Electronic and magnetic properties of metastable $Fe_{22}PdB_6$ and $Fe_{22}PtB_6$ compounds

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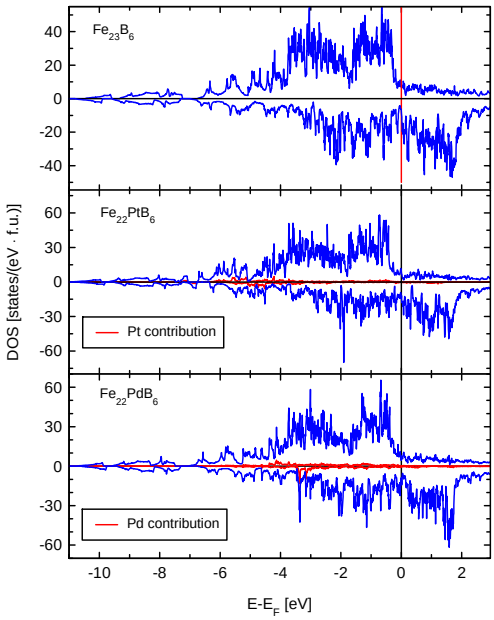
Soft magnets are a very good example of the most successful technical application of nanostructures materials produced by controlled crystallization of amorphous precursors [1]. The soft magnetic behaviour plays an important role in any application involving a change in magnetization.



Our recent investigations of amorphous $(Fe_{100-x}Ni_x)_{81}Zr_7B_{12}$ alloys showed that during the second crystallization stage a magnetically ordered metastable cubic $(FeNi)_{23}B_6$ phase appears and exhibits a $Cr_{23}B_6$-type structure with crystals of a diameter about 23 nm embedded in residual amorphous matrix [2]. In the $Fe_{70}Nb_{10}B_{20}$ alloy this type of phase crystallizes also during the first primary crystallization stage and takes the form of nanosized crystals [3].

The aim of this work is investigation of the influence of additions of Pd and Pt elements on the electronic structure and magnetic moment per atom in a unit cell. High magnetic moments of Fe and Co atoms were found in some unequivalent positions in the investigated cubic crystal structure [4].

In this paper we present *ab-initio* calculations for $Fe_{22}PtB_6$ and $Fe_{22}PdB_6$ alloys performed using the spin polarized tight linear muffin-tin orbital (TB-LMTO) method [5, 6]. The density of electronic states (DOS) calculations is presented in the included Figure and shows the usual electronic behaviour of DOS with small magnetic moments induced on Pt and Pd atoms.

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[4] B. Idzikowski and A. Szajek , Czech. J. Phys. **54** (2004) D59.
[5] O.K. Anderson, Phys. Rev. B **12** (1975) 3060.
[6] G. Krier *et al*., The TB-LMTO-ASA program (source code, version 4.7).

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