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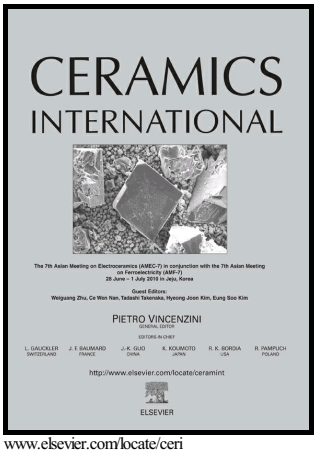

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Pressure dependent mechanical properties of calcium carbides

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The mechanical properties of newly synthesized Ca_2C_3 and Ca_2C under pressure have been studied by using the first-principles calculations with generalized gradient approximation. The equilibrium geometry, elastic stiffness constants, various moduli, and Pugh's ratio of the *C*2/*m* phase of Ca_2C_3 and the *C*2/*m* and *Pnma* phases of CaC_2 are systematically studied. The elastic stiffness constants of *C*2/*m*-Ca_2C_3 under 0 GPa to 30 GPa, *C*2/*m*-Ca_2C under 0 GPa to 7.5 GPa, and *Pnma*-Ca_2C under 7.5 GPa to 30 GPa satisfy the Born−Huang mechanical criteria. The three phases of calcium carbides exhibit ductile characteristics. The surface constructions of bulk and Young's moduli illustrate the mechanical anisotropy of Ca_2C_3 and Ca_2C. Our results are consistent with previously obtained experimental and theoretical data and have significant implications for the application of calcium carbides.

Keywords: Carbides; Mechanical properties; Anisotropic Properties; First-principles calculations

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Declarations of interest: none