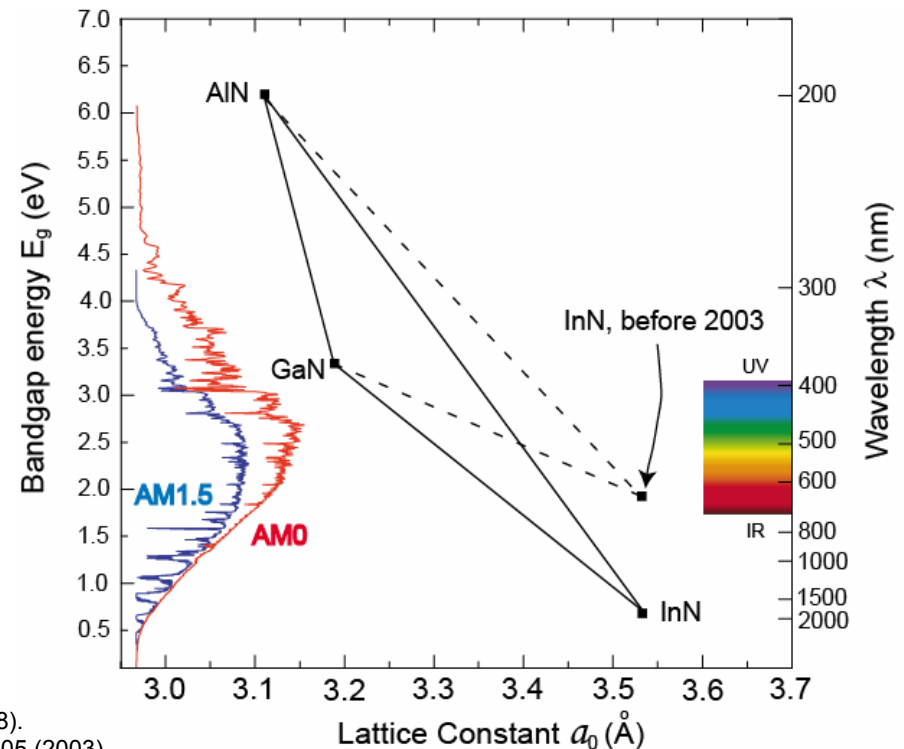


Background

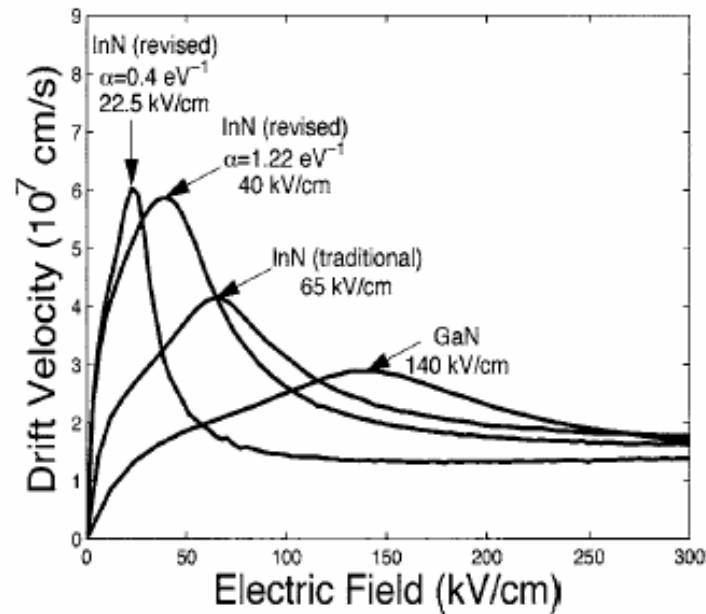
- Among nitrides family (AlN, GaN, InN), InN is still the least explored due to difficulty in obtaining high quality materials
 - Bandgap 1.9 eV \rightarrow 0.65 eV
 - Optical $E_g \sim 0.6$ -0.7 eV
 - Earlier empirical pseudopotential models (EPM) showed 2.0~2.4 eV [1-3]
 - Later using new parameters EPM predicted 0.79 eV⁴
 - Some ab initio studies [5,6] show the $E_g \sim 0.7$ eV and $m^* \sim 0.067m_0$



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2. Y. C. Yeo, T. C. Chong, and M. F. Li, J. Appl. Phys. 83, 1429 (1998).
3. D. Fritsch, H. Schmidt, and M. Grundmann, Phys. Rev. B 67, 235205 (2003).
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Recent works



Valley	Γ_1	A	Γ_2
Number of equivalent valleys	1	1	1
Effective mass	0.11 ^a	1.0 ^b	1.0 ^b
Intervalley separation (eV)	-	2.2	2.6
Energy gap (eV)	1.89 ^c	4.09	4.49
Nonparabolicity (eV^{-1}) ^d	0.419	0.0	0.0

Nonparabolicity coefficient α could be much greater than previous value and m^* should be much lower than before

*Leary etc. *APL* **87**, 222103 (2005)



Recent works (continued)

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Full-zone k·p method of band structure calculation for wurtzite semiconductors

