Modelling of *bcc* multicomponent low dimensional structures composed of transition metals and metalloids

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Bcc multicomponent alloys composed of transition metals and metalloids are interesting from both applied and basic physics. Their ordering processes result in formation of a large class of alloys, some of them having quite extreme characteristics such as large negative magnetoresistance in Fe₂VAl and quenched Co₂Cr_{0.6}Fe_{0.4}Al, semi-magnetic properties in NiMnSb, or semiconductor-like temperature dependence of the resistivity in Fe₂VAl [1 and references therein]. These properties are reflected in the electronic structure of the alloys. On the other hand, it is well known, that a shape and a size of a structure strongly influences on its electronic and magnetic properties. The aim of the study is to show how these geometrical features change electronic densities of states of the bcc multicomponent alloys composed of transition metals and metalloids. Additionally transition from surface to bulk magnetic properties is analyzed.

Band structure calculations of the investigated alloys are carried out within the framework of generalized gradient approximation using FP-LAPW method.

[1] K. Perzyńska, K. Szymański, M. Biernacka, A. Go, W. Olszewski, D. Oleszak, K. Rećko, J. Waliszewski, P. Zaleski, L. Dobrzyński, J.Phys.Soc.Japan 81 064715 (2012).