Lattice defects in fcc Ni from ab initio perspective

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We present a detailed theoretical study of lattice defects (Al and Si impurities, vacancies and the Σ5(210) grain boundaries (GB)) in ferromagnetic fcc Ni focusing mainly on the analysis of structure arrangement, the stability of various configurations and the influence of defects on magnetism. The calculations are performed within the density functional theory using the VASP code [1–3] with projector-augmented plane wave (PAW) potentials [4, 5]. Two possible approaches to equilibration of structure (full relaxation and relaxation with fixed lattice parameters in the GB plane) are presented and discussed.

In case of some configurations containing the interstitial Si impurity and vacancy, the structure equilibration results in the disappearance of vacancy and formation of another configuration with Si in substitutional position. It is confirmed that Si atoms prefer to occupy the interstitial positions at fcc Ni GB and Al atoms, on the contrary, prefer the substitutional ones. Furthermore, the distribution of magnetic moments in structures with and without GB including various point defects is analysed. It is found that there is a slight enhancement of magnetization at the clean GB and in the vicinity of vacancy with respect to bulk Ni (6.9% and 6.1%, respectively). The studied impurities cause the opposite effect, i.e. the decrease of the magnetic moments of neighbouring Ni atoms. The influence of an impurity is larger than the influence of a vacancy. The magnetization varies in the dependence of mutual position of studied lattice defects.

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[1] Kresse G, Hafner J. Phys Rev B 1993;48:13115.
[2] Kresse G, Furthmüller J. Phys Rev B 1996;54:11169.
[3] Kresse G, Furthmüller J. Comput Mater Sci 1996;6:15.
[4] Blöchl PE. Phys Rev B 1994;50:17953.
[5] Kresse G, Joubert D. Phys Rev B 1999;59:1758.