Pre-edge XAFS simulations for the $SrTiO_3$ and TiO_2 crystals

Summer project

Gisel Esperanza Pena Murillo

Universidad Nacional de Colombia
Supervisor: PhD student Ligia Martin Montoya

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X-ray absorption spectroscopy (XAS)

- X-ray absorption spectroscopy (XAS) is a material characterization technique.
- Crystallinity is not required for XAFS measurements.
- Synchrotron radiation surce.
- The absorption coefficient μ, gives the probability that x-rays will be absorbed

X-ray absorption spectroscopy (XAS)

The experimental data show three general features:

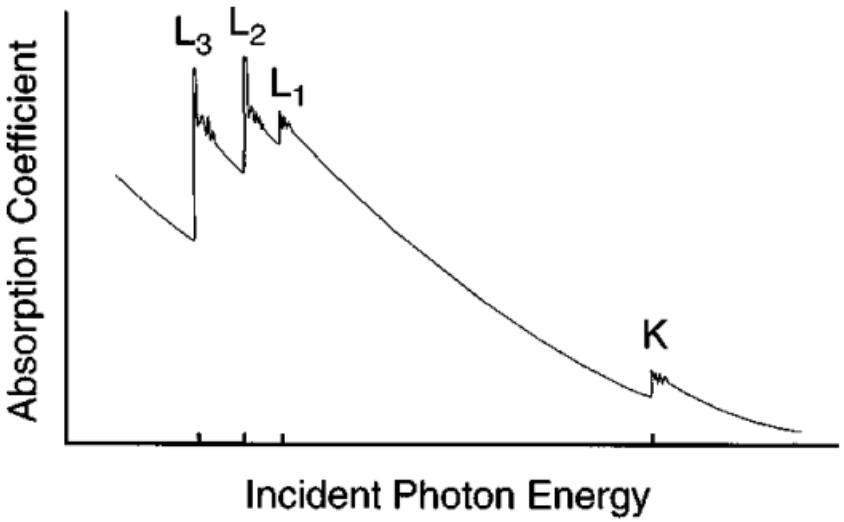


Figure: Absorption edge energy.

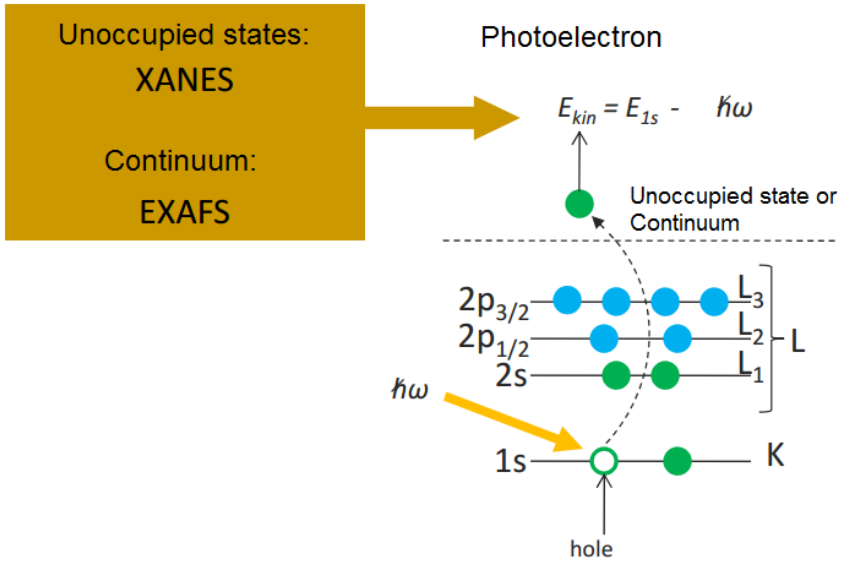


Figure: Photoelectric effect.

