Revisited Stress-Dependent Curie-Temperature in BCC Iron: LSDA+*U* Cleansing of Magnon Ambiguities

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ABSTRACT

This study proposes that the strong correlation of the 3d electrons in Fe is an important key to understanding the stress dependence behavior of Curie temperature (T_c). We proved our proposed hypothesis using density functional theory (DFT) within an LSDA+U (local spin density approximation +U) framework. Applying LSDA+U correction increased both the magnetic moment and magnon energy. The increased magnon energy directly contributed to the higher magnitude of the calculated T_c (compared with LSDA). The acquired T_c (from LSDA and LSDA+U) decreased with increasing unit cell volume; this was consistent with previous studies. Although introducing an on-site Coulomb interaction yielded the same stress dependence trend of T_c compared with the LSDA results, increasing the T_c magnitude was more reasonable under mean-field approximation, suggesting that the strong interaction of the 3d electrons in Fe influenced this phenomenon.

Keywords: Stress dependence, Curie temperature, Body-centered cubic iron, Frozen spin spiral, Magnon, LSDA+*U*

INTRODUCTION

Curie temperature (T_c) is one of the most important and studied factors in magnetic-based applications. The most common material for studying magnetic properties is iron (Fe), because of its high T_c and low cost. The dependence of T_c on stress in Fe, particularly, at room temperature phase (bcc Fe), helps predict the magnetic order in storage devices at actual operational temperatures. Leger and Loriers-Susse (1972) reported the independence of T_c and stress; they showed that the magnetic phase transition remained at a given temperature, even when under stress. However, Morán et al. (2003) produced inconsistent results, concluding that the Heisenberg model might not correctly describe this phenomenon. Later, Körmann et al. (2009) reported good consistency between their calculated and