The electronic and magnetic properties of Nd$_3$Co$_{13}$B$_2$, Nd$_5$Co$_{19}$B$_6$ and Nd$_5$Co$_{21}$B$_4$ compounds

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The Nd$_3$Co$_{13}$B$_2$, Nd$_5$Co$_{19}$B$_6$ and Nd$_5$Co$_{21}$B$_4$ compounds were manufactured as promising systems suitable for fabrication of permanent magnets. They belong to the R$_{m+n}$Co$_{5m+3n}$B$_{2n}$ family with (m = 2n, n = 1), (m = 2, n = 3), and (m = 3, n = 2), respectively [1-3]. The band structure calculations are performed by the tight binding version of the linear muffin-tin orbital method in the atomic sphere approximation (TB-LMTO ASA) [4-5]. The calculated magnetic moments on Co atoms depend on their local environment and vary in the range of 0.2 to 1.67 μ_B/atom. The calculated values of the total magnetic moments are equal to: 24.02 (20.8 [1]), 29.21 (21.5 [2]) and 31.69 (31.1 [3]) μ_B/f.u. for Nd$_3$Co$_{13}$B$_2$, Nd$_5$Co$_{19}$B$_6$ and Nd$_5$Co$_{21}$B$_4$ compounds, respectively, where the experimental values are given in the parenthesis. The main contributions to the total densities of electronic states at the Fermi level are provided by *3d* electrons of the Co atoms.
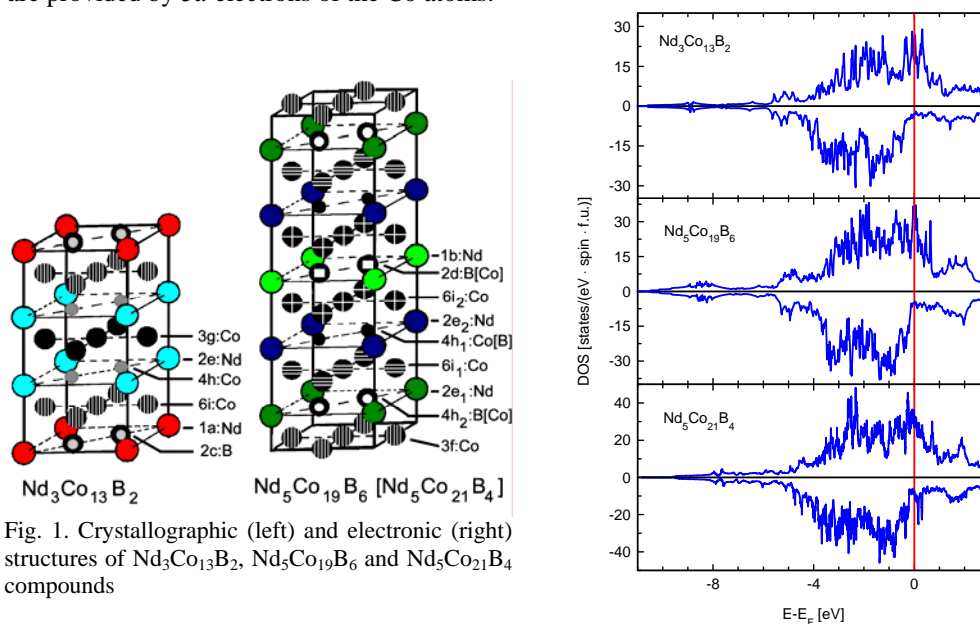

Fig. 1. Crystallographic (left) and electronic (right) structures of Nd$_3$Co$_{13}$B$_2$, Nd$_5$Co$_{19}$B$_6$ and Nd$_5$Co$_{21}$B$_4$ compounds

[1] Y. Chen *et al.*, Appl. Phys. Lett. **74** (1999) 856.
[2] Y. Chen *et al.*, J. Phys.: Condens. Matter **11** (1999) 8251.
[3] W.G. Chu *et al.*, J. Appl. Phys. **90** (2001) 1931.
[4] O.K. Andersen, Phys. Rev. B **12** (1975) 3060.
[5] G. Krier *et al.*, The TB-LMTO-ASA program (source code, version 4.7).

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