Extended X-ray Absorption Fine Structure (EXAFS)

- Corresponds to the oscillatory part of the spectrum.
- The wave behavior of the photoelectron (quantum interference phenomenon)

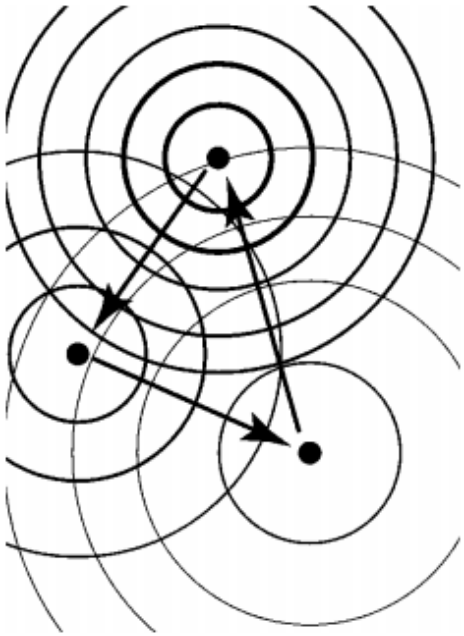


Figure: Scattering by photoelectron with neighboring atoms.

X-ray Absorption Near-edge Structure (XANES)

- Gives information about density of states unoccupied, chemical species and oxidation state.
- In the region of pre-edge dipolar and quadrupolar transitions take place.

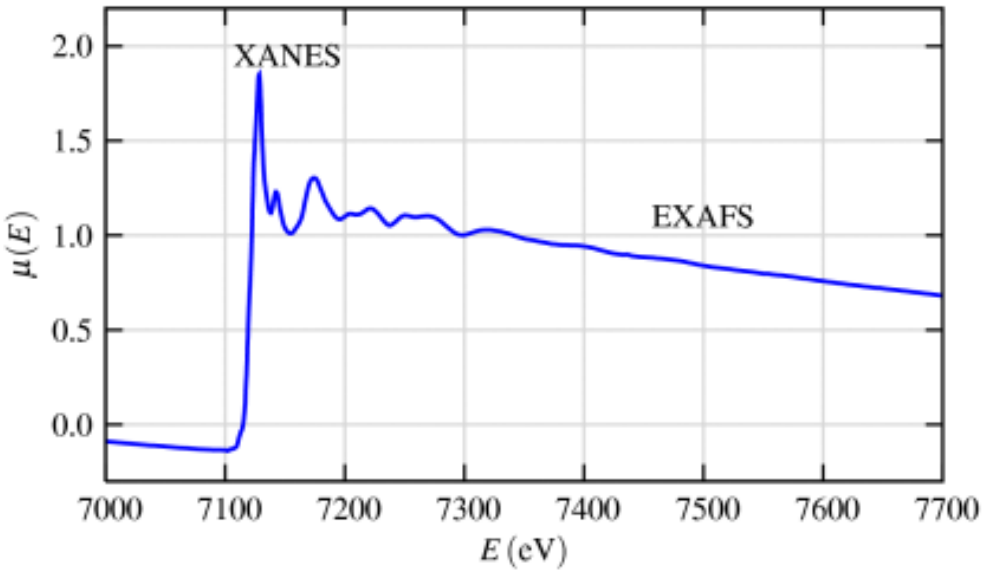
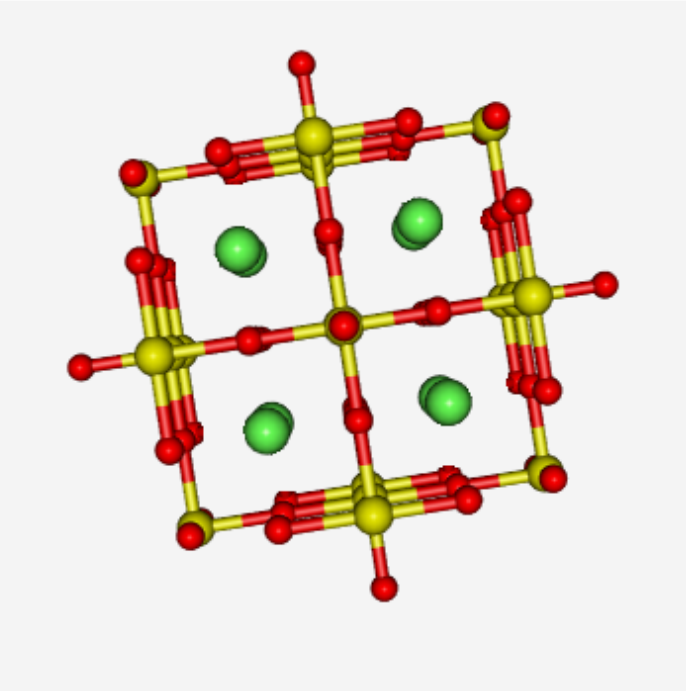


