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Elasticity and anisotropy of Fe_3C at high pressures

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ABSTRACT

Using static electronic structure calculations, we determine the equation of state, the full elastic constant tensor and the sound wave velocities of cementite (Fe_3C) at pressures up to 410 GPa. Fe_3C is ferromagnetic (*fm*) at ambient pressures. Upon compression, the magnetic moment of the Fe atoms are gradually lost and, at around ~62 GPa, Fe_3C becomes non-magnetic (*nm*). We find that the pressure-volume results for the Fe_3C (*fm*) phase are well represented by a Vinet equation of state with K_0^{fm} = 183 GPa, K_0 = 5.9, and V_0^{fm} = 151.6 Å^3 and that of the Fe_3C (*nm*) phase are well represented by a Vinet equation of state with K_0^{nm} = 297 GPa, K_0' = 4.9, and V_0^{nm} = 143.2 Å^3. A third-order Birch-Murnaghan equation of state formulation for the Fe_3C (*nm*) phase yields similar parameters with K_0^{nm} = 304 GPa, K_0 = 4.5, and V_0^{nm} = 143.3 Å^3. At pressures relevant to the Earth's inner core, the full elastic constant tensor of Fe_3C (*nm*) reveals significant P-wave anisotropy (~10%). A crystal preferred orientation with the [110] directions of Fe_3C aligned along the pole axis would be required to explain the inner core anisotropy. Comparing, pure *hcp* Fe and iron carbides with varying stoichiometry, we find that the shear wave velocity decreases linearly with the increasing C content.

Keywords: Fe_3C, magnetic collapse, elasticity, anisotropy, Earth's inner core