First-principles calculations of dislocation-oxygen impurity magnetic interaction in silicon

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Recently, the experimental evidences of magnetic field effect on dislocation-oxygen impurity interaction in silicon [1-2] and other so called magneto-mechanical effects were reported. Today there is no consistent theory to explain these effects. Most researchers explain the presence of the ferromagnetic manifestations of the diamagnetic materials by means of so-called the d_{0} or sp magnetism, in which no traditional magnetic ions are involved. The last has attracted considerable attention due to the possible applications in spintronics.

With first-principles calculations, the possibility of formation of magnetic ordering on the edge dislocation and oxygen impurities as well as the dislocation-oxygen impurity magnetic interaction in silicon are analyzed in presented work.

The atomic structure and electronic spectra of the edge dislocation in crystalline Si are calculated by the density functional theory (DFT) [3] in the generalized gradient approximation (GGA) [4] using the ABINIT package [5]. The atomic structure of the dislocation core is modeled by simulating annealing [6] of 180 Si atoms supercell containing dislocation dipole. Changes in the density of electronic states of the supercell with dislocation dipole as well as the possible formation of magnetic ordering on the dislocation core dangling bonds are discussed. The mechanism of the magnetism can be understood well through Stoner criterion. The spin-polarized calculation of the edge dislocation in crystalline Si confirms the possibility of magnetic ordering on the dislocation core dangling bonds with the spin polarized energy is around 0,015 eV and the uncompensated magnetic moment is 1,25 μ_B per the supercell containing two segments of the dislocation line unit length.

The electronic spectrum of 64 Si atoms supercell with oxygen impurity in the interstitial position is calculated. The atomic positions of atoms in the supercell are modeled by simulating annealing [6]. It is shown that the impurity subband is formed in a vicinity of the Fermi level which can lead to the magnetic ordering according to the Stoner criterion. The uncompensated magnetic moment 1,75 μ_B per the O impurity atom was obtained by the spin-polarized calculation.

Thus the formation of magnetic moments on the dangling bonds in the dislocation core and on the oxygen impurities which leads to the additional magnetic interaction of dislocation-oxygen impurity in silicon are theoretically investigated in this paper. The last has found the experimental acknowledgements [1].

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