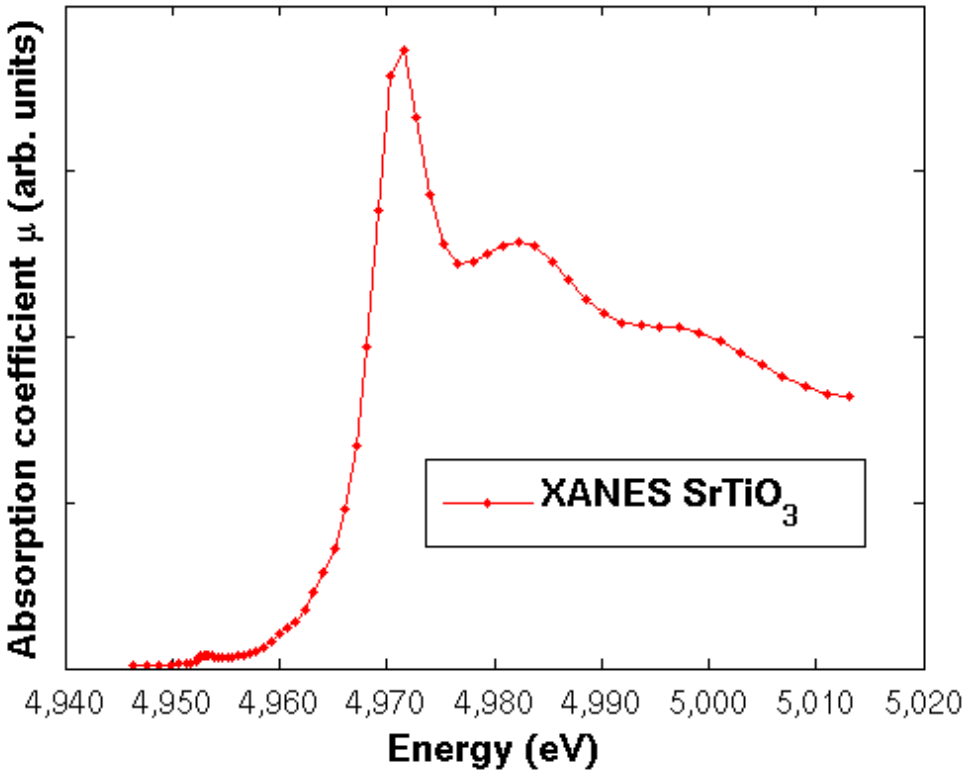
Figure: XANES and EXFAS region.

