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Anomalous thermal expansion in iron-nickel alloys: *ab initio* **calculations and the relation to magnetism** FRANÇOIS LIOT, Department for Computational Materials Design, Max-Planck-Institut für Eisenforschung GmbH, 40237 Düsseldorf, Germany, CHRIS HOOLEY, Scottish Universities Physics Alliance (SUPA), School of Physics and Astronomy, University of St Andrews, North Haugh, St Andrews, Fife KY16 9SS, U.K. — The thermal expansion of ferromagnetic disordered iron-nickel alloys at various temperatures is studied, using an approach based on Ising magnetism and first-principles calculations of the disordered local moment (DLM) type. The theory correctly describes the strong increase of the thermal expansion coefficient with increasing nickel concentration from 0.35 to 0.8 at room temperature. It also reproduces the Invar effect for $x = 0.35$. These results are analyzed, and the effect of the magnetic free energy contribution on the thermal expansion is discussed. Furthermore, a simple relationship between anomalous thermal expansion and magnetism is presented. It is argued that an alloy shows the Invar effect if the concentration of nearest-neighbor iron-iron pairs with antiparallel local moments increases sufficiently rapidly with temperature over a broad temperature interval.

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