

Abstract Submitted
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Ab initio studies of the effect of nanoclusters on magnetostriction of Fe_{1-x}Ga_x alloys¹ HUI WANG, YANNING ZHANG, University of California, Irvine, TENG YANG, Z.D. ZHANG, Institute of Metal Research and International Centre of Materials Physics, Chinese Academy of Sciences, LIZHI SUN, RUQIAN WU, University of California, Irvine — We investigated the effects of B2-like and D0-like nanoclusters on the magnetostriction of Fe-xGa alloys, through systematic density functional calculations. While the B2-like Fe-Ga clusters still undergo slightly tetragonal distortion, D03-like Fe-Ga clusters remain to be cubic in the Fe matrix. Moreover, we found that B2-like nanostructures produce negative magnetostriction whereas D03-like nanostructures give small positive magnetostriction in Fe-xGa alloys. The formation of nanoscale precipitates cannot be the reason for the extraordinary enhancement of magnetostriction of Fe_{1-x}Ga_x alloys.

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