Aluminium Nitride:an overview of the physical properties

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Abstract

Aluminium Nitride exhibits many useful optical,electrical, mechanical, and thermal properties. Here some of them are reviewed and discussed particularly its crystal structure, electronic band structure, optical properties and pressure dependence Raman scattering spectra.

Introduction Semiconductor nitrides have been viewed as a promising materials for their potential use in opto-electronics devices. Aluminium nitride has some outstanding physical properties that have attracted much interest. AlN is tetrahedrally coordinated III-V compound having large band gap 6.3ev. Its hardness, high thermal conductivity, resistance to high temperature attracts a lot for opto- devices. Here we review some of physical properties of AlN to get the insight knowledge of material.

Crystal Structure Heinrich otto, in 1924, first reported AlN to have wurtzite crystal structure with lattice constants range from 3.110 to $3.113A^0$ for a, and from 4.978 to $4.982A^o$ for c. The c/a ratio thus varies between 1.000 and 1.602. The deviation of c/a ratio is probably from lattice stability and ionicity. The wurtzite unit cell is as shown in fig. 1[1]. It contains four unit atoms (2 cation and 2 anions). The basis vectors are $(0,0,0)$, $(\frac{a}{\sqrt{3}},0,\frac{c}{2})$, $(\frac{a}{\sqrt{3}},0,\frac{c}{8})$,$(0,0,\frac{5c}{8})$ where a is the length of hexagonal side, c is the repeat distance along the z-direction. The anions are defined as $\vec{t}_1$,$\vec{t}_2$and cation at $\vec{t}_3$,and$\vec{t}_4$. The reciprocal lattice is also hexagonal. Its direct lattice vectors are defined as $\vec{a} = (\frac{\sqrt{3}}{2}a, -\frac{a}{2}, 0)$,$\vec{b} = (0, a, 0)$,$\vec{c} = (0,0,c)$and reciprocal lattice vectors are $\vec{b}_a = (\frac{4\pi}{\sqrt{3}a}, 0, 0)$, $\vec{b}_b = (\frac{2\pi}{\sqrt{3}a}, \frac{2\pi}{a}, 0)$,$\vec{b}_c = (0, 0, \frac{2\pi}{c})$ The symmetry points of the Brillouin zone are $\Gamma = (0,0,0)$, $K = \frac{2\pi}{a}(\frac{1}{\sqrt{3}}, \frac{1}{3}, 0)$, $M = \frac{2\pi}{a}(\frac{1}{\sqrt{3}}, 0, 0)$, $A = \frac{2\pi}{c}(0,0,\frac{1}{2})$, $H = \frac{2\pi}{a}(\frac{1}{\sqrt{3}}, \frac{1}{3}, \frac{a}{2c})$, $L = \frac{2\pi}{a}(\frac{1}{\sqrt{3}}, 0, \frac{a}{2c})$

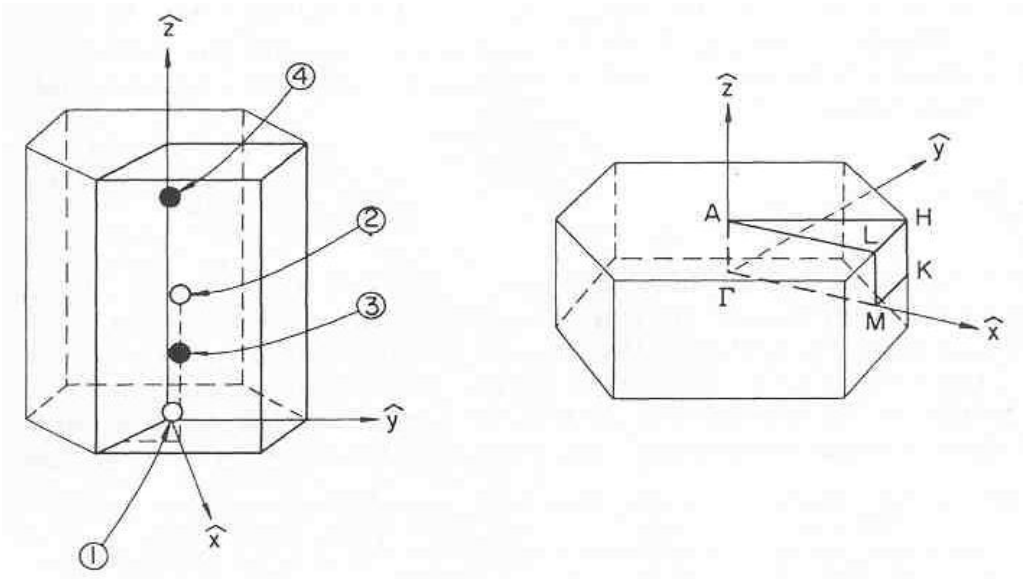

Figure 1: *a) Hexagonal close-packed strucure 1, 2 anions & 3, 4 cations b)Reciprocal lattice with symmetry points of Brillouin zone.*

