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Studies on Electrical and Thermal Transport of InN based on Two Layer Model

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Abstract

InN, a material of huge potential in device applications, is grown on sapphire substrate. But due to the high lattice mismatch between the sapphire and InN, the large number of dislocations develops near the interface between the two materials. However, the density of threading dislocation falls sharply in the bulk layer. The charge density has also similar variation. Therefore, the bulk InN crystal may be treated to be consisting of two layers, one the interfacial layer where the density of dislocations is very high and the layer on the interfacial layer, called bulk layer which has much lower density of dislocation and is considered to be negligible. We have calculated the mobility of InN and Seebeck Coefficient of InN based on the two layer model. We find that the theoretical values of mobility based on two layer model matches quite well with the experimental data. In our model, in the interfacial layer, the dislocation scattering and ionized impurity scattering mechanisms are considered to be the dominating scattering mechanisms while for the bulk layer, the acoustic phonon scattering via deformation potential and piezo electric coupling, ionized impurity scattering and optical phonon scattering mechanisms are considered. The theoretical values of the thermoelectric power of InN, calculated on the basis of two layer model are found to be in good agreement with experimental data.

Keywords: *Dislocations, two layer model, thermoelectric power, mobility*

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INTRODUCTION

The nitrides of the group III metals like Al, Ga and In have been at the centre of huge interest of scientists during last few years [1–3] due to their direct band gap varying from 0.7 eV for InN to 3.5eV for GaN and 6 eV of AlN which facilitates its usage in optoelectronic devices.

The electrical and optical properties of InN have been widely studied for its potential applications in high speed electronic devices and optical devices in infrared region [4–6]. InN has small effective mass and high electron mobility.

The growth of good quality crystalline InN is a matter of great difficulty due to its low dissociation temperature, the high equilibrium vapor pressure of nitrogen molecule and lack of suitable substrate [7].

InN has been grown on sapphire substrate by metal organic chemical vapor deposition (MOCVD) [8] and molecular beam epitaxial method [9]. But due to high lattice mismatch (25%), the large number of dislocations appears in the crystal [10]. To obtain a better quality crystal, InN has been grown on GaN or AlN substrate. C. J. Lu et al. [11] studied InN grown on GaN and AlN substrate and they observed large number of threading dislocations (TD) near the interface. A rapid drop of TD density along the growth direction has also been noticed.

The electron transport of InN is of great research as it is observed by [12] that mobility of the electrons varies significantly with the increase in the width of the crystal. The

variation in electron density is also observed along the growth direction of the crystal.

Hai Lu et al. [10] studied the effect of an AlN buffer layer on the epitaxial growth of InN by molecular beam epitaxy (MBE). They found that by using AlN as a buffer, the electrical property improved a lot in InN. They also observed that Hall mobility increases with the increase in the thickness of the sample. This can be explained by the fact that TD density reduces along the growth line of the crystal.

V. Lebedev [12] studied the effects of dislocations on electrical and electron transport properties of InN film grown by plasma induced molecular beam epitaxial method (PIMBE) on AlN/sapphire pseudo substrate. They have shown that the threading dislocation varies with the epilayer thickness affecting both carrier concentration and electron mobility. They also found that TD is very high near the interface and rapidly decreases along the growth direction. The carrier concentration also decreases rapidly along the growth direction. They developed a relationship between the TD density and carrier density with the thickness of the crystal in the exponential decay form and fitted the variation of mobility with the increase in the thickness taking an exponential growth formula.

The effects of charged dislocations on electron transport of InN have been studied by Miller et al. [13]. GaN, another nitride material has been extensively studied [14–17]. The GaN materials are grown by MBE method or the metal organic chemical vapor deposition (MOCVD) on the sapphire or SiC substrate. Since SiC is very costly, the most affordable substrate is sapphire. But there is also large lattice mismatch between the sapphire and GaN (14%) [18] with 34% [19] mismatch in the thermal expansion coefficient. Due to this large lattice mismatch, large numbers of dislocations develop along the direction of growth of the crystal [20] and cause the scattering of electrons. As a result, the mobility of the electrons gets adversely affected by the presence of dislocations in GaN. The effect of dislocations on dc mobility has been widely studied. Weiman and Eastman [15] have demonstrated that dislocations reduce the dc mobility in GaN. Ng et al. [14] have also shown that dislocations reduce the electron mobility in GaN.
In case of GaN, it has also been observed that the TD density is very high near the interface which reduces very fast along the growth direction of the crystal [21].

