ELECTRONIC STRUCTURE OF $Mg_2Ni_{1-x}Cu_x$ alloys.

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9.7 cm

Magnesium-based alloys are a good material for absorb and desorb hydrogen [1]. The electronic and electrochemical properties of Mg_2Ni alloy have been investigated during the last years [1-2]. Recently Szajek et al.[2] studied the influence of Pd on the electronic structure of Mg_2Ni alloy. In this work we present the change of the electronic structure of $Mg_2Ni_{1-x}Cu_x$ for $0 < x < 0.3$. The band structure was calculated by FPLO5-CPA [3] and KKR-CPA [4] methods. Mg_2Ni has the hexagonal $P6_222$ type structure and Ni atoms occupy two positions: (3d) and (3b) in the unit cell. In our calculations we substituted Cu atoms into Ni site located at 3d and 3b positions. We observe the change of the electronic properties in the Mg_2Ni doped by copper atoms particulary near the Fermi level.

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13.4 cm

Subject category :

3. Magnetic Structure and Dynamics

Presentation mode :

poster

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