



Effects of collapse magnetic under pressure in iron borides

By Gueddouh, Ahmed

Condition: New. Publisher/Verlag: Noor Publishing | First-principles calculations are performed to study pressure effects on structure, magnetic and mechanical properties of Fe_xB ($x=1, 2, 3$) compounds using density functional theory (DFT) within GGA approximation. The three structures are studied in the pressure range from 0 to 90 GPa, in order to predict the critical transition pressure from magnetic to nonmagnetic states (NM) and a possibility of superconductivity in this state was predicted. Mechanical anisotropies in both cases are discussed by calculating different anisotropic indexes and factors. We have plotted the three dimensional (3D) surfaces and planar contours of bulk and Young moduli of Fe_xB ($x=1, 2, 3$) compounds at several crystallographic planes, ((100), (010) and (001)) to reveal their elastic anisotropy. Furthermore, the relationship between crystal structure and material hardness of Fe_xB is also investigated by calculating hardness of Fe-B and B-B bonds using Mulikan population analysis and semi empirical hardness theory. By the elastic stability criteria, it is predicted that Fe_xB are stable up to the selected pressures. | Format: Paperback | Language/Sprache: english | 56 pp.



READ ONLINE

[5.44 MB]

Reviews

An exceptional pdf and also the typeface applied was intriguing to read through. It is definitely simplified but excitement in the 50 % in the ebook. I discovered this ebook from my dad and i recommended this pdf to find out.

-- Jarod Ward

Complete information for publication enthusiasts. It is really basic but shocks inside the fifty percent of your book. I am just delighted to let you know that this is basically the finest book i have read through in my individual lifestyle and might be he best pdf for actually.

-- Elena Runolfsdottir Sr.