RECONSTRUCTION OF THE SPHERICAL ELECTRON MOMENTUM DENSITY DISTRIBUTION IN Mg BY THE MAXIMUM ENTROPY METHOD

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One-dimensional projections of the electron momentum density distribution (Compton profiles - CPs) of single crystal magnesium were measured using high-energy (115.6 keV) synchrotron radiation at the beamline BL08W at SPring-8, Japan [1].

Four special directions in Brillouin zone were chosen for investigations: ΓM, ΓK, ΓA and ΓI (lying between ΓM and ΓK). The total experimental resolution of the measured CPs was equal to 0.12 a.u. Taking into account very small anisotropy [2] of directional CPs of magnesium, one can assume that the electron momentum density distribution $n(p)$ is almost isotropic. Within this approximation the spherical electron momentum density of the valence electrons in Mg was reconstructed using maximum entropy method (MEM).

The experimental resolution is taken into consideration in $n(p) \rightarrow$CP transformation matrix used by MEM algorithm. Thus the reconstructed $n(p)$ is close to the real one. Using smooth electron momentum density (estimated from experimental CPs) as a starting prior in MEM, reconstructed $n(p)$ clearly shows interesting structure below the Fermi momentum.

References

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