Intuition on Behavioural Pattern of PtN having Zinc Blende Structure under Elevated Pressure and Temperature

Madhu Sarwan, Rakesh Kumar Ahirwar, Rajaram Rawte and Sadhna Singh

corresponding author e-mail – madhusarwan@gmail.com

# Abstract. To explain inter atomic interactions involved at high pressures as well as at high temperatures, a phenomenological model extended three body interaction potential at high pressure and temperature (ETBIPHT), has been developed. Based on this model, the study of high pressure phase transition, elastic properties and thermo-physical properties of PtN in zinc blende structure have been studied. To increase the accuracy of model, three- body interactions, van der Waal interactions and zero point energy effect have been included. A strong dependence of temperature on elastic constants C11, C12, C44 is predicted. This is the first attempt where phase transition pressures, volume compression, elastic constants, bulk modulus, Pugh ratio, Poisson ratio, Debye temperatures and anisotropy of PtN have been computed at different temperatures. Also first time the pressure derivative of elastic constants and third order elastic constants of PtN are analyzed. The obtained results are well suited with the available experimental and theoretical results. Our results show that the ductile nature and anisotropic behavior of PtN is maintained even at high temperatures.

# References:

1. P. F. McMillan, Nature Mater. 1 (2003) 19-25.
2. F. Rivadulla, M. B. Lopez, C. X.Quintella, A. Pineiro, V. Pardo, D .Baldomir, M, A. Lopez-Quintal, J. Rivas, C. A. Ramos, H. Salva, Jian-Shi Zhous and J. B. Goodenough, Nature materials (2009) 947-951.
3. E. Gregoryanz, C, Sanloup, M. Somayazulu, J. Badro, G. Fiquet, H. K. Mao, R. J.. Hemley, Nat. Mater, 3 (2004) 294.
4. M. Rabaha, D.Racheda, R. Khenata, N. Moulaya, A. Zenati, Sol. Stat. Comm. 149 (2009) 941-945.
5. R. Yu and X.F.Zhang, Phys. Rev B 72(2005) 054103.
6. F. Penga, H. Fua, X. Yang, Physica B 403 (2008)2851-2855.
7. Xiao- Wei Sun, Qi- Feng Chen, Ling-Cang Cai, Xiang –Rong Chen, Fu-Qian Jing, Chinese Physics Letters 516 (2011)158-161.
8. A. Gour, F. M. Shareef, S. Singh, Phase Tran. 88 (2015)1-15.
9. P. Bhardwaj, S. Singh, Physica A 441 (2016) 158-172.
10. A. Gour, S. Singh, R. K.Singh, J. Alloys. Comp. 468, 438 (2009).
11. R. K.Singh, Many body interactions in binary ionic solids, Phys. Rep. (Netherlands) 85, 259 (1982).
12. M. P. Tosi, F. G. Fumi, J. Phys. Chem. Solids 23(1962)359; M. P. Tosi, Solid State Phys. 16 (1964)1.
13. Madhu Sarwan , Sadhna Singh, J. Alloys. Comp. **550** 150 (2013).
14. Madhu Sarwan , Sadhna Singh, J. Phys. Chem . Solids, **74** 487 (2013).
15. R.K.Singh, S. Singh, Phys. Stat. Sol.(b) 140 (1987) 407.
16. W Chen, J. Z. Jiang, J. Alloys. Comp. 499(2010) 243-254.
17. L. M. Thomas, J.Shanker, Solid State Comm. 96, 417 (1995).
18. J. Shanker, B. P.Singh, K. Jitendra, Cond. Matt. Phys. 11, 681 (2008).
19. B.B. Karki, R.M. Wentzcovitch, S. De Gironcoli and S.Baroni, Phys. Rev. B 61(2000)8793.
20. MJ. Mehl, RJ. Hemley, LL Boyer. Phys Rev B: Condens Matter. 33 (1986) 8685–8696.
21. T. Yamanaka, K. Kittaka, T. Nagai, J Miner Petrol Sci.97 (2002)144–152.
22. R.K. Singh, S. Singh, Phys. Stat. Sol. (b) 140 (1987) 407.