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Investigation of the atomic structure of Zr_2Co_{11} XIN ZHAO, MANH CUONG NGUYEN, LIQIN KE, VLADIMIR ANTROPOV, CAI-ZHUANG WANG, KAI-MING HO, Ames Laboratory, US DOE and Department of Physics and Astronomy, Iowa State University, Ames, Iowa 50011, USA — The compound known as Zr_2Co_{11} is a ferromagnet with high uniaxial anisotropy. Although a lot of experimental work has been done on this compound, its crystal structure is still unsolved. We performed adaptive Genetic Algorithm (GA) search on its atomic structure, in order to have a better understanding of this compound. The validity of our method was verified by locating all the stable phases in Zr-Co alloy system. The search for Zr_2Co_{11} was performed with up to 117 atoms per unit cell and a narrow composition window near 15.38% Zirconium was explored. We found that Zr_2Co_{11} compound has a structure derived from $CaCu_5$ prototype and complex mixed phases can be formed. Simulated XRD and TEM patterns of our models are in agreement with the experimental results. Calculated magnetic properties provide explanations of the high uniaxial anisotropy in this system.

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