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Magnetism effects on structural properties in Al- and Si- substituted Laves phases Fe_2Nb and Fe_2W FRANÇOIS LIOT, MARTIN FRIÁK, JÖRG NEUGEBAUER, Department for Computational Materials Design, Max-Planck-Institut für Eisenforschung GmbH, 40237 Düsseldorf, Germany — Laves phases are promising candidates for the design of new steels with superior mechanical strength. Here we study systematically thermodynamic, structural and magnetic properties in Al- and Si- substituted Laves phase compounds Fe_2Nb and Fe_2W using first-principles density functional methods. Spin polarized calculations predict that substituting Al atoms for Fe atoms in Fe_2Nb is energetically more favorable than substituting Al atoms for Nb atoms. Furthermore, they show that this leads to a significant increase of the lattice constant along the a axis. To investigate the effects of magnetism, non-magnetic calculations are carried out for the same Fe-Nb-Al compounds. Theoretical predictions for the other alloys series, Fe-Nb-Si, Fe-W-Al and Fe-W-Si are presented. This work emphasizes the necessity of taking into account magnetism to understand the structural properties of the ternary alloys.

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