Electronic Energy band Structure The number of theoretical calculations of the electronic energy band structure exist but the energy band structure of AlN was calculated with a orthogonalized linear combinational of atomic orbitals (OLCAO)method with local density approximation (LDA). The resulting band diagram and total density of states (DOS)as shown in Fig 2[2]. Due to hexagonal symmetry of AlN, the top of valence band atΓ point is split into two levels. The order of the levels at the top of the valence band, Γ1 and Γ6, is inverted in AlN. The difference between these levels is 0.2ev. The lowest direct gap in Γ6 $\rightarrow$ Γ1 ($E \perp C$) and Γ1-Γ1 ($E \parallel c$) theoretically are as 6.06 and 5.31ev.[3]

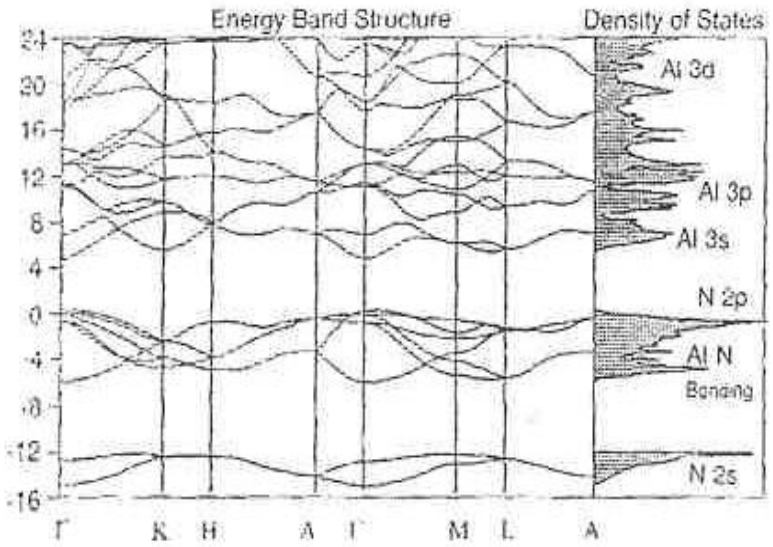

Figure 2: *Energy band structure of AlN.*

Optical Properties:

Yamashita et.al.and Michailin et.al. tried to measure reflectance spectra of AlN in the range from 5.8 to 40ev. But a wide range of wavelength is indespensable for understanding the electronic structure .Loughin et.al.and Guo et. al. had studied optical properties in the interband transition region of AlN from measurements of the fundamental reflectivity spectra. The complex dielectric function $\epsilon(E) = \epsilon_1(E) + i\epsilon_2(E)$,for AlN with $E \perp c$ obtained from the Krammer's Kroning analysis of the reflectance data as shown in fig.3.[4]. The imaginary part of dielectric $\epsilon_2(E)$spectrum in the energy range from 6 to 120ev obtained from KK analysis. According to GUO et.al, the transitions revealed at four critical points peaking at 7.6 8.9,13.0.and 14.8ev and are interpreted as an interband transition from the valence band to conduction band .

From the calculated $\epsilon_2$spectra, the peak position for each transition listed was assigned as in table according to loughin. Assignment of features in the electronic structure of AlN

Energy(ev)	assignment	interband(ev)	predominant orbital character
6.3	$A_{1,1}$ 4.5		
8.0	$\Gamma'_{0.1}$	7.2	
8.7	$A_{1,1}$	9.9	$N2p \rightarrow Al3s$
9.2	$A_{1,1}$	11.5	
10.4	$H'_{2,1}$	12.5	
10.2	$A_{0,2}$	11.1	
14.0	$\Gamma_{1,2}$	13.2	$Al = N \rightarrow Al3p$
25.7	$H_{2,2}$	19	
33.9	$\Gamma_{0,3}$	27-37	$N2p \rightarrow Al3d$

Here the optical response of AlN were resolved into three sets of balanced critical points. Each of the critical points referenced to the band structure of AlN.The first set ranges from the band gap at 6.3-10.4ev, the point at which the transition between the upper valence band and lower conduction band are exhausted . Based on analysis of orbital decomposition of density of states, this set attributes to transition between N2p to Al3s states where there

