Temporary Title: Investigation of Bond Strain Effects on XANES Spectra by Supervised Machine Learning

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Abstract

Your abstract will summarize your thesis in one or two paragraphs. This brief summary should emphasize methods and results, not introductory material.

Executive Summary

Your executive summary will give a detailed summary of your thesis, hitting the high points and perhaps including a figure or two. This should have all of the important take-home messages; though details will of course be left for the thesis itself, here you should give enough detail for a reader to have a good idea of the content of the full document. Importantly, this summary should be able to stand alone, separate from the rest of the document, so although you will be emphasizing the key results of your work, you will probably also want to include a sentence or two of introduction and context for the work you have done.

Acknowledgments

The acknowledgment section is optional, but most theses will include one. Feel free to thank anyone who contributed to your effort if the mood strikes you. Inside jokes and small pieces of humor are fairly common here . . .

Contents

List of Figures

Chapter 1

Introduction

The introduction is one of the most important pieces of your thesis. Here is a place for you to introduce the problem(s) on which you have worked and place them in the larger context of your field. You should aim to ensure that this section is completely understandable to virtually anyone - and certainly anyone with a sophomore-level grasp of physics. Presumably, this will include references to the literature.

In addition to setting your work into context, a second good idea for your introduction is to give a short outline for what the rest of your thesis will discuss. This is often done in the closing paragraph(s) of the introduction with sentences like "In the following chapters ..." and "Chapter 2 discusses ..." Tremendous detail is not required in this outline, but rather just a brief road map for the rest of the document.

1.1 X-ray Absorption Spectroscopy

I want to describe the problem we're trying to solve in this section. So I want to motivate the problem by describing XAFS a little so I can describe the limitations of XANES and why this project is useful. More in-depth explanations can be placed in chapter 2

X-ray absorption spectroscopy measures the absorption of high-energy photons by a sample as a function of energy [1]. The attenuation, or change in transmitted light intensity as a result of inelastic processes is characterized by the Beer-Lambert Law (eq: 1.1) For an incident beam of intensity I_0, the transmitted intensity after interacting with an attenuation/absorption coefficient of μ and a sample of thickness x is:

pick one

$$I = I_0 e^{-\mu x} \tag{1.1}$$

1.1.1 Synchrotron Radiation

I'm not sure where this will end up going, but somewhere I'll have to write about the origin of synchrotron radiation

Synchrotron radiation was first observed by General Electric in Schenectity, New York [2]. First thought of as a side effect particle accelerator experiments, it has since grown to be an incredibly useful source of high-energy electromagnetic radiation. Compared to lab-scale x-ray generation for diffraction experiments, arguably the most important benefit of synchrotron radiation is its high brilliance. Synchrotron radiation creates a highly collimated beam of photons characterized by small divergence and spatial coherence. Additionally, synchrotron radiation is tunable across a wide spectrum (microwaves to hard X-rays) and capable of high flux, useful for short time-scale-dependent experiments or weak scatterers. Synchrotron radiation can be produced in a pulsed structure with great stability, and the incoming photons are highly polarized, either linearly or circularly depending on where the measuremnt lies with respect to the plane of the synchrotron.

frequency range?

1.1.2 XAFS

X-ray Absorption Fine-Structure spectroscopy, or XAFS, refers to the study of absorption spectra created from high-intensity x-ray interactions. As the energy of the incident radiation is increased, the photon's energy will eventually match the binding energy of a core-level electron and an "edge" will be observed. The location of these edges on highly dependent on the chemical and physical structure, as well as the electronic and vibrational state of the material, creating characteristic absorption oscillations.

(Here's a good source to cite a bunch: the 2000 review of XAFS [3]) [4]

absorption edges like fingerprints to identify elements. in 1920 Frische and Hertz observed peak shape, and 40 years later it was learned that this shape can be used to probe the short-range order.1971 e.a. Sterne expalin this effect. Fermi's golden rule. The inelastic interactions of the photon are related to characteristic energies. When the photon energies match the energy difference from the core-electron state to the first unoccupied level, the photon can be fully absorbed (before that only partially absorbed.)

$$\mu(E) = aE^{-3} + bE^{-4} \tag{1.2}$$

$$\mu(E) \propto \sum_{f}^{E_f > E_F} |\langle f|H_{int}|i\rangle|^2 \, \delta(E - E_F - Ef) \tag{1.3}$$

1.1.3 EXAFS

Extended X-ray Absorption Fine Structure (EXAFS)

1.1.4 XANES

1.2 Machine Learning?

Probably want to talk about these papers in this section [5] [6].

Chapter 2

XAFS In Depth

In this section, I can write about XANES to a super in-depth extent, and likely the bulk of this chapter will be about FEFF and FDMNES theoretical calculations

2.1 Theoretical XANES Calculations

Chapter 3

Machine Learning

An explanation of Machine Learning and Neural Networks in general

3.1 Autoencoders if they become useful

Talk about how autoencoders work. Give a nice broad explanation and really go into the math. Include some nice diagrams

Here's [7] a good source to read and model off of. Here [8] is another paper that might be interesting to read. It's about getting noise-free data from the original data using an autoencoder. Neat idea, and could actually be very relevant because they're using geophysical data.

Chapter 4

Results

Here I expect to showcase lots of nice figures and data to show how well the neural network works

4.1 temp

Appendix A

An appendix

Appendices are a good idea for almost any thesis. Your main thesis body will likely contain perhaps 40-60 pages of text and figures. You may well write a larger document than this, but chances are that some of the information contained therein, while important, does *not* merit a place in the main body of the document. This sort of content - peripheral clarifying details, computer code, information of use to future students but not critical to understanding your work . . . - should be allocated to one or several appendices.

Bibliography

[1] D. J. Gardenghi et al., Ph.D. thesis, Montana State University-Bozeman, College of Letters & Science (2012).

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