

Electronic structure of CuIn_5Se_8 studied by angle-resolved photoemission spectroscopy

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CuInSe_2 and related chalcopyrite compounds are recently attracting much attention due to potential applications for thin-film solar cells. Conversion efficiencies up to 19% for solar cells based on polycrystalline CuInSe_2 layers have been reached despite a lack of detailed information on material properties. Indium-rich compounds such as ordered defect compound CuIn_5Se_8 and CuIn_3Se_5 on surface of CuInSe_2 in the typical $\text{CdS}/\text{CuInSe}_2$ heterojunction play an important role for photovoltaic application due to their outstanding photoelectric characteristics [1]. However, the electronic structure of the compound CuIn_5Se_8 and the mechanism of strong localization of the states with the energies close to the Fermi level remained obscure. Knowledge on the stable surface structures of Cu chalcopyrites is very limited due to the difficulties in preparing clean well defined surfaces [2]. The electronic structure of the single crystal CuIn_5Se_8 surface has been investigated by angle-resolved photoelectron spectroscopy (ARPES) and x-ray photoemission spectroscopy (XPS). The samples were cleaved in ultrahigh vacuum of the analyzer chamber. Data have been collected for three different values of the incoming photon energy $h\nu = 20, 25,$ and 30 eV. We found that ARPES spectra along two different high symmetry directions in reciprocal space show existence of four bands. They are situated from 0 to 8 eV below the Fermi energy and have flat dispersions indicating a considerable localization of the electron states. In order to determine the chemical state of the surface and binding energy of the each core-level CuIn_5Se_8 the x-ray photoemission spectroscopy was performed using $\text{Al } K_\alpha$ radiation. The shape of valence-band spectra strongly depends on the exciting photon energies.

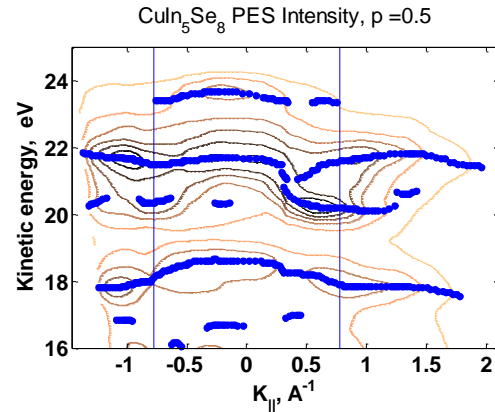


Fig. 1. The diagram of photoemission intensity as functions two variable: a wave vector (parallel a surface, along ΓM direction) and kinetic energy. Greasy curve - the coordinates of maxima of intensity on variable \AA^{-1} , correspond to the law of dispersion of strips. The vertical lines show borders of the first Brillouin zone.

References:

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- [2] Th. Deniozou, N. Esser, Th. Schulmeyer, R. Hunger, Applied Phys. Lett., 88, 052102 (2006)