High temperature behavior of indium nitride

F. Aziz[1], R. Minikayev, P. Piszora, C. Baehtz, H. Teisseyre and W. Paszkowicz[2]
Institute of Physics, Polish Academy of Sciences, Aleja Lotników 32/46, 02-668 Warszawa, Poland.
Email: [1]fizaaz@ifpan.edu.pl , [2]pazk@ifpan.edu.pl

Introduction

Among group III –Nitrides (AlN, GaN, InN), Indium Nitride (InN) gather much attention due to its potential applications in optoelectronic and microelectronic devices. InN crystallizes in a wurtzite-type structure having *P*6$_3$*mc* space group. The properties of InN under specific thermal conditions like variation in stability, thermal expansion coefficient with respect to temperature and resistance to oxidation allowed us to tune the physical properties of these devices. The aim of this work is to present the temperature dependent properties e.g. thermal decomposition of InN, Interaction with air and argon and lattice thermal expansion for a selected temperature range.

Sample description

Material name	Phase	Space group	Lattice parameters a [Å]	Lattice parameters c [Å]	u	B [Å^{-2}]	Zawartość faz składowych, [wag. %]
Material A	InN	P6$_3$mc	3.5393(1)	5.7046(2)	0.377(4)	(In) 0.412(38) (N) 0.21(40)	90.31(1.43)
	In	I4/mmm	3.2545(2)	4.9449(5)	–	0.5	9.41(0.61)
	In$_2$O$_3$	Ia-3	10.131(4)	–	–	0.5	0.28(0.17)
Material B	InN	P6$_3$mc	3.5379(3)	5.7060(6)	0.366(8)	(In) 1.212(96) (N) 1.67(99)	98.51(7.96)
	In$_2$O$_3$	Ia-3	10.13(2)	–	–	0.5	1.49(0.52)

Table 1 Phase components and basic structural parameters of materials A and B at RT.

Thermal stability and decomposition of InN

Material A + Diamond Closed capillary in Ar$_2$

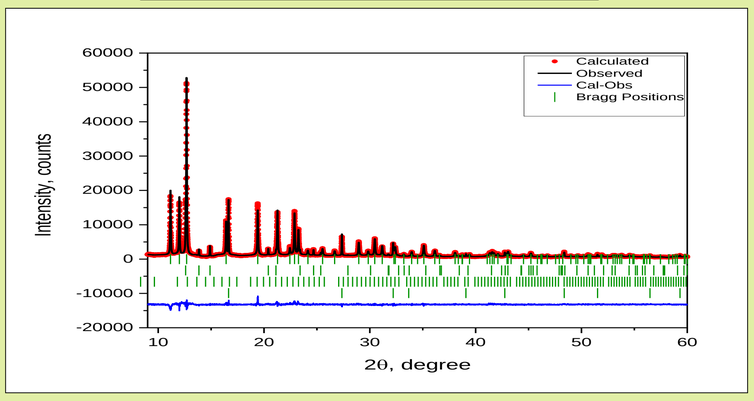

Fig. 1. Refinement results of InN+ Diamond Closed capillary in Ar2 sample at 298K

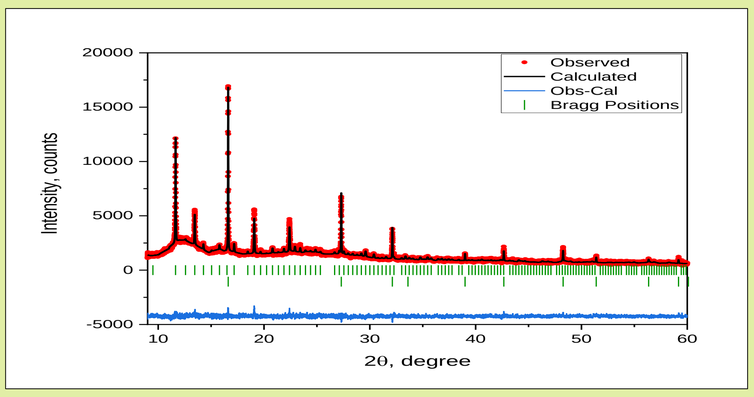

Fig. 2. Refinement results of InN+ Diamond Closed capillary in Ar2 sample at 773K

