

Determination of Al mole fraction in AlGaN by X-ray diffraction and optical transmittance

The Al mole fraction is a critical parameter which determines the emission wavelength in AlGaN light-emitting diodes and the 2-dimensional electron-gas concentration in AlGaN/GaN heterostructures. The bandgap energy versus lattice constant of III-V nitride materials is shown in Fig. 1. The bowing energy of $\text{Al}_x\text{Ga}_{1-x}\text{N}$ is 1.0 eV. The lattice constant is a linear function of Al composition according to Vegard's Law. Determining the bandgap energy allows one to determine the composition using the curve shown in Fig. 1. It is found that the accuracy of determining the Al mole fraction depends on how accurately one can determine the band-gap energy. An error of 50 meV results in ~5% Al mole fraction error.

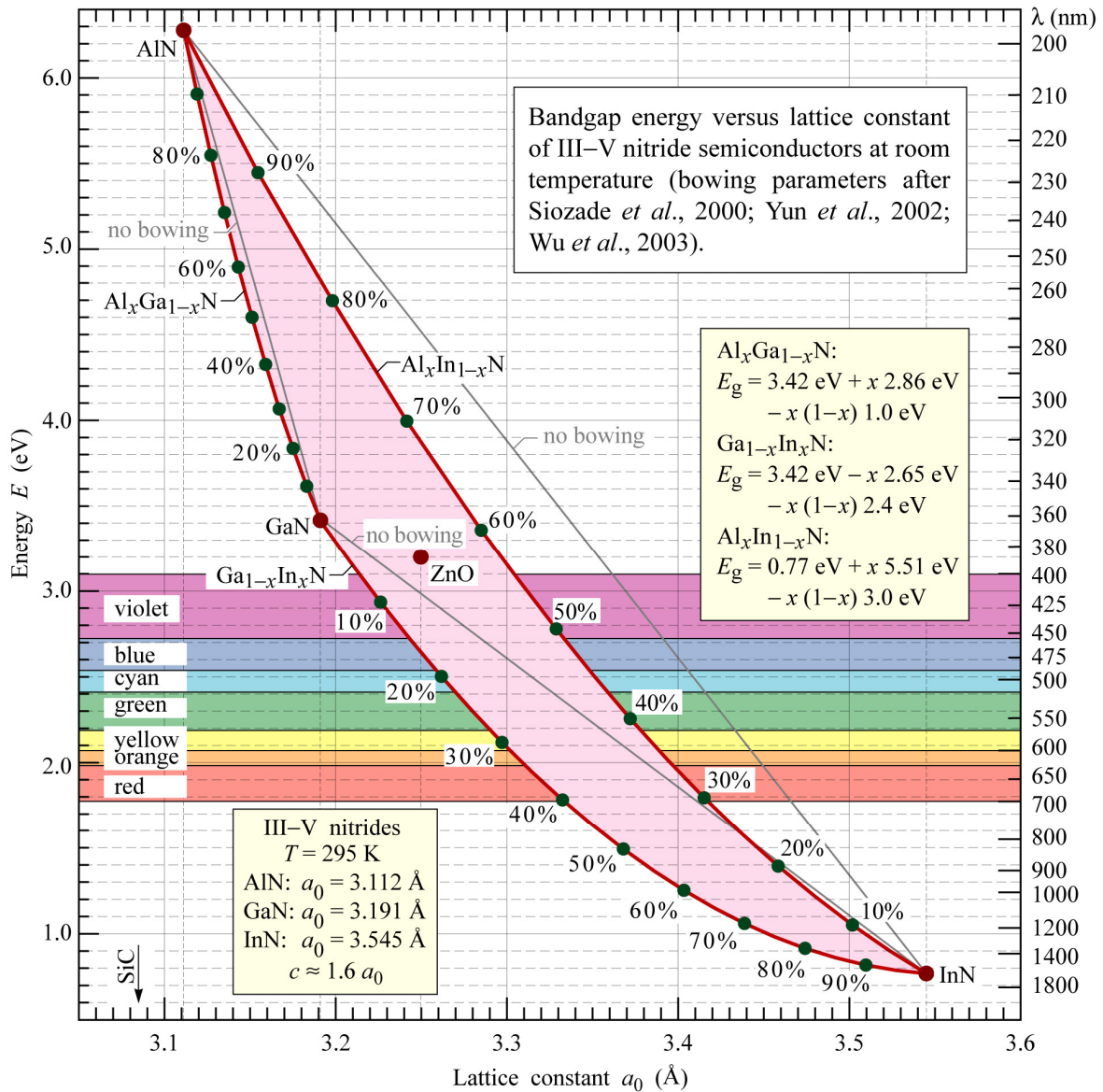


Fig. 1: Nitride band-gap energy versus lattice constant.

