

Abstract Submitted
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Defect Interaction in Iron and Iron-based Alloys¹ HAIXUAN XU, Univ of Tennessee, Knoxville, G. MALCOLM STOCKS, ROGER STOLLER, Oak Ridge National Laboratory — Magnetism has a profound influence on the defect properties in iron and iron-based alloys. For instance, it has been shown from first principles calculations that the helium interstitial occupies the tetrahedral site instead of octahedral site in contrast to all previous work that neglected the magnetic effects. In this study, we explore the effects of magnetism on the defect interaction, primarily interstitial-type defects, in bcc iron and Fe-Cr systems. The magnetic moment change during the interaction of two $1/2 \langle 111 \rangle$ interstitial loops in bcc iron was calculated using the *ab initio* locally self-consistent multiple-scattering (LSMS) method and a significant fluctuation was observed. Adding Cr significantly modifies the magnetic structure of the defects and defect interactions. In addition, the effects of magnetism on the defect energetics are evaluated. This study provides useful insights on whether magnetism can be used as an effective means to manipulate the defect evolution in iron-based structural alloys.

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