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Crystal-field theory and its application on the example of rare-earth borates and intermetallics

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One of important goals of modern physics is creating of new materials with predefined properties [1, 2]. The successes achieved in this direction is related, in particular, with studies of rare-earth compounds whose properties can be varied by creating crystals with the same structure but different rare-earth ions, and by doping light interstitial atoms (hydrogen, nitrogen, carbon) to the crystal (in intermetallics). In this work the crystal-field theory is applied for various rare-earth compounds, including multiferroics and magnetoelectrics [1–4]. A numerical analysis of the magnetic and magneto electric behavior in rare-earth iron borates, aluminum borates and intermetallics in a wide range of external magnetic fields and temperatures is performed. New sets of the crystal-field and exchange parameters are obtained. The magnetization behavior in high magnetic fields is described. The urgency of the work is due, first of all, to the fundamental and applied interest in rare-earth magneto electrics and intermetallics and the wealth of their properties. It is explained by the interaction of two subsystems: rare-earth and iron [1, 2]. Interesting behavior of the magnetization curves in the rare-earth multiferroic $PrFe_3(BO_3)_4$ and the rare-earth intermetallic $NdHoFe_{14}B$ is shown in Fig. 1.

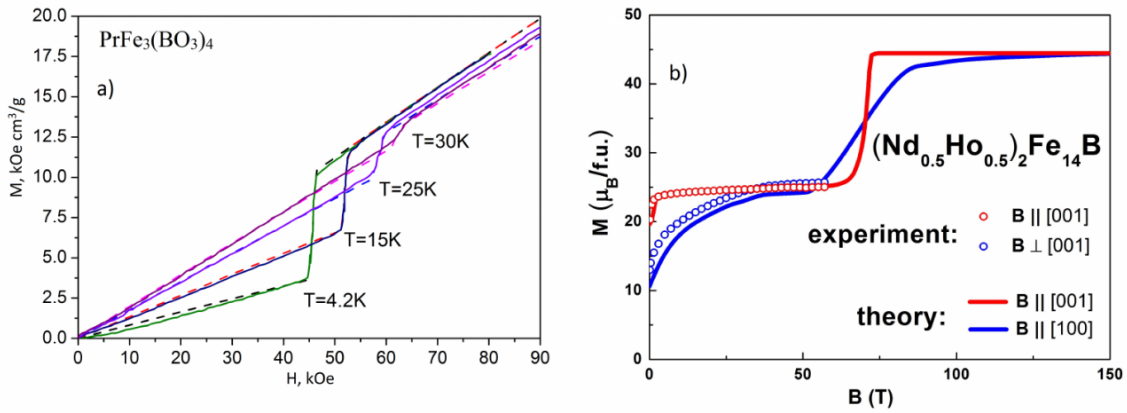

Figure 1: **(a)** Dependences of magnetization in $PrFe_3(BO_3)_4$ on the external magnetic field directed along c-axis at different temperatures (T = 4.2; 15; 25; 30 K). Solid curves are theoretical results, and dashed curves are experimental data [1]. It is shown that the transition from the antiferromagnetic phase into the angular one is the spin-flop transition (second-order). **(b)** High-field theoretical magnetization curves plotted using fitted crystal-field parameters for $(Nd_{0.5}Ho_{0.5})_2Fe_{14}B$. Solid curves are theoretical results, and dots are experimental data.

References

[1] N. V. Kostyuchenko, PhD thesis (2016).
[2] N. V. Kostyuchenko et al. Physical Review B, Vol. 92, p. 104423 (2015).
[3] A. M. Kadomtseva et al. Physical Review B, Vol. 89, No. 1 p. 014418 (2014).
[4] N. V. Kostyuchenko et al. IEEE Transactions on Magnetics, Vol. 50, issue 11 (2014).