

Abstract Submitted  
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**First Principles Studies of the Magnetic Properties of Alnico Permanent Magnet Materials**<sup>1</sup> BALAZS UJFALUSSY, Research Institute for Solid State Physics & Optics, Budapest, GERMAN SAMOLYUK, KHORGOLKHUU ODBADRAKH, G. MALCOLM STOCKS, Oak Ridge National Laboratory, Oak Ridge, TN 37831 — Until the advent of rare earth based magnets Alnico was one of the highest energy product hard magnets available. Recently, interest in this system has been rekindled as system whose properties and utility may be further enhanced but does not contain rare earth elements. Recent experiments on Alnico alloy suggest that there is no sharp interface between the disordered bcc FeCo magnetic phase and the ordered B2 NiAl non-magnetic phase; thereby undermining our understanding of the large coercivity of this material. By utilizing several electronic structure methods we first study the issue of the effect of substitutions of additional elements into B2 NiAl phase. We also calculate the magnetic moment distribution across the interface and examine the magnetic ground state. These calculations suggest that the magnetic structure of the B2-phase as well as the interface is much more complex than previously thought.

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