Summer Student Programme

2013

A Detailed Absorption Spectrum of $SrTiO_3$

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Abstract

In this project, the structure factors for a $SrTiO_3$ crystal was calculated on the Mathematica platform. The pre-edge region data derived from FEFF is fitted to the structural data to get the detailed absorption spectrum, including the dipole and quadrupole transitions.

Introduction

X-rays are indispensible atoms probes and therefore used in the study of the structure of matter using diffraction. An incident beam of X-ray interact with atoms in the following ways- scattering due to atomic scattering centres, and absorption. The diffraction patterns produced due to scattering electrons can be used to reconstruct the crystal structures.

Scattering by an electron

An elementary scattering object is a free electron. The ability of an electron to scatter is expressed as scattering length which is given by,

$$r_o = \frac{e^2}{4\pi\varepsilon mc^2} \text{ Å}$$

This is called the Thompson scattering length.[1]

Scattering from a Crystal

A crystalline material is characterized by a lattice and a base(atom or molecule associated with each point in the lattice). In crystals with parallel planes separated by a distance d, x rays scattered in certain directions will be in phase and others will be out of phase. The condition for the constructive interference, Bragg's Law, is

$$n\lambda = 2dSin\theta$$

The quantity that expresses the amplitude and phase of the reflection of an x ray diffracted beam in a crystal, is the structure factor F(hkl). The F(hkl) values are complex numbers that express both the amplitude and phase of the reflection off of the (hkl) family of planes – structure factors are the quantities that is essential to obtain for each of the reciprocal lattice points. The set of structure factors that we obtain for a crystal are the data that we use to model the unit cell contents.

Theories of X-Ray Diffraction

Three broad theories are used to explain the intensities observed in diffraction studies of x rays- Geometrical theory, Kinematic theory, and Dynamical Theory. Geometrical theory gives an idea of the directions in which diffracted rays appear. This leads to the development of the concept of structure factors.[2] The Kinematical theory considers scattering from each volume element to be independent of the other and finally the Dynamical Theory takes into account all the wave interactions with the crystal. [3]

$SrTiO_3$ Crystal

Strontium Titanate is an oxide of strontium and titanium. This belongs a space group: Pm3m, cubic with unit cell constants a= 3:9050A and atomic positions: Sr (0, 0, 0); Ti: (0.5, 0.5, 0.5); O: (0.5, 0.5, 0); O: (0.5, 0, 0.5); O: (0, 0.5, 0.5).

Mathematica Description

The Mathematica crystallography package written by Dr. Martin Tolkhien makes calculations on the basis of the Dynamical Theory of Diffraction. The package sets up the crystal, calculates the real and imaginary parts of the structure factors.

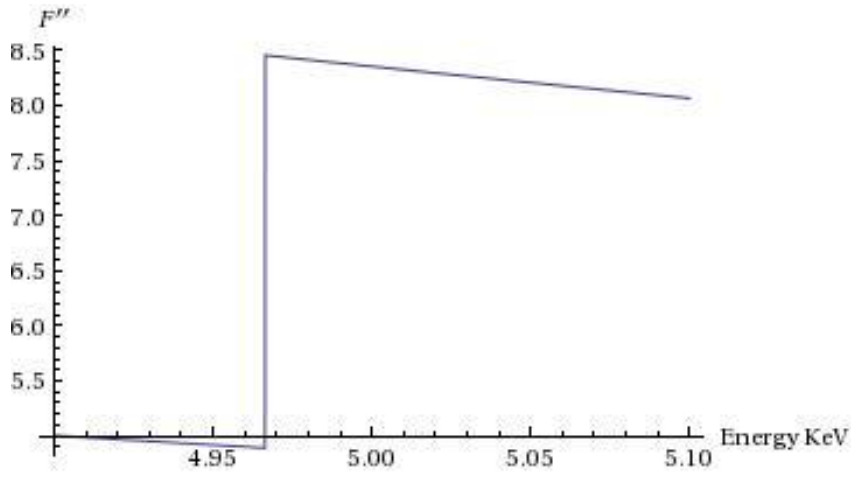

Fig.1: The Imaginary Part of Structure factor. The K-edge of Ti is a t 4.9 KeV

The pre-edge region data containing the fine structure derived from the programs FEFF is as shown below.