Look and Molnar developed the two layer model [19, 20] considering n-GaN as consisting of two layers, where one layer interfacing the substrate with large dislocations and the other layer with negligible dislocations. With the two layer model, he could explain the mobility of n-GaN which matches quite well with the experimental data. Shrestha et al. [23] calculated the thermal conductivity and the Seebeck coefficient of n-GaN applying the two layer model.

There is a striking similarity on the TD distribution pattern in GaN and InN crystals. In both the cases, the density of TDs reduces rapidly along the growth direction of the crystals. So the two layer model proposed by DC Look for GaN can also be applied to study the electrical and electronic behavior of InN. We find here that the theoretical values of mobility and thermoelectric power of InN calculated based on two layer model fit quite well with the experimental data [13].

THEORETICAL FORMULATIONS

The schematic presentation of the two layer model is shown in the Figure 1.

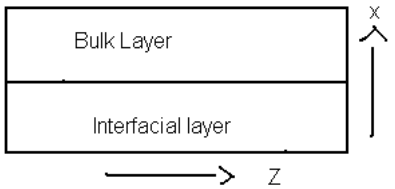

Fig. 1: *Two Layer Model of InN.*

The threading dislocations are along x-direction whereas the longitudinal magnetic and the electric fields are applied along z-direction (longitudinal configuration). The edge dislocations introduce acceptor centers along the dislocation lines which capture electrons from the conduction band in an n-type semiconductor [23]. The dislocation lines become negatively charged and a space charge is formed around it. The resulting potential

field scatters the electrons and reduces the mobility of the electrons [24]. According to the two layer model, the combined current is the sum of the total currents through the layers, hence

$$I_{com} = I_{int} + I_{bulk} \quad (1)$$

where, I_{int} ,I_{bulk} are currents in the interfacial layer, bulk layers and and I_{com} represents the combined current of the crystal as a whole. The combined conductivity σ_{com} is obtained as

$$\sigma_{com} = \frac{(a\sigma_1 + \sigma_2)}{(a+1)} \quad (2)$$

where, σ_1 and σ_2 are the conductivities of the bulk layer and the interfacial layer and a is the ratio of the width of the bulk layer and the interfacial layer.

If we denote S_{com} as the combined Seebeck coefficient, then the combined Seebeck coefficient is given by [23]

$$S_{com} = \frac{(S_1\sigma_1 a + S_2\sigma_2)}{(\sigma_1 a + \sigma_2)} \quad (3)$$

where, S_1 and S_2 are the thermoelectric power of the layer 1 and layer 2 [25] and

$$S = \frac{\xi}{\nabla_z T} = \frac{1}{eT}\left[\frac{\langle E\tau\rangle}{\langle\tau\rangle} - E_F\right] \quad (4)$$

Here τ represents total relaxation time. For the interfacial layer, we have considered dislocation scattering and the ionized impurity scattering and as for the bulk layer, we have considered ionized impurity, polar optical, piezo electric and acoustic potential scattering mechanisms. We have calculated the combined mobility and thermoelectric thermo electric power of InN crystal and found that the calculated values of mobility and thermo electric power match quite well with experimental values. The parameters used for InN are indicated in the Table 1.

Table 1: *Values of Parameters of InN.*

Item	Unit	InN
Density	Kgm^{-3}	6810
Longitudinal sound velocity	ms^{-1}	5200
Static dielectric constant		10.3
High frequency Dielectric constant		6.7
Effective mass		$0.06m_o$
Piezo Electric constant ε_{14}	Cm^{-2}	0.375
Lattice constant, a	Angstr	3.54
Lattice constant, c	Angstr	5.70

RESULTS AND DISCUSSIONS

We have considered here the samples as referred in Miller et al. [13]. Here we have considered the two layers to find the variation of mobility with the width of the InN crystal. For the interfacial layer, we have considered only the dislocation scattering and ionized impurity scattering while for the bulk layer we have considered the acoustic deformation scattering, piezo electric scattering, and polar optical scattering and ionized impurity scattering.