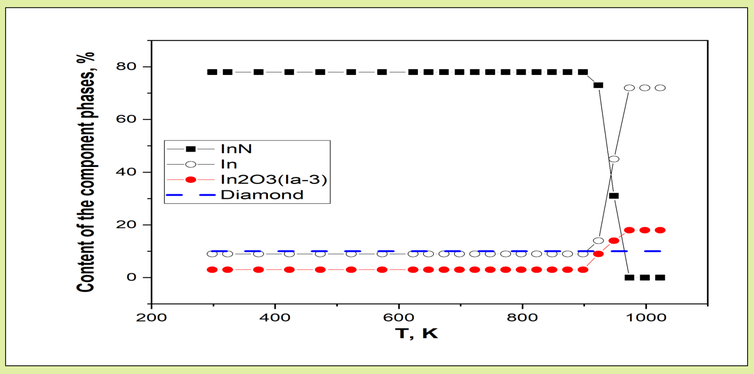

Fig. 3. Phase content as function of temperature

Material B + Diamond Opened capillary

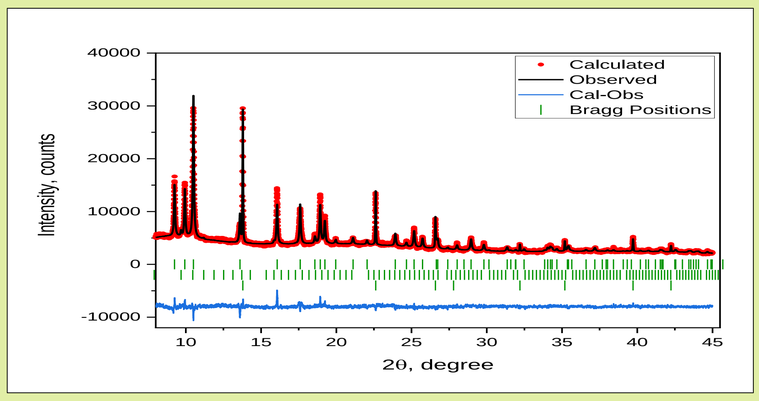

Fig. 4. Refinement result of InN+ Diamond Open capillary sample at 298K

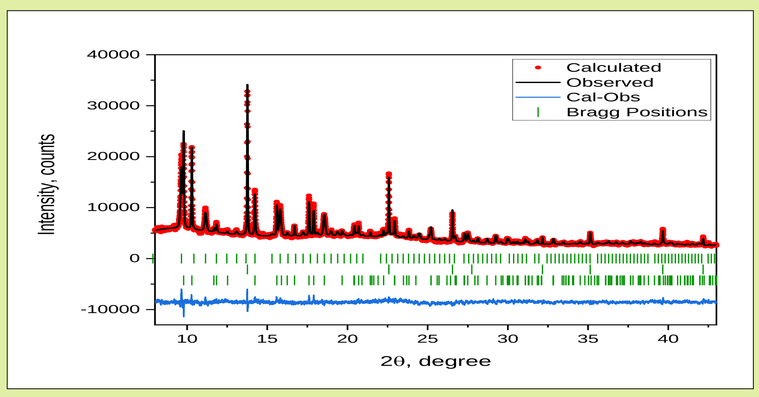

Fig. 5. Refinement result of InN+ Diamond Open capillary sample at 813K

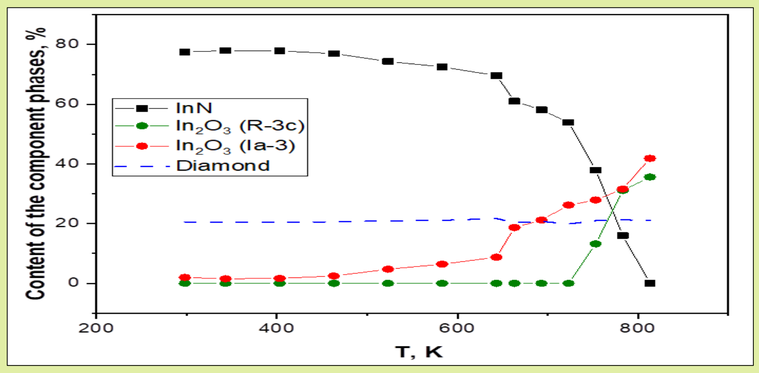

Fig. 6. Phase content as function of temperature

Material A + Diamond Flat sample holder