Parameteres in the FEFF input file *feff.inp*

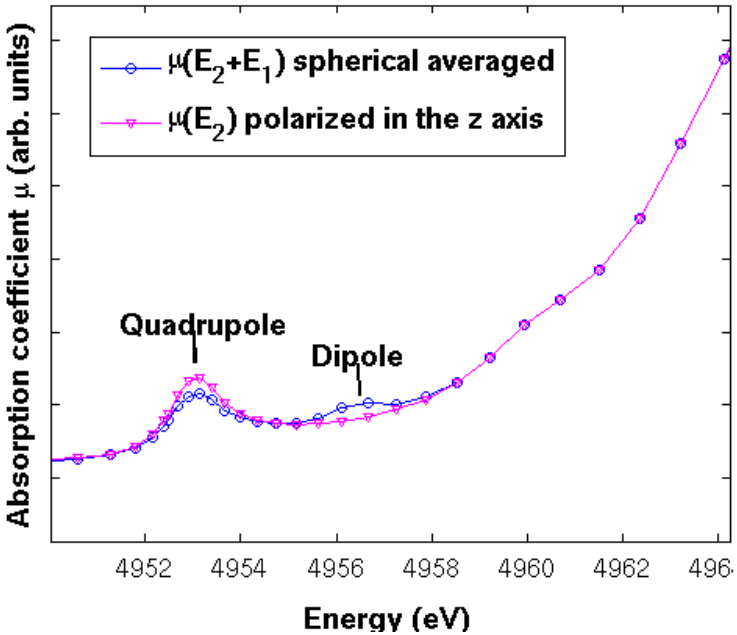
- FEFF 9.6 can do XANES simulations.
- The CARD is a keyword to specify which rutine FEFF will run.
- The SCF to do XANES calculations.
- By defult FEFF does a spherical average over the crystal/It could be implemented the electric field direction.

