Bulk electronic structure of Ni_2MnGa studied by density functional theory and hard x-ray photoelectron spectroscopy

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Results of a combined study employing density functional theory (DFT) using the experimentally determined modulated structures in the martensite phase and bulk-sensitive hard x-ray photoelectron spectroscopy of stoichiometric single-crystalline bulk Ni_2MnGa alloy will be presented in this talk. We show that there is an excellent matching between the experimental valence band (VB) features and the theoretical VB spectra calculated by DFT for both the martensite and austenite phases, with the experimentally determined structure. We further establish the existence of a charge density wave (CDW) state in the martensite phase from the shape of the VB near the Fermi level (EF). This shows (i) a transfer of spectral weight from the near EF region to the higher binding energy side resulting in a dip-peak structure in the difference spectrum that is in excellent agreement with DFT and (ii) presence of a pseudogap at the EF that is portrayed by fitting the near EF region with a power-law function. Detailed analyses of the results of electronic structure calculations help in understanding the experimental results. The present study explains the electronic origin and the role of the atomic modulation in hosting the CDW state in the martensite phase of bulk stoichiometric Ni_2MnGa alloy.