

Abstract Submitted
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The interaction of Cr and Ni solute atoms with core of screw and edge dislocation in bcc Fe¹ YURI OSETSKY, ODBADRAKH KHORGOLKHUU, GERMAN SAMOLYUK, DON NICHOLSON, ROGER STOLLER, MALCOLM STOCKS, Oak Ridge National Laboratory — Mobility of dislocations controls the plasticity in metals. Density functional theory (DFT) is an effective tool in providing *ab initio* information on the energetic and magnetic properties of defects including dislocations and its interaction with other defects. We present DFT calculations on atomic properties of $1/2 \langle 111 \rangle$ screw and $1/2 \langle 111 \rangle (110)$ and $1/2 \langle 111 \rangle (112)$ edge dislocations in Fe-Cr/Ni system. The periodic quadrupole approach was applied to model the core dislocation structure, core interaction with Cr/Ni solute atoms. The size of supercell changes from 130 atoms for screw to 1800 atoms for edge dislocations. We investigated sensitivity of the binding energy of impurity atoms with a dislocation to lattice relaxation and size of modeling supercell. It was demonstrated that magnetic moment of solute atoms is ordered in the same direction as that of Fe matrix atoms for the case of Ni and in the opposite direction for Cr. Binding energy was found to be very sensitive to magnetic ordering.

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