Contribution ID: **54** Type: **oral**

Electronic structure and magnetic properties of UNi1/2Sb2 compound

Tuesday, 30 March 2010 11:25 (20 minutes)

Electronic structure and magnetic properties of UNi1/2Sb2 compound
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The UNi1/2/2Sb2 compound crystallizes in the tetragonal HfCuSi2 type structure with space group P4/nmm [1]. The single crystals studied order antiferromagnetically below 161 K, with the effective magnetic moment 3.17 ⊠B[1].
We present results of ab-initio band structure calculations based on full potential - linearized augmented plane wave (FP-LAPW) implemented in WIEN2k code [2]. Calculations based on experimental lattice constants and Wyckoff positions [1]. The spin polarized calculations were done for parallel and antiparallel magnetic moments arrangements. For antiferromagnetic calculation we prepared double supercell, the Wyckoff positions of uranium atoms were splitted into two nonequivalent sorts: U1 and U2. The antiferromagnetic solution was not assumed in advance. The starting magnetic moments on uranium atoms had opposite signs because of initial splitting. The system reached, iteration by iteration, selfconsistent solution, which was antiferromagnetic state. Starting from the local (spin) density approximation (L(S)DA) we verified either the orbital polarization (OP) correction or the LSDA+U approach with Coulomb repulsion energies U from 0 to 3 eV for the uranium 5f-electrons.
Calculated magnetic moments confirm antiferromagnetic ground state and collinear magnetic sequences. Total LSDA magnetic moment on uranium atom amount to 0.88 ⊠B .

Fig. 1 Crystalographic structure and DOS plots for UNi1/2Sb2 compound.

References

[1] Z. Bukowski et al. Intermetallics 12, 1381 (2004).
[2] P. Blaha et al., WIEN2k_7.3, An Augmented Plane Wave + Local Orbitals Program for Calculating Crystal Properties, Karlheinz Schwarz, Techn. Universität Wien, Austria, 2007.

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Session Classification: Theory and Spectroscopy II

Track Classification: Theory, electronic structure