15:15	Poster	2

Reconstruction of the 3D electron momentum density distribution in Mg by the maximum entropy method

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Three-dimensional electron momentum density (EMD) distribution (ρ^{3D}) for valence electrons in hexagonal Mg was reconstructed by the maximum entropy method (MEM) using four one-dimensional experimental projections of the ρ^{3D}, the so-called Compton profiles (CP's). The high-resolution (0.12 a.u.) CP's were measured with the use of synchrotron radiation at SPring-8 (station BL08W) [1]. Before being used in reconstructions, the experimental profiles were deconvoluted with experimental resolution function by the MEM method.

The two-step MEM reconstruction procedure was applied. First, deconvoluted one-dimensional EMD distribution (ρ^{1D}) was reconstructed in the isotropic approximation using averaged experimental Compton profile and the Schülke model of the EMD in the correlated electron gas [2] as a *prior* (initial information). The result of this reconstruction was then interpolated into 3D momentum space and was used as a *prior* in ρ^{3D} reconstruction together with four deconvoluted experimental CP's.

The two-dimensional EMD distributions in the hexagonal plane (ρ^{2D}) were also calculated as a line integral of the ρ^{3D} along the *Z* (ΓA) axis. In order to observe the electron occupancy (in ***k*** space), Lock-Crisp-West (LCW) folding procedure [3] into the first Brillouin zone was then applied. The results ($\rho^{2D\text{-}LCW}$) were compared with the MEM reconstruction based on the five theoretical CP's (Korringa-Kohn-Rostoker method [4, 5]) and adequate reconstruction results using Cormack's method [6, 7] (Fig. 1). The both methods were compared with the calculations based on the free electron model.

The advantage of MEM in the EMD reconstruction with insufficient experimental information was affirmed despite of the low quality of the reconstructed ρ^{3D}. The reconstruction results, based on the experimental Mg profiles, showed that we are able to observe even small distortions of the Fermi surface in the regions of Brillouin zone boundaries. There are subtle but clear differences between the results obtained by the maximum entropy and the Cormack's methods in the observed electron occupancy.

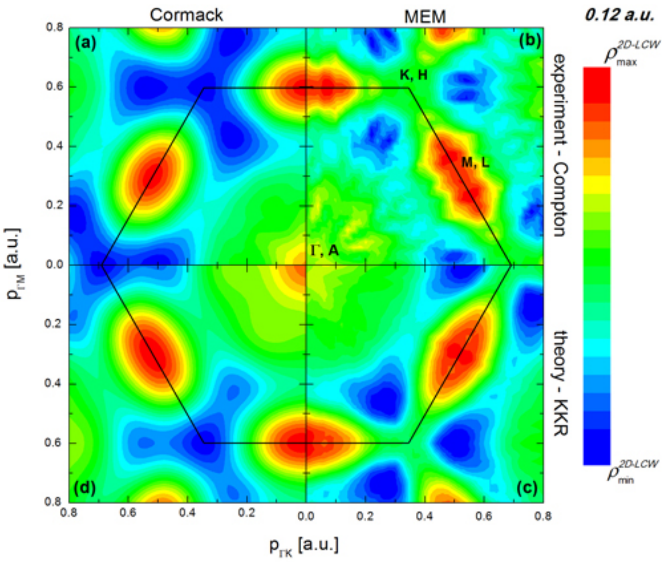

Figure 1 The $\rho^{2D\text{-}LCW}$ densities reconstructed by the Cormack method (a, d) and MEM (b, c). (a, b) panels show the reconstruction results based on the experimental CP's and (c, d) panels show the results based on the theoretical (KKR) CP's. The locations of the special high-symmetry points projected to a MΓK plane are marked on (b).

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