Full Potential Multiple Scattering calculations for trigonal Se K-edge XANES

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Topological insulator is a noble type of material that has conductivity on the surface but is an insulator in the bulk region. Selenium is a typical element used for topological insulator materials, so that Se has attracted growing attention.

Trigonal Se (t-Se) has a highly anisotropic crystalline structure (See Fig.1), which consists of helical chains of covalently bounding atoms with three atoms per turn, which are in turn bound together into a hexagonal lattice. In t-Se, the chains form the primary structure, and the inter-chain interactions between the chains produce the secondary structure. [1]

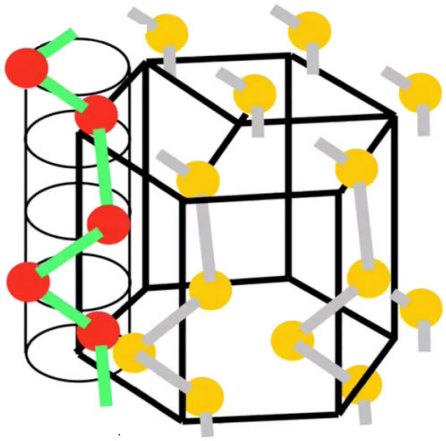

Figure 1 The structure of Trigonal Se. [2]

Our aim is to study the local structure of nano particles of Se atoms. Since there is no long range periodic order, X-ray Diffraction can not be used for this study. While X-ray Absorption Near Edge Structure (XANES) can be used to investigate a structure with middle range order, so that it is adequate for our aim.

We calculated XANES of Se K-edge with Muffin-tin approximation which employs spherically averaged charge density and potential of atomic sites. This Muffin-tin result was not satisfactory, indeed for such low dimensional systems like t-Se case, the MT approximation is known to give very poor results. Hence we have done full-potential calculations by FPMS code [3]. We will show preliminary results with the experimental spectra.

References

[1] H. Ikemoto, A. Goyo, T. Miyanaga *J. Phys. Chem. C* **115(7)**, 2931-2937 (2011)

[2] https://www2.kek.jp/ja/newskek/2008/janfeb/tellurium.html

[3] K. Hatada, K. Hayakawa, M. Benfatto and C. R Natoli, *J. Phys.: Condens. Matter* **22**, 185501(2010).