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Sensitivity of the Stacking Fault Energy in FeMn Alloys on the Local Environment: a First-Principles Study ALEXEY DICK, TILMANN HICKEL, JÖRG NEUGEBAUER, Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany — An in-depth understanding of the physical processes that may influence the stacking fault energy (SFE) is necessary for a knowledge-based optimization and engineering of high-Mn-steels. We have performed a first-principles study of the SFE in austenitic FeMn-alloys, which are prototype structures for realistic high-Mn-steels. The relevant atomic configurations have been identified by combination of the cluster-expansion methodology and the concept of special quasirandom structures based on the density functional theory calculations. Employing either the axial interaction model and/or explicit calculations of the generalized SFE surfaces we show that the value of the SFE sensitively depends on type of the chemical and magnetic ordering in the system. We further show that the SFE can be changed not only by varying the composition of the FeMn-alloy or its temperature, but also by admixing different chemical elements or by controlling local strain fields.

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