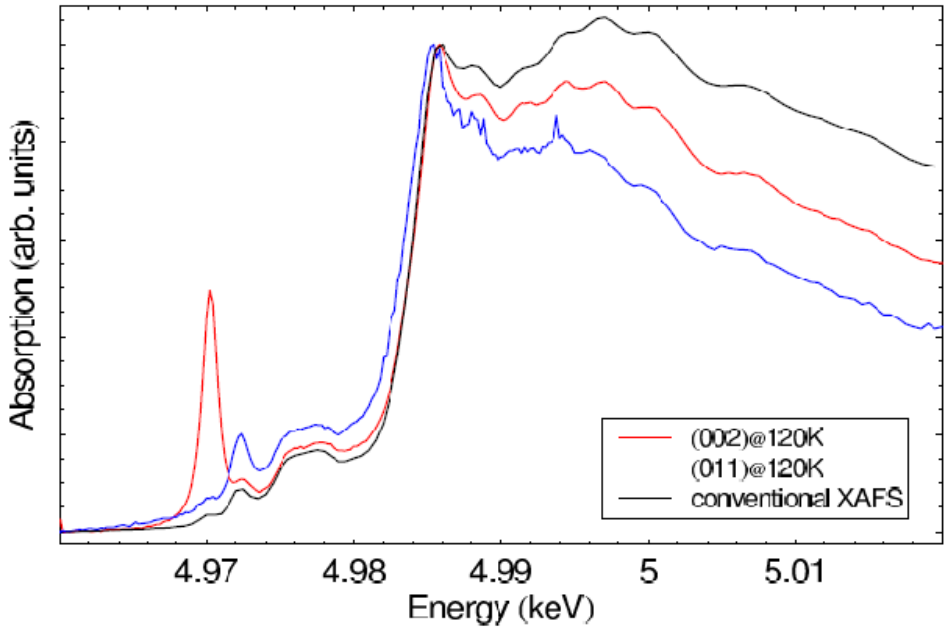
$SrTiO_3$ Crystal



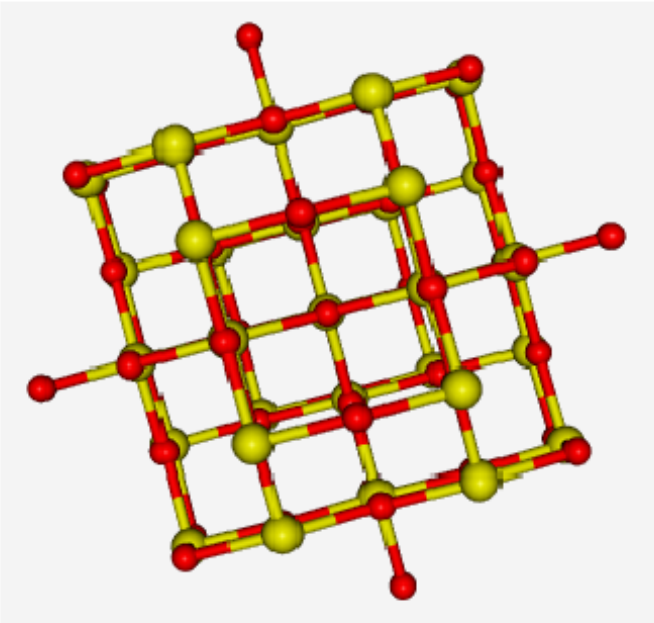


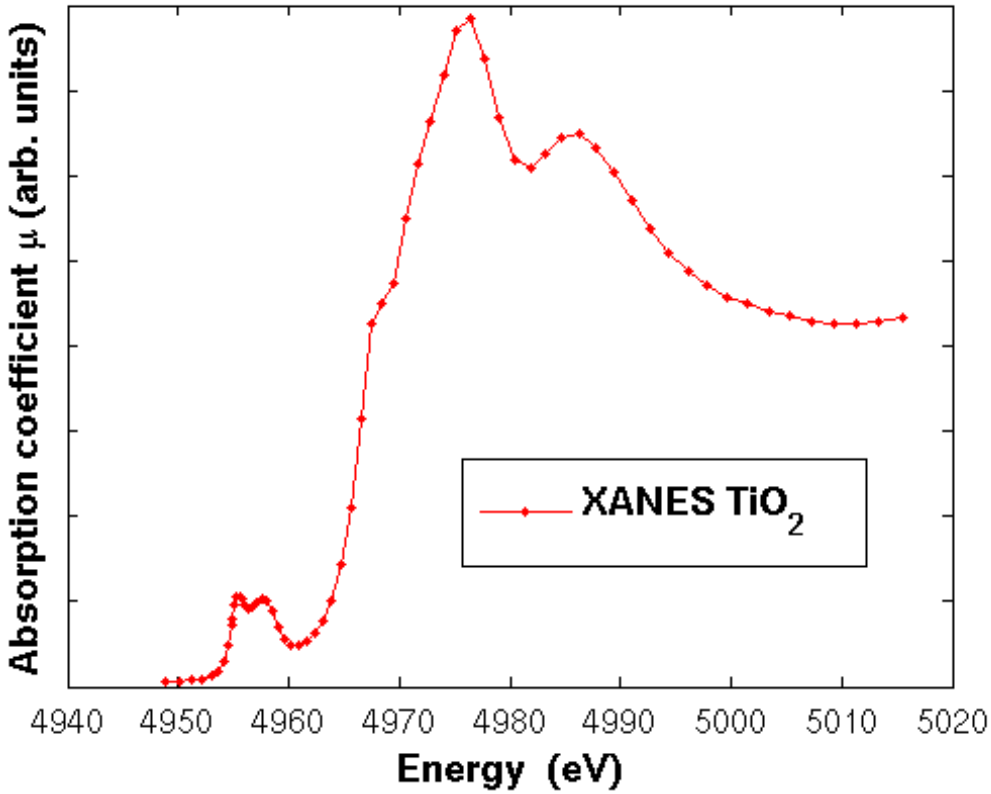
$SrTiO_3$ Crystal



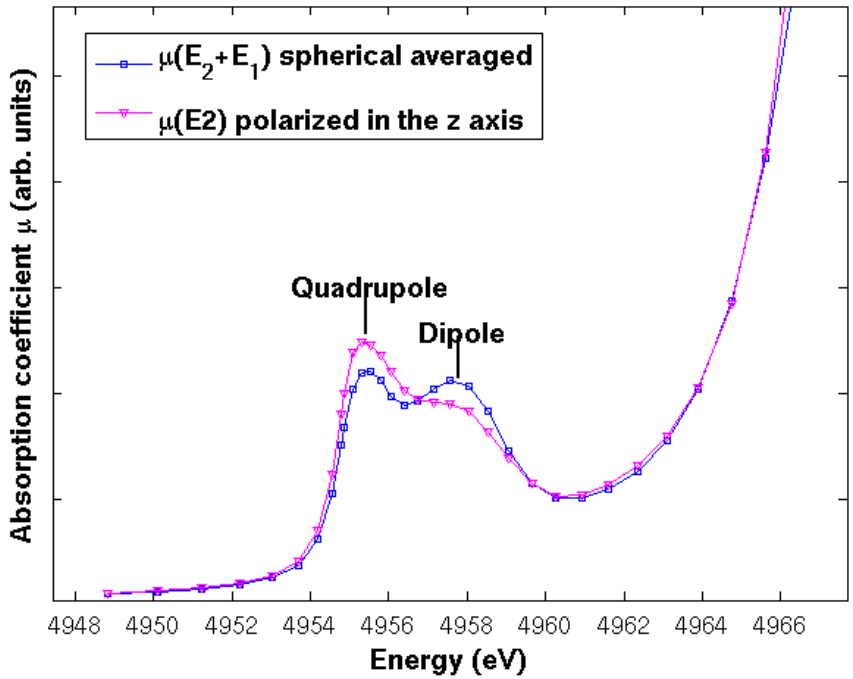


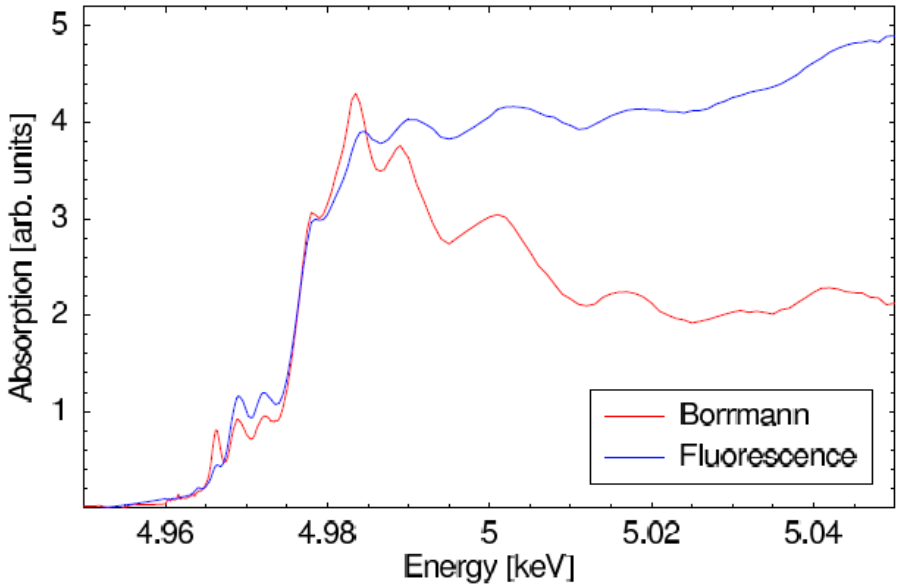
TiO_2 Crystal





TiO_2 Crystal





Conclusions

- FEFF is in fact a suitable program to simulate the pre-edge region of XAFS.
- The direction of polarization makes the quadrupole transition peak increases.
- There is an energy shift between the experimental and the theoretical quadrupolar peak could be a calibration problem with the monochromator.

Acknowledgments

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References

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[4] http://cars9.uchicago.edu/ newville/adb/search.html