- **Metals and Alloys**

The studies on the local structure of materials seem to be rare because of the complexity of the problem. There is only limited information available on the investigations of materials in terms of the local structure. It is quite obvious that numerous research papers are being published every year based on powder as well as single crystal X-ray diffraction data. But, the structures reported using those data are only average structures. Since, the analysis of local structure needs highly precise data up to maximum possible Bragg angle, attempts to refine the data in terms of the atomic pair distribution function (PDF) are limited. Because of the complexity of the problem, tasks of acquirement of precise X-ray data from the samples, and the computational incapabilities, many crystallographers do not routinely try this approach. But the present researcher is keen in collecting precise data sets and carry out an analysis and stabilizing the methods of complex crystallographic problems. Hence using the available expertise, precise powder and single crystal X-ray data are collected for some important materials, especially metals and alloys (as test cases) and the data are being analyzed in terms of PDF in addition to the determination of the average structure using Rietveld full profile analysis. Though many structural works have been carried out based on Rietveld refinement technique, the analyses based on PDF are only a handful. For example, Billinge and Thorpe, F. Frey, Proffen and Welberry, Neder *et al.,* Billinge *et al.,* to quote a few [1,2,3,4,5].

It is clear that the refinement of local structure is not so common but it is the actual tool for elucidating the actual internal atomic level nature of materials. The routine analysis of Rietveld profile fitting is being reported frequently. Knowing the precise local nature of the systems is very important in modern day applications. Because, small scale technologies including nanotechnology, deal only with local structure. Hence a study using the local structure analysis becomes essential and timely.

The main objectives of the proposed research work will be the following;

1. Characterization of the bulk materials (some important metals and semiconductors and series of solid solutions) in terms of the measurements of thermal conductivity, electrical conductivity, thermal expansion, density measurements, micro hardness measurements and other physical characterization.
2. X-ray powder and single crystal data collection of the above characterized materials and the (average) structure determination using full profile fitting methods and full matrix least squares refinement.
3. Development of the necessary computer programs and software and stabilization of the programs.
4. Elucidation of the local structure using the PDF (Pair Distribution Function) analysis.
5. Comparison of the local and average structural properties and a try for the correlation of these properties with the bulk (average) physical properties.

The proposed research work will reveal the local structural properties of many materials, which are not studied in these lines. New understanding of the existing materials will be gained in terms of the local structure. The physical properties of the material will be understood in the lines of the local and average structure of that material. Many novel aspects on the bonding characters of metals and semiconductors will be studied. A clear understanding on the atomic level properties of the metals and semiconductors will be gained. This proposed research will give a clear understanding of the bonding features, scattering power of the local supposed to be/and new atoms/impurities happened to be at the locality. These properties can be properly utilized for the proper engineering of the technologically important materials. The present work will give an advancement of knowledge about the (1) local structure (2) average structure and (3) physical properties of the metals and semiconductors which will be very useful in technological applications and the interpretation of the existing ideas these systems. The methods/techniques for the above mentioned studies would be stabilized which can be implemented for any future system of materials. Good quality samples will be obtained and studied for their physical characteristics. Then the quality of the samples will be checked. Then, the X-ray powder data collection will be carried out. Some important tasks to be carried out are given here.

(1). <u>Physical Characterization:</u>

As mentioned earlier, the physical characterization of the samples will be carried out and some of these measurements will be based on the thermal conductivity, thermal expansion of the sample and electrical conductivity. The results will be analyzed during the later stages after the elucidation of the local structure using Pair Distribution Function analysis.

(2). <u>Quality assessment</u>

The quality of the samples will be tested using X-ray photographic techniques like Laue pattern recording,

oscillation technique, etc. Then fine samples with highest quality will be selected for X-ray data collection.

(3). Average Structure

The average structure of the chosen materials will be studied using Rietveld refinement technique as well as using single crystal X-ray data. Very precise step scan powder data up to maximum two theta values will be utilized for the purpose. Since PDF needs reflections up to maximum possible extent, special request will be made to the data collection centers to oblige this fact. The refined structure will be analyzed in terms of the isotropic and anisotropic thermal parameters, atomic positions, bond length between atoms, etc. A clear understanding of the average structure will be gained.

(4). Local Structure

The local structure of the material will be studied using Pair Distribution Function analysis. Preliminary programs will be written and stabilized for the purpose. Then using standard programs, the pair distribution function will be calculated. The observed PDF will be obtained from the observed powder X-ray data. The Observed and calculated PDF's will be matched and refined. The refined parameters will be analyzed and compared with those of the average structure and also the physical characteristics obtained through physical quantities measured earlier.

References

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