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On the high pressure behavior of body-centered cubic iron FLORIN APOSTOL, SHEN QIU, PAUL MARCUS, Florida Atlantic University — The high pressure–high temperature behavior of iron is of current interest for geophysical reason, i.e., the earth's core is believed to be iron at high p and T. The value of the pressure at which the rigid lattice of body-centered-cubic ferromagnetic iron goes unstable was recalculated by newer methods. We give some thermodinamic arguments in support of our procedure, which minimizes the Gibbs free energy at constant pressure rather than internal energy at constant volume, and then finds elastic constants as second derivatives of G with respect to strains. The calculations used WIEN2k band-structure program and a minimum path program that makes a series of jumps in structure based on the local slope and curvature of G at a point in structure space. Errors are pointed out in several recent papers that found values different than ours, mainly due to neglect of the pressure correction required when elastic constants are calculated in a system under finite pressure by differentiation of the energy rather than Gibbs free energy.

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