Several approaches are widely used to determine Al mole fraction of AlGa_xN epitaxial layers. The first approach to be discussed here uses X-ray diffraction. The ω -2 θ scan can tell the Al mole fraction based on the peak position shift of the AlGa_xN layer from reference peak position. Generally the AlN or GaN peak position is used as reference peak and the Al mole fraction can be easily evaluated from Vegard's law. For instance, for Al_xGa_{1-x}N, the difference of angle θ of AlN and GaN is $\Delta\theta_0$, the angle shift of Al_xGa_{1-x}N from GaN is $\Delta\theta$, then the Al mole fraction can be given as:

$$x = \frac{\Delta\theta}{\Delta\theta_0} \quad (1)$$

But there are several limitations for this method. Firstly, a simple structure is needed in order to determine the Al mole fraction of one layer. Secondly, the resolution is affected by the full width at half maximum. Thirdly, if the ternary is pseudomorphically strained, such as the MQW layer and superlattice layer, it is very difficult to evaluate the alloy composition from the ω -2 θ scan directly. The elastic deformation of lattice due to the strain needs to be considered.

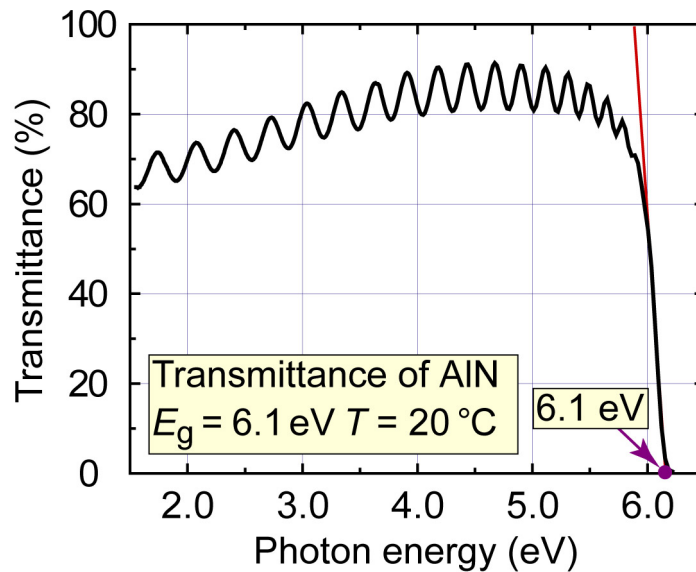


Fig. 2: The optical transmittance curve of an AlN layer grown on sapphire.

The second approach to be discussed here is optical transmission measurements. A transmission spectrum of an AlN layer is shown in Fig. 2. Due to strong band-edge absorption, a sharp cut-off is observed at around 6.1 eV. Hence, the band-gap energy can be evaluated from

the cut-off wavelength. Since the band-gap energy is related to Al mole fraction by using curve in Fig. 1, the Al mole fraction can be determined. The band-gap energy is evaluated by following the tangent method: A tangent line is drawn through the cut-off edge, and extended to intersect the x-axis (i.e. energy axis). The intersection-point value is attributed to the band-gap energy. The Al mole fraction measured by transmission curve is compared with that obtained by XRD, as shown in Fig. 3.

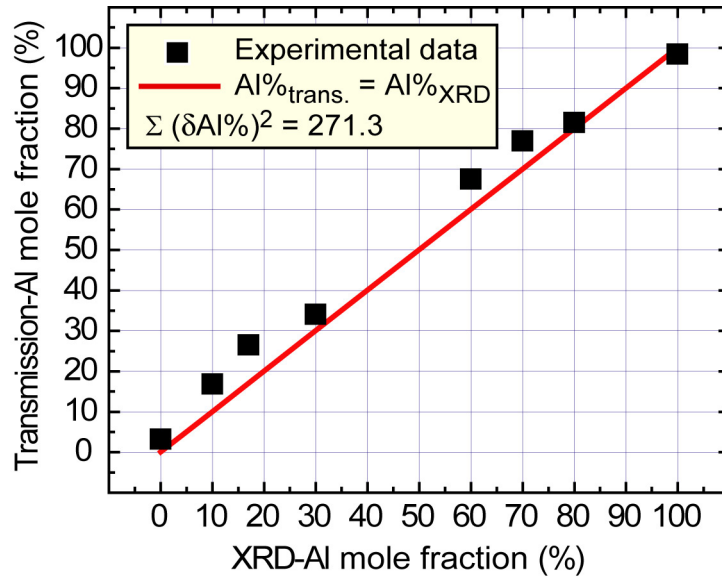


Fig.3: Al mole fraction determination by using transmittance and XRD methods.

The solid line in Fig. 3 stands for same Al mole fraction obtained from transmittance method with XRD method. From Fig. 3, it is found out easily that the Al mole fraction determination by using the transmittance method is consistent with XRD results and thus can be used as an alternative method.

The disadvantage of this method is that only the Al mole fraction of the layer with the smallest band-gap can be evaluated. The accuracy of this method depends on the sharpness of the cut-off edge in the optical transmittance spectrum.