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First principles study of thermodynamic, structural and elastic properties of eutectic Ti-Fe alloys LI-FANG ZHU, MARTIN FRIÁK, JÖRG NEUGEBAUER, Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Str. 1, 40237, Düsseldorf, Germany — Ti-based alloys have been suggested for commercial applications with a great potential due to their high strength and good corrosion resistance. The strength of these materials can be even further increased if bulk nano-structured eutectic alloys are produced. Motivated by experimental results showing eutectic Fe-Ti alloys decomposing into the FeTi compound with B2 structure and β -Ti alloys with varying Ti concentration, Ti-Fe alloys covering a broad range of Ti concentrations were studied using density functional theory within generalized gradient approximation. Our formation energies correctly predict the experimentally observed phases and explain their stability in terms of a sensitive concentration dependence of the density of states at the Fermi level. Further, single-crystalline elastic constants as well as polycrystalline moduli are predicted employing Hershey's homogenization. Based on these results we discuss the effect of local lattice strain on the thermodynamic phase stability and elastic properties in nano-structured eutectics.

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