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Anharmonicity alters the stability of Fe_7C_3 at the conditions of the Earth's core ZAMAAN RAZA, NINA SHULUMBA, OLLE HELLMAN, Linkoping Univ - Linkoping, LEONID DUBROVINSKY, Universitat Bayreuth - Bayreuth, IGOR ABRIKOSOV, Linkoping Univ - Linkoping — Recently, a new orthorhombic phase of iron carbide (Fe_7C_3) with an unusually high Poisson's ratio was discovered experimentally, raising the possibility that it may be important at the Earth's core. However, calculations of the Gibbs free energy in the quasiharmonic approximation suggested that it would be metastable with respect to the well known hexagonal phase at the pres sure and temperature of the Earth's core. We present new anharmonic calculations of the Gibbs free energy using the temperature-dependent effective potential (TDEP) method, which suggest that the orthorhombic phase is more stable at the conditions of the Earth's core. Anharmonicity is shown to be important at relatively low temperatures, and has a decisive effect on the phase diagram. Moreover, we show that Fe_7C_3 decomposes to form Fe_2C and Fe_3C over a narrow region of the phase diagram between the orthorhombic and hexagonal phases.

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