Appendix A

Compton Scattering Measurements

To study the electron momentum densities and electronic properties of materials, we present a brief description of these techniques, like X-ray Compton scattering, γ-ray Compton scattering, synchrotron radiation based high resolution Compton scattering, electron Compton scattering and positron-annihilation method.
INTRODUCTION

In 1923, A. H. Compton [1,2] discovered the inelastic scattering of X-ray which is known as Compton scattering for which he got the Nobel Prize in Physics. Within last forty years, Compton scattering has undergone considerable renewed interest in predicting the electronic structure and other related properties of crystalline solids [3,7]. It is an experiment probe which measures directly the distribution of momentum of electrons in metal. It must be emphasized that analysis in position and momentum space are complimentary and whichever space is considered is chosen only for the convenient of the use. The Compton scattering method is very sensitive to the loosely bound valence states as their contribution is confined near the Compton peak due to the lower electron momentum. The Compton profile is simply a projection of the three dimensional electron momentum distribution on to the scattering vector $\vec{k}$. The most important use of Compton profile and momentum density measurements is as test ground for various band structure schemes. Band structure serves a role of finger prints in estimation of electronic properties of any materials. Because of this significance, the band structure calculations of material had ever remained a chief target of researchers in the field of materials science.

Department of Physics, Sardar Patel University is a place of repute in material scientists due to its contribution to the research in the field of crystal growth. Crystal growth and characterizations of large number of technologically important as well as new materials have been scored in the history of Department of Physics and is still continued. Several researchers of this department are also working in the field of theoretical band structure calculations. Therefore, the experimental study of Compton profile of the material synthesized at the department will serve as a bridge between the experimental and theoretical research.
continuing in our Department. Looking to this important of Compton scattering, we have decided to perform the Compton scattering measurements on the grown crystals as a part of work which is presented in this appendix. Experimental facility required to perform Compton scattering measurements, the Compton spectrometer is already set up at the M. L. Sukhadia University, Udaipur by a group of researcher under the guidance of Prof. B. L. Ahuja. Preliminary studies of Compton scattering measurement made by us on the 2H-MoSeTe single crystal is presented here and the remaining studies like band structure calculations are in progress at the Compton scattering laboratory at M. L. Sukhadia University, Udaipur.

Hypothesis which Compton scattering experiment most clearly highlights is the idea that the individual photon of frequency $\nu$ should carry a momentum

$$p = \frac{E}{c} = \frac{h\nu}{c}$$  \hspace{1cm} (A1)

Where h is Planck’s constant. In this type of experiment, we have an incoming photon of energy of $\omega_1$ colliding with stationary particles (electron of mass m). After the collision, the photon transfers some of its momentum to the electron which recoils with certain momentum. With its momentum reduced, the photon then emerges with lower energy of $\omega_2$. A basic diagram of Compton scattering is shown in figure A1.
Figure A1 Schematic diagram of Compton scattering. $\omega_1$ and $\omega_2$ refer to incident and scattered X-ray energies.

Here to analyze the collision, the conservation of energy and momentum are used. One can get a very popular relation namely wavelength shift formula as

$$\Delta \lambda = \lambda_2 - \lambda_1 = \frac{h}{mc}(1 - \cos \theta)$$

(A2)

Here, $\lambda_1$ and $\lambda_2$ are incident and scattered photons wavelengths respectively and $\theta$ is the scattering angle.

**X-ray Compton scattering**

Before high energy $\gamma$-rays and energy dispersive detectors, X-rays were the basic radiation in the Compton spectroscopy. CuK$_a$, MoK$_a$, AgK$_a$, lines were mainly used in such experiment. The X-ray scattering was suitable only in low Z elements ($Z < 20$). In X-ray experiments, scintillation and proportional counter were mainly used for the detection of scattered radiations. The count rate of the spectrometer was very low so a large number of data points were needed for an accurate determination of the line shape. Since X-ray sources were not mono
energetic due to which Compton spectra overlapped which could not be eliminated properly by using filters or a good quality monochromators. The incident radiations had very low energy, which were only suitable for light materials. Also at the X-ray energies, the ratio of Compton to photoelectric cross section is very small. The step-scan method used in this process was very time consuming. Therefore, this method almost failed and it is no more in use.

