New insights into intrinsic anomalous Hall effect from Fe(001) angle resolved photoemission

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The anomalous Hall effect (AHE), i.e. the occurrence of the transversal voltage when a longitudinal current flows through the ferromagnetic sample placed in the magnetic field, has been the subject of numerous experimental and theoretical studies, however, a complete picture of the AHE, which combines the roles of intrinsic and extrinsic scattering-related mechanisms has emerged only relatively recently [1]. The intrinsic contribution to AHE is described in terms of the Berry-phase curvatures and it is therefore an intrinsic quantum-mechanical property of a perfect crystal [2]. The intrinsic contribution to AHE depends therefore on the details of the electronic band structure of a ferromagnet in the vicinity of the Fermi level. It is established, that the intrinsic contribution dominates in the moderately conducting ferromagnetic samples, such as thin films [1].

In this contribution we will present results of the combined experimental and theoretical study, where we use angle-resolved photoemission spectroscopy to determine, which of the theoretical ab initio methods of describing the electronic band structure of bcc Fe is the closest to the experimentally obtained band structure. The experiments are performed on Fe(001) films deposited on Au(001) at cryogenic temperatures and the theoretical methods that we use are local density approximation (LDA) and the generalized gradient approximation (GGA) and GGA corrected with many-body perturbation theory in the GW approximation.

We find the best agreement between the experimental results and the photoemission simulation based on the initial state band structure given by the GW method. In the next step, we use the GW band structure with the experimental Fermi level position to calculate the value of the intrinsic AHE in bcc Fe, and we find a value of $\sigma_{xy} = 845$ S/cm, which is much closer to the experimentally measured value of $\sigma_{xy} \approx 1000$ S/cm [4] than previously available results based on GGA band structures. This finding improves our understanding of not only the anomalous Hall effect itself, but also of other related phenomena, such as the anomalous Nernst effect and shows that highly-precise results of these transversal transport properties require a very accurate evaluation of the electron structure beyond the conventionally used GGA to the exchange-correlation functional used in DFT.

References:

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