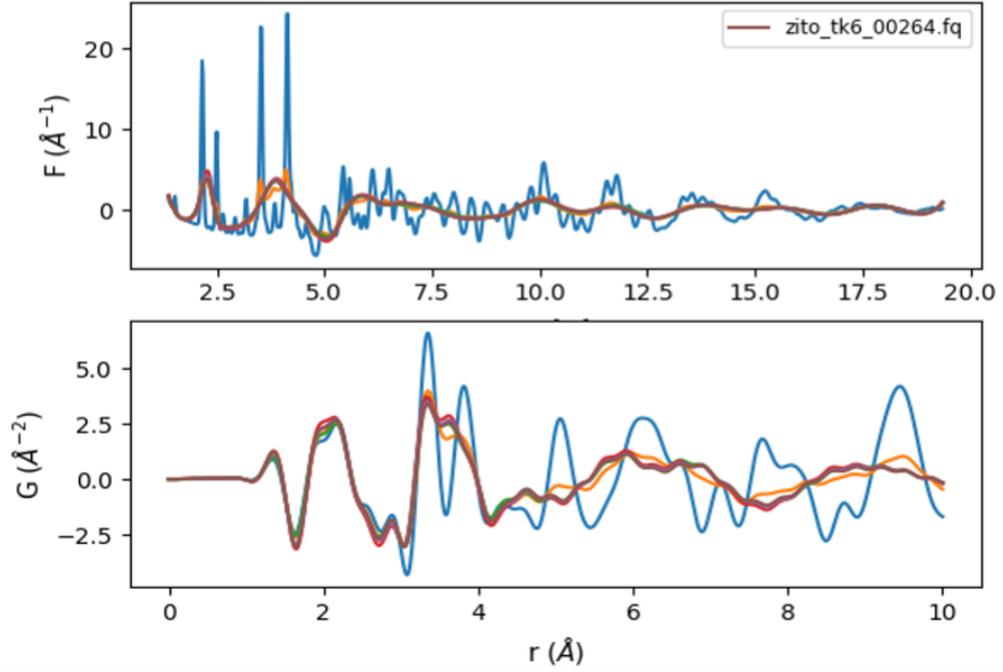


Fig. 6. Graph of multiple measurements of reciprocal space data (top) and real space data (bottom) overlaid.  $F(Q)$  represents the measured scattering intensity as a function of the wave vector (related to  $I(Q)$  in Eq. 3.3, specifically  $F(Q) = \frac{I(Q)}{\langle b \rangle^2} - 1$ , and  $G(r)$  is the Fourier transform as shown in Eq. 3.4 [7]

These two graphs are Fourier transforms of the other. Only from the bottom graph physical structural information such as bond length and coordination number can be extracted.

### 3.3 Results of PDF

Matlab code is used to extract structural information from the Fourier transform obtained from pdfgetx3. The bond length corresponds to the position of a peak in the radial-distribution function. The integrated area of a peak is related to the coordination number. The full-width at half maximum (FWHM) has information about the distribution of bond lengths in the sample. A wide peak corresponds to

a larger distribution, as in the case of amorphous samples. The FWHM typically decreases as the sample becomes more crystalline.

# Chapter 4

## Comparison of Methods

In this chapter I will discuss the benefits and drawbacks to using either method in an experimental setting, and the kinds of results that the experiments can produce.

### 4.1 Benefits and Drawbacks: EXAFS

Because the x-ray scattering factors of the elements are proportional to the number of electrons, elements adjacent in the periodic table cannot be distinguished in a typical XRD experiment. However, EXAFS allows the differentiation of elements of a similar atomic weight and electron count. Additionally, EXAFS works for both crystalline and amorphous samples.

When only local atomic ordering is present, such as in an amorphous TCO, the EXAFS signal produces usable data due to the interaction of photoelectrons and scattered x-rays from the absorbing and neighboring atoms, respectively. Therefore, information about local atomic order is obtained when studying a range of crystalline and amorphous samples. Due to how an EXAFS signal is obtained, information about local structure of the absorbing atom is the only data that is obtainable. Atoms farther away from the absorbing atom produce a much weaker

signal, resulting in the first coordination shell being the only one that can be reliably interpreted for most amorphous samples.

## 4.2 Benefits and Drawbacks: PDF

Similarly to EXAFS, the PDF technique does not require long-range atomic ordering, so it works for both short- and long-range order. This is good for experiments with amorphous TCOs, like the study on ZITO to which I contributed, since the series of samples included both amorphous and crystalline ones. Because the scattering patterns only form from atomic pairs, the actual atomic periodicity is not required, as the pair will be represented independent of its relation to other pairs.

Another unique property of the PDF method is that all the information about each pair exists, and although amorphous samples lose significance of data as  $r$  values increase, crystalline samples still have usable information as values of  $r$  increase, since a given atomic pair's average separation is more predictable.

A downside to the PDF method is that because the bond lengths of different pairs such as indium-oxygen, tin-oxygen, and zinc-oxygen can be very close to each other, one intensity peak could have contributions from all three of these pairs, making it hard to separate the contributions of each individual pair for ZITO. In EXAFS, because the x-ray energy is fine tuned to be near the absorption edge of a particular atom like indium, only the peak created by indium-oxygen in this example would be obtained, since the absorption edge of tin or zinc is not the same as indium.

A corollary of this fact also presents a problem: if two unique atomic pairs (say, indium-indium and indium-oxygen) had a very similar separation, the center of their peaks would lie very close to each other. The resulting peak would be a convolution of the two pairs. This is a drawback for both EXAFS and PDF with certain samples.

# Chapter 5

## Conclusion

Both EXAFS and PDF methods are contemporary methods that yield similar results, but whose theory and experimental measurements are very different. Fundamentally, both of the methods depend on the scattering of x-rays to convey information about the atomic structure of a material. EXAFS measurements use finely tuned x-ray energies that correspond to the absorption edge of a particular element, causing information about that element and its pairs to be the most visible. This allows for a more detailed insight into what specific intensity the peak of a coordination shell is at, exactly how wide it is, etc. However, in the amorphous TCO case, information past the first coordination shell was lost.

A PDF measurement, on the other hand, uses energies in great excess of the absorption edges of the material's elements, which in turn allows for information about each coordination shell to be recorded. However, since many shells such as indium-oxygen, zinc-oxygen, and tin-oxygen in ZITO are very close to each other, it can be difficult to tell the contribution from each individual element to the total intensity vs radial distance.

Both methods have yet to show how further iterations of amorphous semiconductors such as other TCOs and nitrides differ from other semiconductors mechanically and electronically. Ideally, both techniques should be used to obtain

complementary structural information of the samples.

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