Structural Analysis of Al, Ni, and Cu Using the Maximum Entropy Method, Multipole and Pair Distribution Function

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The average and local structures of the metals Al, Ni, and Cu have been elucidated for the first time using the MEM (maximum entropy method), multipole and PDF (pair distribution function). The bonding between the constituent atoms in all these systems is found to be well pronounced and clearly seen from the electron density maps. The MEM maps of all three systems show the spherical core nature of the atoms. The mid bond electron density profiles of Al, Ni, and Cu reveal the metallic nature of the bonding. The local structure using the PDF profile of Ni is compared with that of previously reported results. The R value in the present work using low Q XRD data for the PDF analysis of Ni is close to the value in the literature using high Q synchrotron data. The cell parameters and displacement parameters are also studied and compared with the reported values.

Key words: Metals; Rietveld; Maximum Entropy Method; Pair Distribution Function; Multipole; Local Structure.