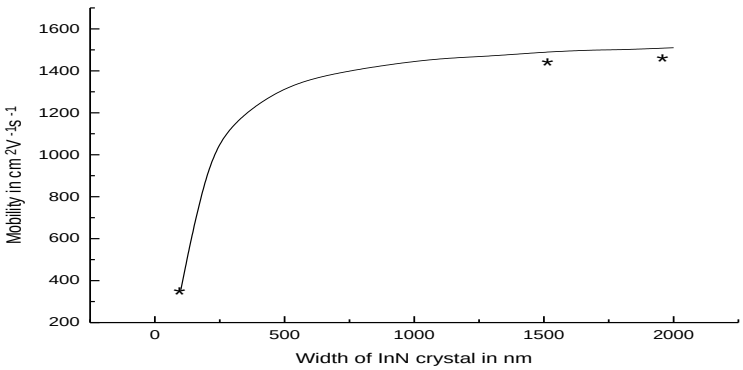

Fig. 2: *The Variation of Mobility with the Thickness of the InN Crystal.*

In Figure 2, the variation of mobility with the width of InN crystal based on two layer model has been shown. Here the width of InN crystal consists of the interfacial layer of 100 nm and balance is the varying width of the bulk layer. Lebedev [12] developed the exponential variation formula, according to which the maximum mobility works out to be 4400 $cm^2V^{-2}s^{-1}$. But experimentally, the maximum mobility is found to be 1520 $cm^2V^{-2}s^{-1}$ at 300 K. From the Figure 2, we find that the theoretical values of mobility are very close to the experimental data and the mobility attains maximum value near 1500 $cm^2V^{-2}s^{-1}$. Here the temperature is considered to be 300 K. The density dislocation of the interfacial layer is considered to be $4x10^{14}$ cm^{-2}. The electron density of the interfacial layer and bulk layer are $6x10^{18}cm^{-3}$ and $4x10^{17}cm^{-3}$, respectively.

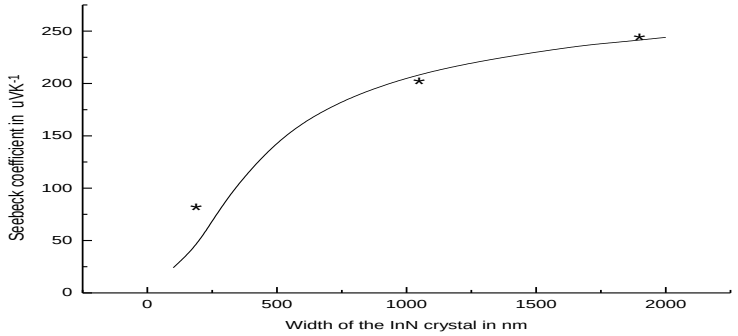

Fig. 3: *The Variation of Absolute Values of Seebeck Coefficient with the Width of the Crystal at 300 K.*

In Figure 3 the variation of the theoretical absolute values of the thermoelectric power with the width of InN crystal calculated on the basis of two layer model with the width of the InN crystal has been shown. The value of Seebeck coefficient also increases with width of the InN crystal and finally approaches a steady value 250 μVK^{-1}. The theoretical values match quite well with the experimental values [13].

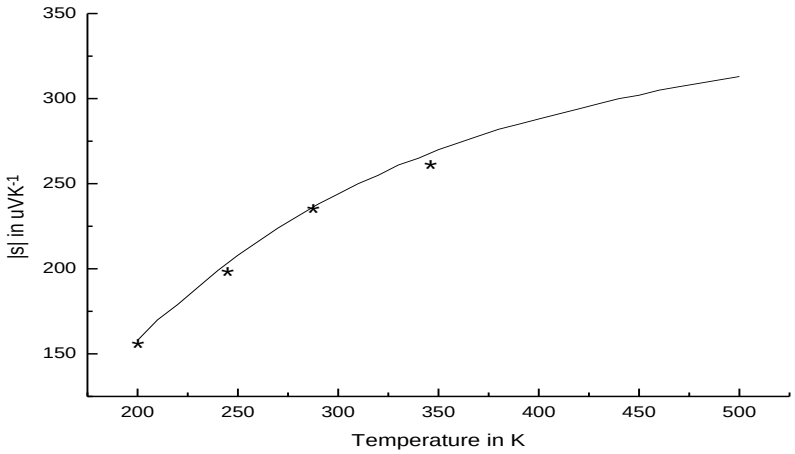

Fig. 4: *Variation of Absolute Values of Thermoelectric Power with Temperature.*

In Figure 4, the variation of the theoretical values of thermoelectric power of InN calculated on the basis of two layer model with temperature has been shown. The theoretical values have been compared with experimental data [13] and are found to agree quite well near. Here we have taken the ratio between width of the bulk layer and interfacial layer as 19:1.

CONCLUSIONS

InN grown on sapphire or other substrate develops large numbers of dislocations at the interface. The dislocations affect the electrical properties of InN significantly. The theoretical values of mobility and thermo electric power of InN calculated based on two layer model are in good agreement with the experimental data. Dislocations in InN crystal have adverse effect on the mobility and thermoelectric power as well.

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