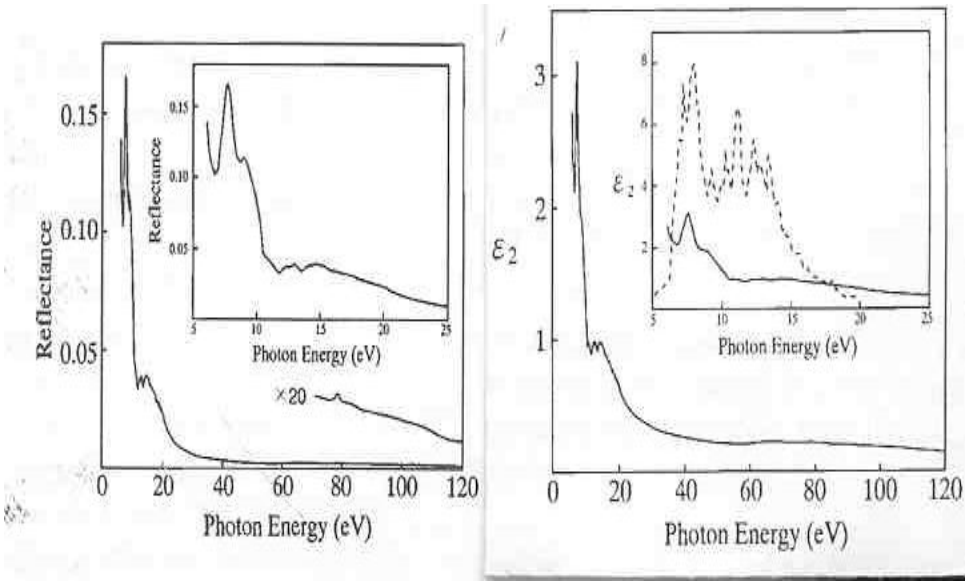

Figure 3: *Spectral dependence of reflectance and imaginary dielectrics function for AlN.*

is a sharp minimum in the optical response at 8.7 ev.above 10.2 ev. A divergent peak at 14.ev is seen and a broad interband maximum centered at 12.57ev. This is identified with transition between Al=N bonding states and Al3p antibonding states. At higher energies ,it is difficult to resolve into discrete form but has some 33.8 ev from N2s to Al3d transition.

Raman scattering

AlN crystallizes in the hexagonal wurtzite structure with four atoms in the unit cell .There are six raman active phonons two E_2, $E_1(TO)$, $E_1(LO)$, A_1 (TO) and A_1 (LO). Single crystals of AlN were grown by high-pressure ,high temperature synthesis with nitrogen as a pressure transmitting medium and got the Raman scattering spectra of AlN at ambient pressure as shown in fig [4] .

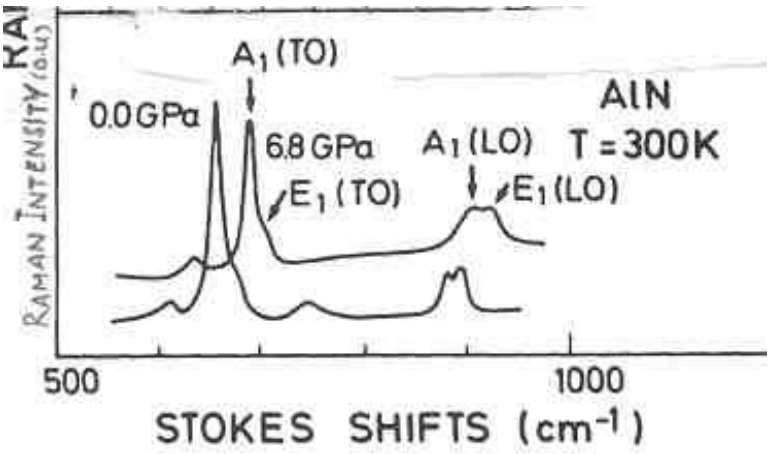

Figure 4: *First order Raman spectra of AlN.*

The results for E_2 mode is 241 cm^{-1}, $A_1(TO) = 607cm^{-1}$, $E_2^2 = 660$ cm^{-1} and $E_1(LO) = 924$ cm^{-1}. The Raman peaks show a linear dependence with pressure in the measurement range and the solid line is due to the least square fits using the equation:

$$\omega_{LO}(E_1) = (895 \pm 2) + (4.0 \pm 0.2)p \quad (1)$$
$$\omega_{TO}(E_1) = (671.6 \pm 0.8) + (4.84 \pm 0.09)p \quad (2)$$
$$\omega_{LO}(A_1) = (882 \pm 2) + (3.8 \pm 0.2)p \quad (3)$$
$$\omega_{TO}(A_1) = (659.3 \pm 0.6) + (4.97 \pm 0.06)p \quad (4)$$

with ω_{TO} cm^{-1} and ω_{LO} cm^{-1} and p in GPa.Since AlN is anisotropy, the pressure dependence equation are found by taking an average frequencies as

$$\omega_{LO} = (893 \pm 2) + (3.9 \pm 0.2)p \quad (5)$$
$$\omega_{TO} = (667.5 \pm 0.7) + (4.88 \pm 0.08)p \quad (6)$$

