

Abstract Submitted
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The modification of core structure and Peierls barrier of $1/2\langle 111 \rangle$ screw dislocation in bcc Fe in presence of Cr solute atoms GERMAN SAMOLYUK, YURI OSETSKY, ROGER STOLLER, DON NICHOLSON, GEORGE MALCOLM STOCKS, Oak Ridge National Laboratory — Mobility of screw dislocations controls low temperature plasticity in bcc metals including ferritic alloys. Density functional theory (DFT) is an effective tool in providing parameter-free information on the energetic and magnetic properties of defects including screw dislocations. We summarize DFT calculations on atomic properties of $1/2\langle 111 \rangle$ screw dislocations in Fe-Cr system. The periodic quadrupole approach was applied to model the core dislocation structure, core interaction with Cr solute atoms and to estimate their effect on Peierls stress and barrier. The binding energy of Cr impurity atoms with a screw dislocation and its effect on the dislocation core structure are discussed and the importance of magnetism in the effects of Cr on screw dislocation mobility is demonstrated. This work was supported by the Center for Defect Physics, an Energy Frontier Research Center funded by the US Department of Energy, Office of Science, Office of Basic Energy Sciences.

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