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Multi-scale study of martensite stability in Fe-based solid solutions ALEXANDER UDYANSKY, JOHANN VON PEZOLD, ALEXEY DICK , JÖRG NEUGEBAUER, Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Str. 1, 40237, Düsseldorf — Martensitic phases refer to tetragonal states of interstitial solid solutions. We study such Fe-based dilute phases by combining atomistic modeling with the reciprocal space microscopic elasticity theory (MET), which allows us to account for long-ranged elastic interactions between impurities. The short-range chemical interactions, as well as the parameters entering the MET are obtained by density functional theory (DFT) calculations. This approach allowed us to compute temperature/interstitial concentration phase diagrams and provided a direct insight into the stability limits and formation mechanisms of martensite: specifically, tetragonal states are predicted to be preferred even at low impurity concentrations of carbon, nitrogen and oxygen due to a thermodynamically driven orientational ordering of the interstitials. Moreover, both the structural type of the tetragonal state and the transition temperature were found to sensitively depend on the local strain state of the system.

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