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On structural, elastic and dynamic stability of rare earth nitrides: First principle calculations B.D. SAHOO, K.D. JOSHI, S.C. GUPTA, Bhabha Atomic Research Centre, Mumbai, India - 400085 — The structural stability of LaN and CeN under hydrostatic compression has been analysed theoretically. For LaN the comparison of enthalpies calculated at various pressures for rocksalt type (B1), tetragonal (B10) and CsCl type (B2) structures suggests that the B1 phase will transform to B10 structure at $\sim$ 20 GPa, in line with the experimental value of 22.8 GPa. Additionally, we predict the B10 to B2 phase transition at higher pressure of $\sim$ 165 GPa. Similar transition sequence has been predicted for CeN also with the B1 to B10 and B10 to B2 transition pressures calculated as 53 GPa and 198 GPa, respectively. However, the static high pressure EDXRD measurements on CeN by Olsen et al. report direct B1 to B2 phase transition at $\sim$ 65 GPa. To resolve this discrepancy, we have performed lattice dynamic calculations on these structures. The phonon spectra calculated at zero pressure correctly shows B1 phase to be dynamically stable and B10 and B2 to be unstable. At 65 GPa the B1 phase becomes dynamically unstable and the B10 emerges as a dynamically stable phase whereas B2 still remains unstable, supporting theoretical finding. Further, our results are substantiated by calculated ADXRD pattern of B10 and B2 phases.

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