ABSTRACT

In the present work, a gamma-ray Compton spectrometer using a 200 mCi $^{241}$Am point source and an HPGe detector has been designed and built for the study of Compton profile and electron momentum density of some solids. Using 59.54 keV incident photons from the $^{241}$Am source, Compton profiles of a number of solids viz. Al, $\beta$-SiC, TiN, VN, TiB$_2$, VB$_2$ (all polycrystalline) and mixed KCl$_x$Br$_{1-x}$ (x=0.2, 0.5, 0.83 and 1.0) single crystals have been measured. Attempts have been made to interpret the Compton profile data in terms of existing models for a better understanding of the electron momentum density as well as related bonding properties.

The present Compton profile of Al is in good general agreement with the earlier reported experimental data. However, the present measurement has established for the first time better agreement between gamma-ray and high resolution X-ray data. On the theoretical side the APW calculation is seen to provide much better agreement with the experimental data than the tight binding LCAO and the interacting electron gas model calculations.

Compton profile of $\beta$-SiC is reported for the first time and reasonable agreement is obtained with the existing theoretical data. As suggested earlier, valence Compton
profile of $\beta$-SiC scaled according to the lattice momentum is found to be very similar to those of other covalent solids of similar crystal structure i.e., diamond and Si.

As regards TiN and VN reasonable agreement is obtained with theoretical estimates based on some recent band structure calculations. Present results indicate that bonding in TiN is very similar to that in TiC while in VN it is somewhat different. The difference in bonding properties of VN could be explained as due to a relatively higher occupancy of the metal 3d state compared to the non-metal 2p state.

The unit area valence Compton profiles of TiB$_2$ and VB$_2$ scaled according to the Fermi momentum are found to be almost identical. This is due to the underlying similar nature of bonding resulting in similar crystal structures.

For KCl$_x$Br$_{1-x}$ single crystals measurements were carried out along the (100) direction. The present results show, within statistical error limits, an almost linear variation of electron momentum density with the composition parameter $x$. Autocorrelation functions determined from the Compton profile data are found to yield a linear dependence of the lattice constant with $x$ in conformity with Vegard's law. Our result on KCl is in reasonable agreement with the earlier reported results.