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Magnetic moment collapse induced by high-pressure in semi-borides TM_2B (TM = Fe, Co). A first-principles study

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ABSTRACT

The high-pressure effects are investigated on the structure, magnetic phase transition, and anisotropic elastic properties of the 3d transition-metal semi-borides TM_2B (TM = Fe, Co) by using the generalized gradient approximation (GGA) within the framework of density functional theory (DFT). At equilibrium spin polarization, calculations show that the Fe_2B and Co_2B compounds are ferromagnetic (FM). In the applied pressure range from 0 to 90 GPa, the magnetic moment of Fe_2B and Co_2B slowly decreases and then abruptly drops to zero at 85 GPa, indicating a state transition from the ferromagnetic to the nonmagnetic (NM) state (a first-order quantum phase transition). The collapse of the magnetic moment is accompanied by an abrupt change in the lattice parameters and elastic constants. In addition to this phenomenon, the density of states (DOS), and anisotropic elastic properties are presented at 0 GPa and at the critical transition pressure. Furthermore, I have plotted the three-dimensional (3D) surfaces and planar contours for the Young and bulk moduli of the compounds at several crystallographic planes, ((100) and (001)) to reveal their elastic anisotropy. On the basis of anisotropic elastic properties, I have predicted the easy and hard axes of magnetization for the TM_2B compounds.

1. Introduction

The coating is produced via the process of boriding (or boronizing), which includes the deposition of boron and an additional heat treatment, e.g. in the form of a thermochemical process to form the boride layers [1]. The boriding process offer excellent surface properties such as high hardness, increased wear and corrosion resistance and the stability of mechanical properties at high temperature [2–4]. The transition metal borides stand out due to their considered practical importance and fundamental interest for science, technology and industrial applications. Iron borides(FeB/Fe_2B) in particular, are widely used as hard and protective coatings on steel surfaces for improved wear and corrosion resistance of the material [1,5].

Cobalt boride (CoB /Co_2B) coatings were developed on the surface of a CoCrMo alloy using the powder-pack boriding process at temperatures between 1223 and 1273 K using different exposure times for each temperature [6].

Furthermore, the magneto-structural interaction is an important phenomenon in magnetic practical materials, hence, the magnetism of some borides plays a crucial role for the development of memories for mass storage. An example of this can be found in spintronics which are an integration of magnetic materials, in order to realize nanosized devices with better features.

The presence and nature of unconventional magnetic phases of semi-borides may be clarified by tuning them systematically with the help of an external parameter such as pressure. One can obtain much information on structures from the behavior under pressure. For example, magnetic collapse is a widely observed phenomenon, as a transition from a ferromagnetic state to the nonmagnetic state

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