PROPERTIES OF THE UFe_5Sn COMPOUND: ELECTRONIC STRUCTURE AND X-RAY PHOTOEMISSION

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9.7 cm

Recently synthesized compound of the composition UFe_5Sn crystallizes in the orthorhombic $CeCu_5Au-$type structure having $Pnma$ space group [1]. The unit cell has complex structure, 28 atoms in the unit cell: the iron atoms occupy four inequivalent sites, and uranium and tin occupy one type of site, each. The distance between uranium atoms, equal to 4.89 Å, is well above Hill limit ($\sim$ 3.4 Å) and suggests the possibility of an appreciable uranium magnetic moment. Also magnetic moments located on the iron atoms should be distinct because of different local environments for inequivalent sites. The electronic structure has been studied by the tight binding version of the linear muffin-tin orbital method in the atomic sphere approximation (*TB LMTO ASA*). The iron magnetic moments are antiparallely oriented to the uranium moments. The photoemission spectra, calculated from densities of electronic states, are compared with experimental ones [2].

Work supported by the KBN Grant No. 2 P03B 023 22

[1] A.P. Gonçalves, M. Godinho, H. Nöel , *J. Solid State. Chem.* **154** (2000) 551

[2] A. Bajorek, G. Chełkowska, R. Troć, Proceedings of the PM'02

13.4 cm

Subject category :

7. Computations of Electronic Band Structures

Presentation mode :

poster

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