

Abstract Submitted
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Atomic structure and magnetic properties of HfCo₇ alloy MANH CUONG NGUYEN, XIN ZHAO, 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 — Low energy atomic structures of HfCo₇ alloys were searched by adaptive generic algorithm with unit cell up to 48 atoms. We found some different motifs existing in other magnetic systems in low energy structures for unit cell with 16 and 32 atoms. When the unit cell size is bigger than 40 atoms, we observed structures with phase separation into pure hcp Co and Hf₂Co₇ in agreement with phase diagram. Magnetic properties calculations were performed to investigate the relationship between the structure motifs and magnetic properties. The magnetization and Curie temperature of low energy structures are close to those of hcp Co and for some structures, a magnetic anisotropy larger than that of hcp Co were found. We will discuss more on how calculated intrinsic magnetic properties can explain the observed permanent magnet properties and how to improve the magnetic properties of HfCo₇ alloy.

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