The mode Gruneisen parameters can be determined by the equation

$$\gamma_i = -\frac{\delta \ln \omega_i}{\delta \ln V} = \frac{B_o}{\omega_i}\frac{d\omega_i}{dp} \quad (7)$$

where the ω_i s are given phonon modes[LO (Γ) and TO (Γ)]and Bulk modulus $B_o = 218$ Gpa. The calculated value of mode Gruneisen parameters of the zone center phonons are $\gamma_{TO} = 1.6$ and $\gamma_{LO} = 1.0$.

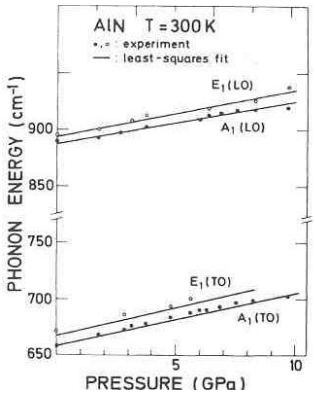

Figure 5: *Dependence of LO(Γ) and TO(Γ) phonon frequency.*

Other properties The phonon structure(lattice vibration spectra) of AlN has been subject of numerous investigations. Since the hexagonal wurtizite structure has four atoms per unit cell, there are 12 branches, 3 acoustic and 9 optical modes at k$\approx$ 0. The three acoustic branches are essentially zero at k $\approx$ 0. The zone center(k=0) transverse optical(TO) and longitudinal optical(LO)phonon energies are determined from its infrared reflectivity measurements shown in fig [6] using dispersion theory. The zone center values of LO and TO effectively form the limits of restrahlen band. Since as the angle between propagation vector and c axis of a uniaxial crystal decreased from 90^0, the width of band decreases for the extraordinary ray.The longer wavelength moves to shorter wavelength side when strongly convergent light is used. Therefore it suggests that λ (LO) $\sim$ 10.8 μ and $\lambda(TO) > 13.5\mu$ the zone photon energies are LO $\sim 115mev$ and TO < 92 mev . Similarly, the other measured parameters ϵ_∞ and ϵ_0 are 4.84 and 9.14 respectively. The temeperature dependent

band gap is given as $E_g = E_g(o) - 1.799 \times 10^{-3}\frac{T^2}{T+1462}(ev)$ where T is the temperature in degrees K(0¡T¡300)[Guo and yoshida(1994)] and the value is 6.13ev. as shown in fig[6]. **Applications**AlN is very promising materials for high power/temperature electronic de-

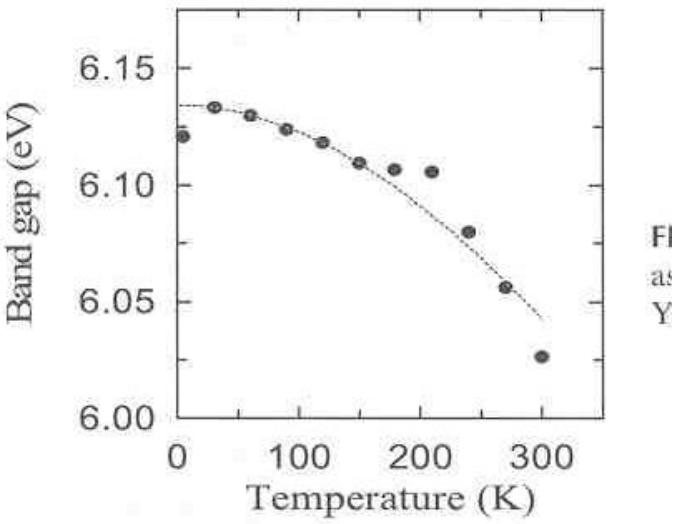

Figure 6: *optical band gap of AlN as function of temperature.*

vices. This material has 6.2ev band gaps so it can be used for UV region. Specifically, It is suitable for surface acoustic wave devices ,UV detectors ,laser diodes for digital data read -write application and much more.

Some basic parameters at 300k	
crystal structure	wurtzite
No. of atoms in cm^{-3}	9.58 $\times 10^{22}$
Density ($gmcm^{-3}$)	3.23
Debye temperature(k)	1150
Electrical properties :mobility of electrons	300
holes	14
Refractive index	2.15
Thermal conductivity ($Wcm^{-10}C^{-1}$	2.85
Specific heat	0.6

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