**γ-ray Compton scattering**

Use of γ-ray Compton in scattering overcame many limitations of X-ray scattering, like low energy, multiple energy input, large bremsstrahlung contribution in data and failure of Impulse Approximation for high Z materials. $^{137}$Cs, $^{51}$Cr, $^{57}$Co, $^{203}$Hg and $^{198}$Au are the main candidates for γ-ray sources as shown in Table A1. Since γ-rays are highly monochromatic, one can obtain a desired energy of incident photons. $^{241}$Am source has half-life of 458 years which made it the most popular source for the Compton spectroscopy.

In the Compton Profile Lab, people are employing $^{241}$Am and $^{137}$Cs γ-ray sources to study the electron momentum densities. Schematic self-explanatory diagram of $^{137}$Cs γ-ray Compton spectrometers is shown in figure A2. In this Compton spectrometer, single or polycrystalline samples can be held vertically in the sample chamber and are exposed by γ-rays (662 keV).

This Compton spectrometer is based on a $^{137}$Cs source which emits photons of energy 661.65 keV. The S-S distance is 380 mm. The incident beam scattered inelastically on the sample through $160^\circ$ is detected by a high purity planar Ge detector (Canberra GLP0510P) kept at a distance of 548 mm from the sample. The channel width of the multichannel analyzer (Genie 2000, Canberra) is approximately equal to 0.035 a.u. on
the momentum scale and the overall momentum resolution of the spectrometer is 0.34 a.u.

Figure A2 Schematic sketch of 20 Ci $^{137}$Cs Compton spectrometer. Various components of the spectrometer are: (1) Steel chamber (1150 mm x 350 mm x 400 mm) divided into two parts, (2) Lead partition to separate source housing and scattering chamber, (3) $^{137}$Cs source, (4) HPGe crystal, (5) Collimator before the detector capsule, (6) Sample position (7) Port for evacuation, (8) Additional window for Compton scanning, (9) Volume seen by detector and (10) Beam stop for additional biological shielding. Other abbreviations: S1 - S3: Collimating slits and LB: Lead blocks. Standard electronics used in the detection process is also shown.
### Table A1
A quick comparison of $\gamma$-ray and X-ray based Compton spectrometers (CS).

<table>
<thead>
<tr>
<th>Parameter</th>
<th>X-ray CS</th>
<th>$\gamma$-ray CS</th>
</tr>
</thead>
<tbody>
<tr>
<td>Source energy</td>
<td>5 - 30 keV</td>
<td>10 - 1000 keV</td>
</tr>
<tr>
<td>Energy resolution of the detector</td>
<td>5% (for &lt; 100 keV)</td>
<td>1% (for &lt; 100 keV)</td>
</tr>
<tr>
<td>Purity of beam</td>
<td>Mixing of $K_{\alpha1}$ and $K_{\alpha2}$ lines and bremsstrahlung background etc.</td>
<td>Monochromatic source e.g. $^{241}$Am = 59.54 keV $^{137}$Cs = 661.65 keV</td>
</tr>
<tr>
<td>Ratio of Compton to photoelectric cross-section</td>
<td>Smaller</td>
<td>Higher</td>
</tr>
<tr>
<td>Monochromator</td>
<td>Required to separate out the proper energy from the source (multi-energy nature).</td>
<td>Not required</td>
</tr>
<tr>
<td>Applicability</td>
<td>Applicable to light elements say for $Z &lt; 25$.</td>
<td>For low and high $Z$ materials</td>
</tr>
</tbody>
</table>

Above table A1 shows the comparison of $\gamma$-ray and X-ray based Compton spectrometers (CS).

Compton scattering measurements of MoSeTe have been successfully measured using above described set up. To do this, a pellet of MoSeTe material with 2 mm thickness and 20 mm diameter was prepared by pressing at 6 ton. The raw data were accumulated over a period about 284 hrs to yield an integrated Compton intensity of about $3.6 \times 10^{17}$ photons.
Figure A3 Difference between the isotropic experimental and convoluted theoretical (spherically averaged) Compton profiles using the various schemes of the LCAO and the SPR-KKR for MoSeTe single crystal.

To extract the true Compton profile from the measured intensity distribution, the data were corrected for detector efficiency, background correction, instrumental resolution, multiple scattering, Compton cross-section, etc. Figure A3 shows the Compton profiles computed from PP-DFT-LDA, PP-DFT-GGA and PP-B3LYP are found to be very close to each other for 2H-MoSeTe single crystals. In the low momentum range, $p_z < 3.0$ a.u., we observe significant deviations between all the PP based models and the corresponding experiment. An overall poor agreement between the SPR-KKR calculations and experimental data for MoSeTe is observed [8-10].
REFERENCES