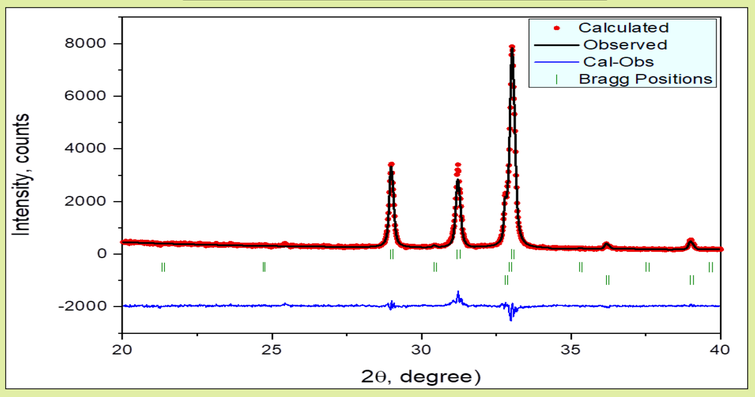

Fig. 7. Refinement results of InN+ Diamond Open sample at 298K

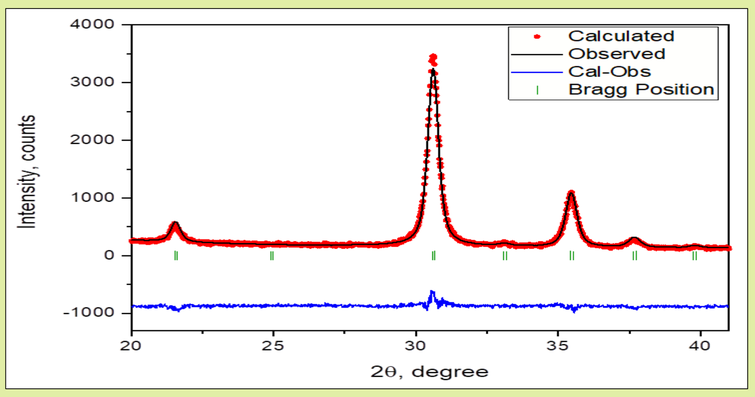

Fig. 8. Refinement result of InN+ Diamond Open sample at 998K

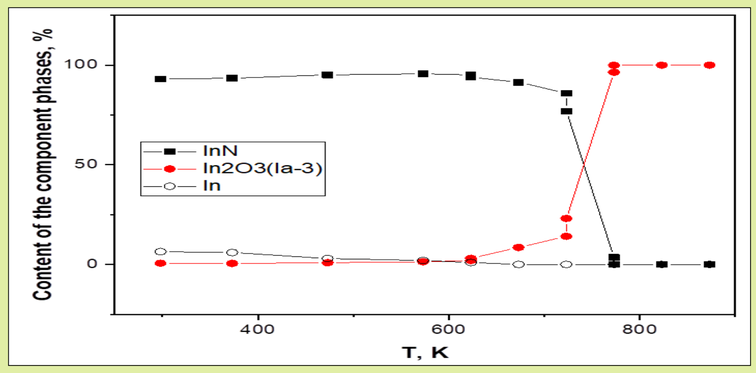

Fig. 9 Phase content as function of temperature

Lattice parameters and thermal expansion coefficients

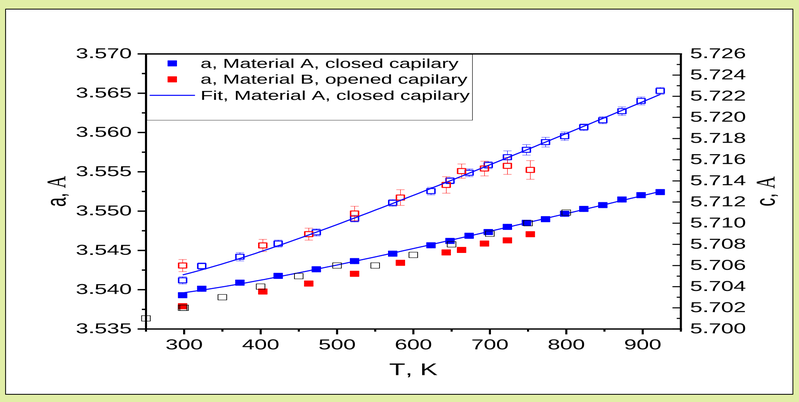

Fig. 10. Comparison of Temperature dependence of lattice parameters of all samples with literature.

