

I obtained my Ph.D. degree based on the studies on some semiconductors viz., GaAs, GaP, InP, InSb, Si & Ge on the lines of their anharmonic thermal vibration, anomalous dispersion effects and the bonding charges. Since then I was working as a CSIR Research Associate at School of Physics, Madurai Kamaraj University, Madurai – 625 021, until December 1997. I was offered a Post-Doctoral Fellowship and Lectureship at the Centre for Interdisciplinary Research, Tohoku University, Sendai, Japan, from January 1998 to March 2000.

Abstract of Ph.D. thesis (March 1988 – November 1993)

During my tenure as a Research Student, I was studying the harmonic, anharmonic thermal vibrations and the charge transfer in III-V compound and elemental semiconductors, Si & Ge. In non-centrosymmetric structures, due to the site symmetry of the atoms there is a possibility of anharmonic thermal vibration even at room temperatures. So, I studied the individual anharmonic thermal vibrations in the technologically important III-V compound

semiconductors. Moreover, the direction of charge transfer in these materials is always controversial. Reports are available for the direction of charge transfer to be in both ways i.e. from III to V and V to III. My precise investigations revealed that the direction of transfer is from III to V only. This was accomplished by precise X-ray data collection using Enraf-Nonius CAD-4 diffractometer and full-matrix least-squares refinement of the observed structure factors. I developed all the softwares used for the above in FORTRAN. Since all the above compounds are non-centric, I have made a thorough investigation of the anomalous dispersion effects. I have also studied the defect structure of some mixed semiconductors like $Ga_{1-x}As_x$ with various x values using scanning electron microscopy (SEM). Further, defect characterization of KCl with dilute Cd^{++} impurities was also carried out.

Post-Doctoral work at School of Physics, MKU (December 1993 – December 1997)

After my Ph.D., I continued my research work on semiconducting systems on the lines of the amount of charge transferred from III-V atoms, the thermal vibrations of the core and valence electrons in Si, Ge, diamond & LiF. Precise estimation of the imaginary part of the anomalous dispersion correction term of the heavy atoms Ga, As, In and Sb was done. Further, the tetrahedral distortion of fluorine atom in CaF_2 was also investigated using X-ray data. Research work done at Japan as a Research Associate & Lecturer (January 1998 – March 1999)

I gained knowledge in the analysis of the modulated structures (both commensurate and incommensurate) using the concept of super space groups. As a part of my research work on the modulated structures, I carried out the structural analysis on $1T-TaS_2$ which is incommensurately modulated at room temperature due to CDW (Charge Density Wave) formation. During the period when I was helping a Post-Graduate student in the Department of Applied Physics, Tohoku University, Japan, powder X-ray data were collected for $1T-TaS_2$ at the Centre for Interdisciplinary Research of the same university using a newly installed Rigaku X-ray Powder Diffractometer. This was equipped with a superconducting magnet to reach magnetic fields up to 5 tesla and with a cryostat to reach liquid He temperature. This data set was analyzed assuming a five-dimensional space group symmetry. The computer program used for the analysis (PREMOS) was modified extensively by me and used for obtaining the modulated structure and numerical parameters. In order to study the magnetic behavior of $1T-TaS_2$, single crystals were grown and subjected to a magnetic field (up to 5 tesla) perpendicular and parallel to the c-axis. The variation in the phase transition temperature was analyzed. $1T-TaS_2$ has a nearly commensurate phase (NC) at room temperature. This phase has been solved with an R_w factor as low as 12 %, using higher dimensional crystallography and using the precise data collected on the above powder diffractometer. All the satellite reflections up to the third order, arising out of the structural modulation have been indexed. Further, I studied the precise bonding electron density distribution of GaAs, CdTe and ZnTe using the versatile MEM (Maximum Entropy Method) technique. The optimum conditions for the collection of precise intensity data were standardized by collecting as much as 13 data sets each containing about 1000 reflections both at room and low temperatures (300, 220, 200 K). These data sets were collected using an Rigaku AFC5R diffractometer with rotating anode. The final MEM electron density maps were very precise and indicate a charge transfer from III to V in GaAs (mixed covalent and ionic nature), a highly ionic nature in CdTe and ZnTe. The program for the initial refinement of the observed structure factors was written and standardized by me in FORTRAN. I have also started working on some CMR (Colossal Magneto Resistance) materials, $La_{1-x}Ca_xMnO_3$, which involve charge and orbital ordering at specific compositions and magnetic transitions from anti-ferromagnetic to ferromagnetic.

Research work done at Japan as a Visiting Researcher (November 1999 – March 2000)

The work on the data collection and analysis using MEM has been finalised and fresh data sets have been collected at 300, 250, 200 and 170 K. The obtained MEM maps are very precise indicating a charge transfer from Ga to As in GaAs. These results are confirmed, comparing with the results from the refinement of the amount of transferred charge. Theoretical calculations of the electron densities are being carried out to compare the experimental results. In order to study the phase transitions in $1T-TaS_2$ at lower temperatures (a commensurate phase (CCDW) below 190 K and a triclinic phase (TCDW) at around 225 K on

heating and also on cooling) efforts are undertaken. Powder data have been collected at these temperatures to study the modulated structures in this two dimensional layered compound. It is planned to subject these phases to the magnetic fields upto 5 Tesla and to study the effect of the field, particularly in the TCDW phase, on which a complete structural analysis has not been made so far.