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First principles determination of the rhombohedral magnetostriction of $Fe_{100-x}Ga_x$ and $Fe_{100-x}Al_x$ ($x < 20$) alloys[1]

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— Extensive efforts have been dedicated to investigate the extraordinary magnetostriction of Galfenol ($Fe_{100-x}Ga_x$) and Alfenal ($Fe_{100-x}Al_x$) alloys, which are very promising magnetostrictive materials for various applications such as sensors, transducers and spintronic devices. In contrast to the strong response of the tetragonal magnetostriction (λ_{100}) to the Ga/Al concentration (x), the rhombohedral magnetostriction,λ_{111}, vs. x curves for both FeGa and FeAl alloys show negative and steady values for $0 < x < 15$. Strikingly, the sign of λ_{111} changes at x = 18, a concentration that corresponds to the first peak of λ_{100}-x curves. Through highly-accurate full potential linearized augmented plane-wave method (FLAPW), our theoretical results nicely reproduce the main features of experimental λ_{111}-x curves, except the opposite sign of λ_{111} of pure Fe. Detailed analyses on the structural and electronic properties of Galfenol provide deeper understandings of the origins of the sign change, as well as the large magnetostriction anisotropy in these alloys. Possible reasons on the disagreement between the calculated and observed rhombohedral magnetostriction of bcc Fe will also be given.

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