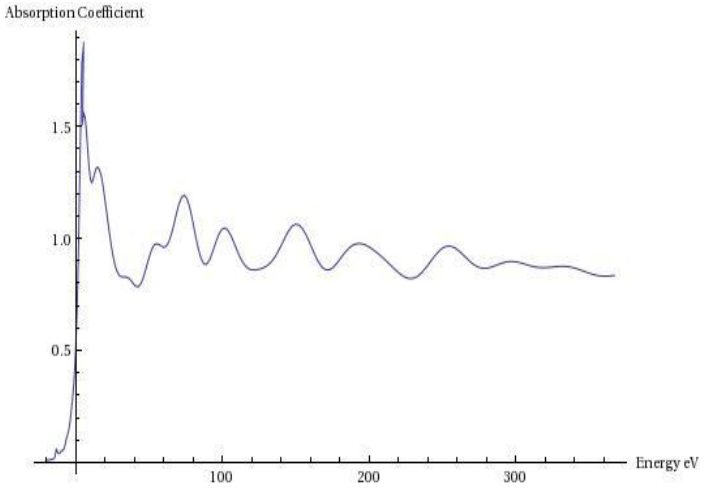

Fig2: The Absorption coefficients from FEFF

To fit the FAFF data onto the existing imaginary part of the structure factor, the scales are adjusted so that the spectra are coincident at the peak in dipole absorption and far from the edge.

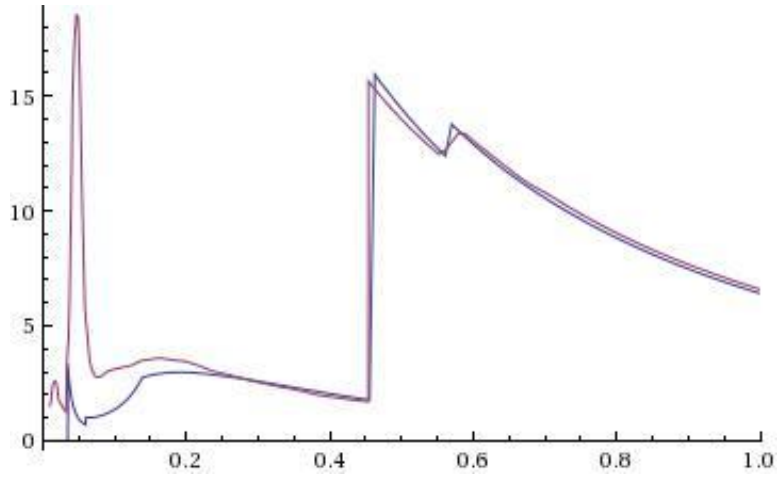

Fig.3 - The Detailed absorption spectrum including the pre edge characteristics from FAFF.

Conclusion

With this, the next step is to calculate in the high energy range for a complete picture. Using that, the real part of the structure factor can be calculated using the Kramers-Kroning relationship.

Acknowledgements

I wish to place on record my sincere gratitude to Dr. Martin Tolkhien for giving me an opportunity to learn concepts and tools that were very new to me and helping me out every step of the way. I would also like to thank Torsten Laurus for helping me getting started with the Summer Program, and Ligia Andrea Martin Montoya for her encouraging words. I would also like to thank Gisel Pena, my colleague and a fellow summer student for a memorable time. Last, but certainly not the least, I would like to thank my family and my friends for their constant support in all my endeavours

References

[1] Elements of Modern X-Ray Physics, *Jens Als-Nielsen, Des McMorrow,* Wiley Publication

[2] Introduction to the Dynamical Theory of Diffraction , *P.P. Ewald*, Acta Cryst, A25, 1969

[3] Dynamical Diffraction of X-Rays by Perfect Crystals, *Boris W Batterman, Henderson Cole,* Reviews of Modern Physics Vol36, July 1964.