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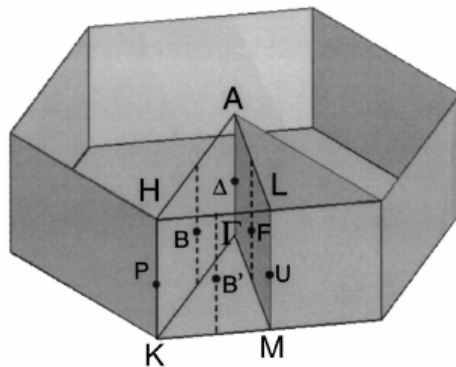
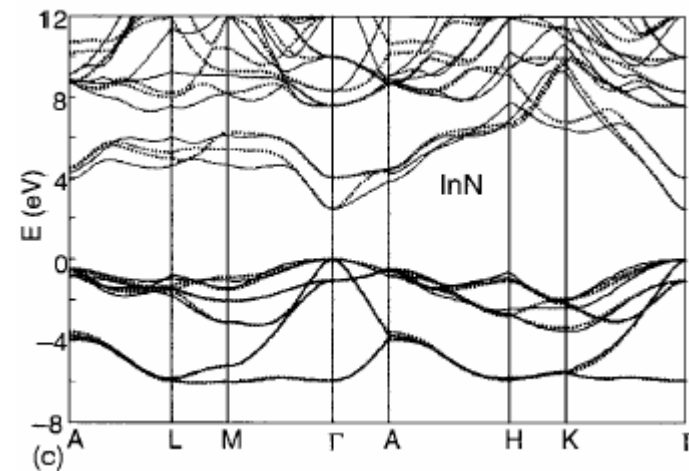


FIG. 1. High-symmetry points of the Brillouin zone in wurtzite. The line from Γ to K is termed T and that from A to H is S ; points along both have the symmetry of the point B . The R line along $A-L$ and the Σ line along $\Gamma-M$ comprise points with the same symmetry as point F ; after Rashba (Ref. 24).

$$H u_{n,k} \equiv \left[H_0 + \frac{\hbar}{m} \mathbf{k} \cdot \mathbf{p} + \frac{\hbar^2 k^2}{2m} \right] u_{n,k} = E_n(\mathbf{k}) u_{n,k},$$



My work

- Nearly free electron band of InN
 - The crystal potential is vanishingly small
 - Plot electron energy band in reduce zone

$$E = \left(\frac{\hbar^2}{2m}\right)k^2 = \left(\frac{\hbar^2}{2m}\right)(k + G)^2$$

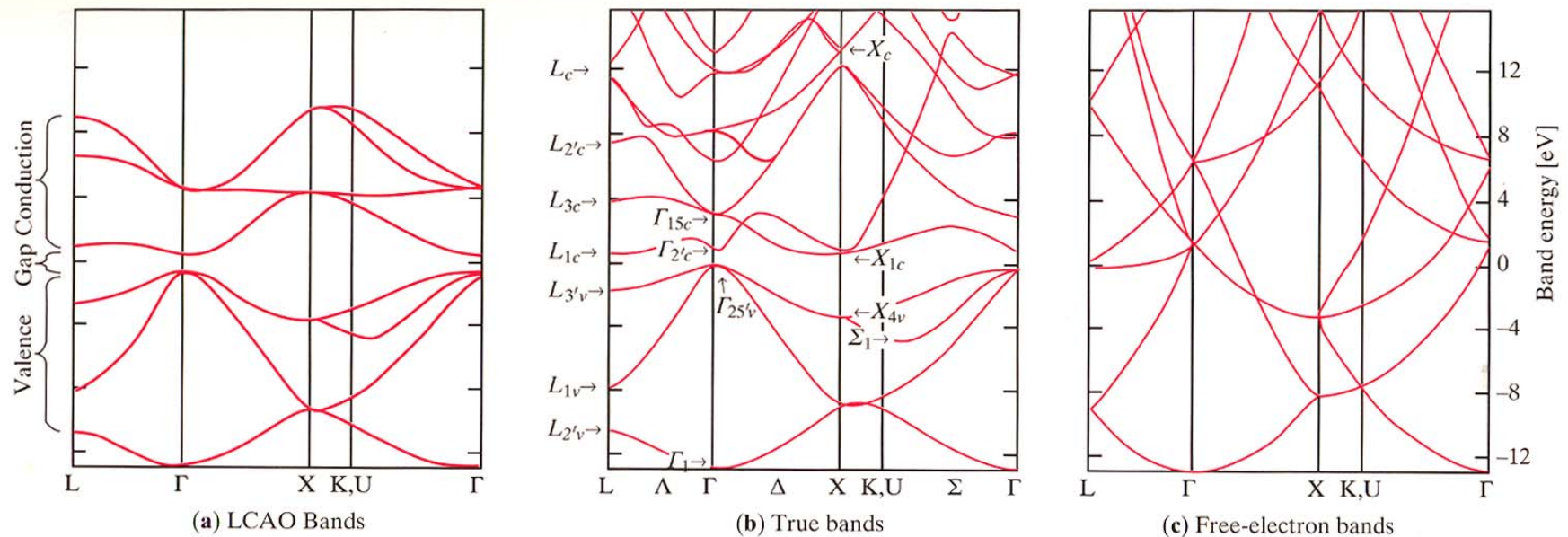


Fig. 2.25. A comparison between the band structure of Ge calculated by (a) the tight-binding method, (b) the empirical pseudopotential method, and (c) the nearly free electron model [Ref. 2.24, p. 79]



My work

- Method to simulate the band structure of InN

Tight binding method, or Linear combination of Atomic orbits (LCAO)	Describe entire valence and conduction band	Empirical technique. Use atomic function a basic set of bloch function
Pseudopotential method	Describe entire valence and conduction band	Divide wave function to a mooth part (pseudo-wave) and an osillatory part
k·p (perturbative techniques)	More accurate describe near band edge	Begin with known band structure, using the perturbation theory to predict band structure away from high symmetry points