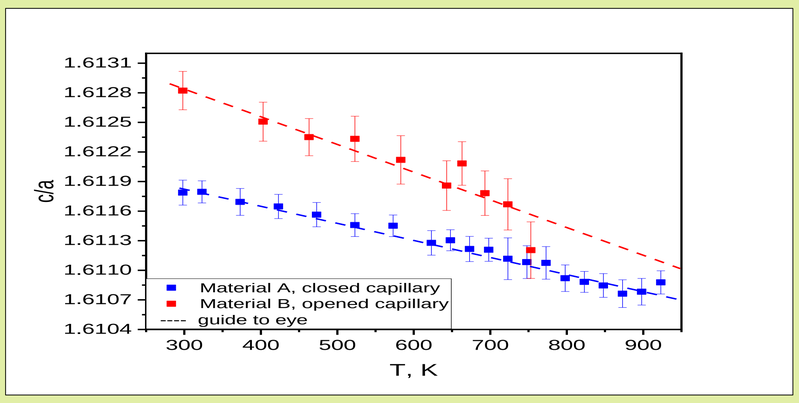

Fig.11. Comparison of Temperature dependence of c/a with literature

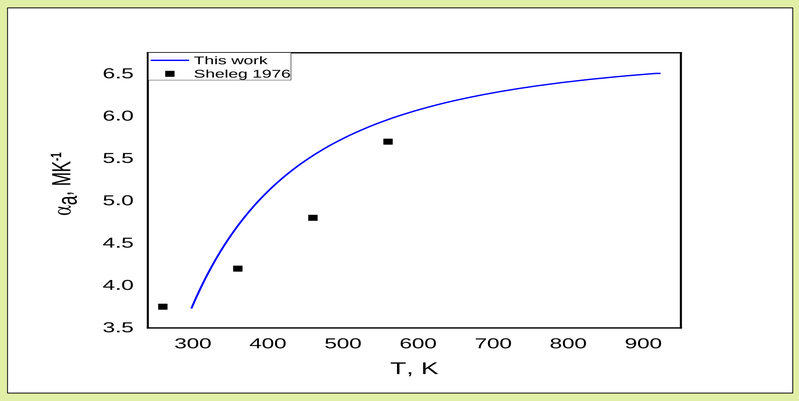

Fig. 12. Comparison of Temperature dependence of α_a of InN with literature

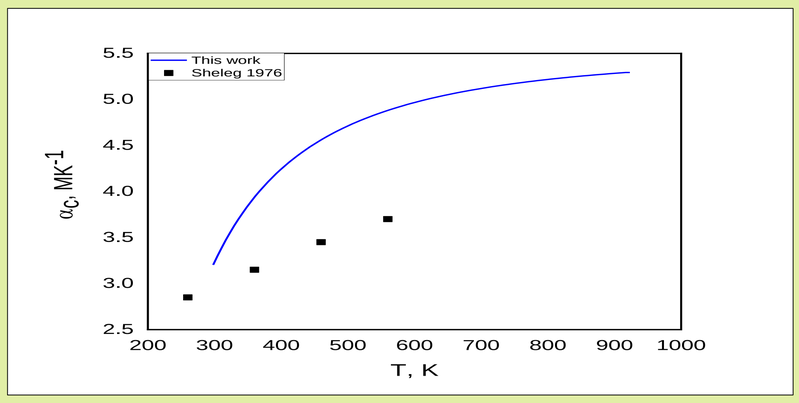

Fig.13. Comparison of Temperature dependence of α_c of InN with literature

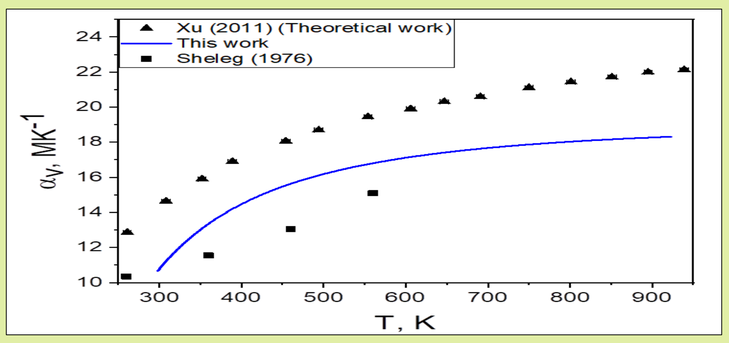

Fig.14. Comparison of Temperature dependence of α_v of InN with literature

Summary

- Within the studied temperature range (298-850 K) InN is observed and products of its decomposition and oxidation.
- Due to heating there is a variation in lattice parameters: a relative change of ~ 0.36% in “a” and ~ 0.29% in “c” direction.
- III-V nitrides exhibit low thermal expansion values. The TEC values of InN are comparable with the experimental data of Sheleg et al. (1976) and theoretical (DFT) ones by Xu et al. (2011).
- The TEC at room temperature (3.7 MK^{-1} for α_a, 3.2 MK^{-1} for α_c, and 10.6 MK^{-1} for α_v) are in agreement with literature data 3.826 MK^{-1} [1], 2.67 MK^{-1} [1], 10.3 MK^{-1} [1] (or theoretical 12.86 MK^{-1} [2]) for α_a, α_c and α_v respectively.
- The decomposition and oxidation of InN depend on the experimental condition applied.
