The effect of vacancies on grain-boundary segregation in *fcc* ferromagnetic Ni

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This work presents a detailed ab initio study of interactions between grain boundaries (GB), impurities X (X = Al, Si) and vacancies (Va) in *fcc* ferromagnetic nickel. As a basis of our calculations, supercells containing 60 or 120 atoms, containing the tilt $\Sigma5(210)$ GB, were used. The calculations were 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 structures (full relaxation and relaxation with fixed lattice parameters in the GB plane) are presented and discussed.

The analyses of the following phenomena are provided: the influence of the lattice defects on structural properties of material such as lattice parameters, the volume per atom, interlayer distances and atomic positions; the energies of formation of particular structures with respect to the standard element reference states; the stabilisation/destabilisation effects of impurities (in substitutional (s) as well as in tetragonal (iT) and octahedral (iO) interstitial positions) and of vacancies in both the bulk material and material with GBs; a possibility of recombination of $Si^{(i)}$-Va defect to $Si^{(s)}$ one with respect to the Va position; the total energy of formation of GB and Va; the binding energies between the lattice defects and their combinations; impurity segregation energies and the effect of Va on them; magnetic characteristics in presence of impurities, vacancies and GBs. As there is very little experimental information on interaction between impurities, vacancies and GBs in *fcc* nickel, most of the present results are theoretical predictions which may motivate future experimental work.

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