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Second harmonic generation and high pressure ferroelectricity in $PbTiO_3$ MUHTAR AHART, ALEXANDER F. GONCHAROV, P. GANESH, R.E. COHEN, RUSSELL J. HEMLEY, Carnegie Institution of Washington — We performed measurements of second harmonic generation (SHG) in single-crystal $PbTiO_3$under hydrostatic pressure up to 60 GPa and polycrystalline samples up to 100 GPa at room temperature. The SHG effect is a nonlinear optical effect resulting from a nonlinear dependence of the polarization on the electric field and it strongly couples to ferroelectric order parameters. The integral intensity of SHG in the material is remarkably sensitive to pressure and its intensity decreases monotonically with pressure below 12 GPa. The SHG shows weak intensity with no obvious dependence on pressure above 12 GPa. The integral intensity of the SHG can serve as an order parameter that is responsible for the pressure induced phase transition in $PbTiO_3$ crystals. To understand the experiment results, we also performed first-principles density functional calculations using both plane-wave and tight-binding methods and phonon band-structure calculations. We find the ground state to have zone-boundary distortions, with a small polarization. The energy differences between the competing phases are within $\sim$ 1-6 meV/at. suggesting a low Tc at higher pressures, which would be consistent with observed room temperature SHG measurements. This work is supported by the ONR (N000140210506) and the Carnegie/DOE Alliance Center (CDAC) (DF-FC03N00144).

Muhetaer Aihaiti
Carnegie Institution of Washington

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