- in argon atmosphere (closed capillary), the decomposition starts at ~900 K accompanied by c-In$_2$O$_3$ formation due to oxidation of liquid In (decomposition product).
- The decomposition of InN in air starts at ~600 K and InN disappears completely at ~800 K.
- In air atmosphere (case of open capillary), the rh-In$_2$O$_3$ phase is present along with c-In$_2$O$_3$ (but only c-In$_2$O$_3$ gorms for open holder sample).

References

[1] Sheleg, A.U., and Sevastenko, V.A. (1976) “Investigation of thermal expansion of indium and gallium nitrides,” Vestsi Akad. Navuk BSSR, No. 3, 126-128
[2] Li Chun. X, Ru-Zhi. W, Xiadong. Y, Hui. Y (2011), "thermal expansion of AlN, GaN, InN : fISRAT PRINCIPLE PHONON CALCULATIONS" J. Appl. Phys. 110,043528
[3] Paszkowicz, W. (1999). “X-ray powder diffraction data for indium nitride,” Powder Diffr. PODIE2 14, 258–260
[4] Paszkowicz, W., Adamczyk, J., Krukowski, S., Leszczynski, M., Porowski, S., Sokolowski, J. A., Michalec, M., and Lasocha, W. (1999). “Lattice parameters, density and thermal expansion of InN microcrystals grown by the reaction of nitrogen plasma with liquid indium,” Philos. Mag. A PMAADG 79, 1145–1154. pma, PMAADG
[5] Rodriguez-Carvajal, J. (2001). “Recent developments of the program FULLPROF,” Newslett. IUCr Commission Powder Diffr. PODIE2 26, 12–19. pdj, PODIE2