Synchrotron X-ray powder diffraction investigation of the crystal structure of $HoCo_{12}B_{6-x}C_x$

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Rare earth-transition metal borides are of significant interest due to their diverse structural and magnetic properties, which make them promising candidates for advanced functional materials [1]. Within this class, the $HoCo_{12}B_6$ compound was selected for detailed investigation due to its structural stability and unusually low magnetic ordering temperature [2-6]. This compound exhibits a rhombohedral structure, based on the hexagonal $SrNi_{12}B_6$-type structure, with a space group R-3m. Since carbon is chemically similar to boron and has a comparable atomic radius, it is a logical candidate for partial substitution without drastically altering the crystal framework [7]. In this study, we focus on the structural evolution of the $HoCo_{12}B_{6-x}C_x$ series with increasing carbon content, aiming to determine the solubility limit of carbon and evaluate the effects of substitution on lattice parameters and magnetic behaviour.

X-ray diffraction measurements using synchrotron radiation were performed at room temperature at the ROBL beamline (BM20) of the European Synchrotron Radiation Facility (ESRF). These high-resolution data enabled precise determination of lattice parameters and phase composition. The results demonstrate a linear decrease in the lattice constants and unit cell volume with increasing carbon content up to x = 0.8, after which a stabilization is observed. Rietveld refinement confirms the trends observed by both XRD methods, while SEM-EDX analysis verifies the elemental composition and homogeneity of the samples.

The synchrotron data reveal a near-isotropic lattice contraction, with the a and c parameters decreasing at similar rates. The contraction rate of the unit cell volume is approximately 0.5% per C/f.u. up to x = 0.8. Importantly, the c/a ratio remains nearly constant throughout the substitution range, indicating uniform shrinkage of the unit cell. Comparison with laboratory XRD shows more pronounced variation in the c parameter, while synchrotron XRD provides enhanced accuracy and signal-to-noise ratio. These findings offer insight into the structural effects of carbon incorporation in $HoCo_{12}B_6$ and lay the groundwork for further magnetic property investigations.

[1] E. Burzo, Rare Earths-Transition Metals-Boron Compounds: Basic Properties to Technical Applications, Springer International Publishing, Cham, 2023. https://doi.org/10.1007/978-3-030-99245-3.

[2] L.V.B. Diop, O. Isnard, Spin reorientation and magnetic structure of $HoCo_{12}B_6$ ferrimagnetic compound, J. Phys.: Condens. Matter 27 (2014) 026004. https://doi.org/10.1088/0953-8984/27/2/026004.

[3] L.V.B. Diop, Z. Arnold, J. Kamarád, O. Isnard, Pressure dependence of the magnetic properties and phase diagram of $HoCo_{12}B_6$ ferrimagnetic compound, Journal of Magnetism and Magnetic Materials 476 (2019) 106–110. https://doi.org/10.1016/j.jmmm.2018.12.042.

[4] J.M. Cadogan, S.J. Campbell, X.L. Zhao, H.S. Li, P.W. Thompson, Spin reorientation in HoCo12B6, in: M.F. Thomas, J.M. Williams, T.C. Gibb (Eds.), Hyperfine Interactions (C), Springer Netherlands, Dordrecht, 2002: pp. 119–122. https://doi.org/10.1007/978-94-010-0281-3_30.

[5] F. Mesquita, S.G. Magalhaes, P. Pureur, L.V.B. Diop, O. Isnard, Electrical magnetotransport properties in $RCo_{12}B_6$ compounds (R = Y , Gd, and Ho), Physical Review B 101 (2020) 224414. https://doi.org/10.1103/PhysRevB.101.224414.

[6] M. Mittag, M. Rosenberg, K.H.J. Buschow, A magnetization study of $RCo_{12}B_6$ intermetallics, Journal of Magnetism and Magnetic Materials 82 (1989) 109–117. https://doi.org/10.1016/0304-8853(89)90070-X.

[7] E.T. Teatum, J.T. Waber, COMPILATION OF CALCULATED DATA USEFUL IN PREDICTING METALLURGICAL BEHAVIOR OF THE ELEMENTS IN BINARY ALLOY SYSTEMS., Los Alamos National Lab. (LANL), Los Alamos, NM (United States), 1968. https://doi.org/10.2172/4789465.