Atomistic modelling of twin structures in Heusler alloys

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In this work ab initio calculations of twin structures with a periods of 1-1, 2-1, 2-2, 2-3, 2-4, 2-5, 2-6, 2-7, 3-3, 4-4, 5-5, 6-6, 7-7 and 8-8 of the $Ni_2Mn_{1.75}In_{0.25}$ alloy were performed using the Vienna Ab initio Simulation Package (VASP) software [1] in the approximations of the GGA-PBE functionals [2]. The arrangement of excess Mn atoms in the lattice was made by two way. First, the excess of Mn atoms sequentially arrangements along the long axis of lattice. Second, it was calculated using the ATAT software package [3]. The plain waves cutting energy was 460 eV. The convergence criteria for total energy were set at the level of 10^{-8} eV. According to the obtained data, second structures have a lower total energy than first one. It is shown also that second structures more stable relatively to segregation. However, the structural characteristics of alloys after geometric optimization for both manners of distribution of excess Mn atoms in the In sublattice practically do not differ from each other. From all considered structures the 3-3 twin one has lower energy.

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