Deeper insight into crystal structure and magnetic properties of $(Fe_{0.7}Co_{0.3})_2B$ alloys with $5d$ atom substitutions

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If the theoretical and experimental methods provide complementary information on the system studied, their appropriate combination provides the data allowing a comprehensive interpretation of the phenomena taking place in the investigated system. We applied this approach, combining ab-initio calculations and various experimental techniques in the search for new alloys that could be used for production of rare-earth free permanent magnets. Our first-principles calculations for the substituted $(Fe_{0.66}Co_{0.28}W_{0.06})_2B$ and $(Fe_{0.66}Co_{0.28}Re_{0.06})_2B$ alloys showed about 15% decrease in magnetic moment, relative to that of $(Fe_{0.7}Co_{0.3})_2B$, also showing a twofold increase in magnetocrystalline anisotropy energy for the alloy with Re. To confirm experimentally these results, fully amorphous ribbons of $(Fe_{0.7}Co_{0.3})_2B$ and $(Fe_{0.675}Co_{0.275}X_{0.05})_2B$ (X = W, Re) were obtained by the melt-spinning method. Differential scanning calorimetry results indicate the highest temperature of the first crystallization peak (T_p = 574°C), and consequently the highest thermal stability, for the $(Fe_{0.675}Co_{0.275}Re_{0.05})_2B$ alloy. All of the investigated alloys were isothermally annealed at two different temperatures. The XRD patterns provide evidence of crystallization of the $(Fe,Co)_2B$ phase after isothermal annealing with a slightly different lattice parameter depending on the alloy composition. The Re substituted alloy shows the highest saturation magnetization from among the investigated samples, equal to 1126 emu/cm^3. The Mössbauer spectra of the annealed alloys consist of two sextets for $(Fe_{0.7}Co_{0.3})_2B$ or three sextets for the alloys doped with Re and W. The third sextet is related to the localization of Fe atoms in additional defect positions.

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