Ab-initio study of elastic and structural properties of layered nitride materials

George Simiyu Manyali*

School of Physics and DST/NRF Centre of Excellence in Strong Materials,

University of the Witwatersrand,Johannesburg 2050,South Africa

Abstract

Layered nitride materials in the form of Carbon nitride (C_3N_4) was speculated nearly 22 years ago. It has various structural forms ranging from layered graphitic to superhard structures. Using first principles calculations based on density functional theory, the structural and elastic properties of these phases are determined. Elastic constants, bulk and shear moduli of cubic phases are compared to that of diamond. From the work it is evident that, although the compressibility of some of the superhard phases may be better than diamond, the shear modulus indicates that C_3N_4 is not harder than diamond in contrast to what has been speculated ealier. The graphitic hexagonal, rhombohedral as well orthorhombic phases are soft as indicated by their bulk and shear moduli, which are similar to that of graphite. Other elastic properties such as the Young modulus and Poisson's ratio as well as the Raman and infrared vibrational frequencies are also presented in this dissertation.

KEYWORDS: DFT, C_3N_4, SUPERHARD, GRAPHITIC.