Strain effects on structural properties of ScN, YN, LaN, and LuN materials

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*RE*N materials (*RE* = Sc, Y, La, and Lu) exhibit the Rock Salt (RS, NaCl) ground state phase. However, the investigations based on the density functional theory (DFT) considered a stability of the hexagonal BN-like structure (hBN) in ScN [1], which differs from the wurtzite (WZ) ground state of group III nitride materials. A tendency toward flattening the WZ bilayer in Sc-bearing nitrides was further confirmed by the experimental studies of structural properties of $Sc_xGa_{1-x}N$ alloys [2].

In this presentation, the structural properties of *RE*N materials under nonhydrostatic strain are investigated with the DFT-based methods. The structural relaxations for possible phases of *RE* nitrides (RS, WZ, ZB, hBN) with various volumes of a unit cell are performed within the local density approximation. The findings presented here support previous predictions that tensile strained *RE*N systems may adopt the hexagonal structures of boron nitride. Further elongation of the in-plane lattice parameters stabilize the WZ phase in *RE*N materials, which is unstable under hydrostatic conditions. A strain-induced occurrence of WZ phase in *RE*N systems may intentionally be employed for fabrication of high quality ternary *RE*N and group III nitride alloys and some heterostructures formed from such materials.

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[1] N. Farrer, L. Bellaiche, *Phys. Rev. B* **66**, 201203(R) (2002).
[2] C. Constantin, H. Al-Brithen, M. B. Haider, D. Ingram, A. R. Smith, *Phys. Rev. B* **70**, 193309 (2004).