One of the problems introduced by heterostructures is the resistance caused by the heterointerface. It has been shown that heterostructure band discontinuities can be eliminated by grading of the semiconductor chemical composition (e.g., Al composition in $Al_xGa_{1-x}N$ layers) in the vicinity of the heterostructure. Prior to the growth of the grading layer, one needs to design the growth parameters, such as the growth rate and the growth time, the desired thickness and the target Al composition.

General calculation:

The growth rate of an $Al_xGa_{1-x}N$ layer is given by

$$\begin{aligned} g_{\text{AlGaN}} &= g_{\text{AlN}} + g_{\text{GaN}} = g^*_{\text{AlN}}\,\Phi_{\text{V,TMAl}} + g^*_{\text{GaN}}\,\Phi_{\text{V,TMGa}} \\ &= g^*_{\text{AlN}}\,\Phi_{\text{V,TMAl}} + g^*_{\text{GaN}}\,(\Phi_{\text{V,total}} - \Phi_{\text{V,TMAl}}) \end{aligned}, \tag{1}$$

where $\Phi_{\text{V, TMAl}}$ is the volume flow rate of TMAl, $\Phi_{\text{V, total}}$ is the total volume flow rate, and g^* is the growth rate at unit volume flow rate of the MO precursor.

The Al molar fraction is obtained by

$$x = \frac{g_{\text{AlN}}}{g_{\text{AlN}} + g_{\text{GaN}}} = \frac{g^*_{\text{AlN}}\,\Phi_{\text{V,TMAl}}}{g^*_{\text{AlN}}\,\Phi_{\text{V,TMAl}} + g^*_{\text{GaN}}\,(\Phi_{\text{V,total}} - \Phi_{\text{V,TMAl}})}. \tag{2}$$

The volume flow rate of TMAl can be expressed in terms of the Al molar fraction x by solving Eq. (2) for $\Phi_{\text{V, TMAl}}$

$$\Phi_{\text{V,TMAl}} = \frac{g^*_{\text{GaN}}\,\Phi_{\text{V,total}}}{\dfrac{g^*_{\text{AlN}}}{x} + g^*_{\text{GaN}} - g^*_{\text{AlN}}}. \tag{3}$$

The growth rate g_{AlGaN} of the $Al_xGa_{1-x}N$ layer can be obtained in terms of the Al molar fraction x by inserting Eq. (3) into Eq. (1)

$$g_{\text{AlGaN}} = \frac{g^*_{\text{GaN}}\,g^*_{\text{AlN}}\,\Phi_{\text{V,total}}}{g^*_{\text{AlN}} + (g^*_{\text{GaN}} - g^*_{\text{AlN}})\,x}. \tag{4}$$

The thickness of the $Al_xGa_{1-x}N$ layer is

$$D = \int g_{\text{AlGaN}}\,\mathrm{d}t\,. \tag{5}$$

If a linearly graded layer is desired, the Al molar fraction x will change linearly with the thickness D, which means

$$\frac{\mathrm{d}x}{\mathrm{d}D} = \frac{\Delta x}{\Delta D} = \frac{x_2 - x_1}{D_0} = C\,. \tag{6}$$

Here x_1 and x_2 are the Al molar fraction at the two ends of the $Al_xGa_{1-x}N$ grading layer, D_0 is the thickness of the grading layer, and C is a constant.

Eq. (6) can be rewritten as

$$\frac{\mathrm{d}x}{\mathrm{d}t}\frac{\mathrm{d}t}{\mathrm{d}D} = C \;\Rightarrow\; \frac{\mathrm{d}x}{\mathrm{d}t}\left(\frac{\mathrm{d}D}{\mathrm{d}t}\right)^{-1} = C \;\Rightarrow\; \frac{\mathrm{d}x}{\mathrm{d}t} g_{\mathrm{AlGaN}}^{-1} = C \;. \tag{7}$$

Elimination of g_{AlGaN} from Eq. (4) and Eq. (7) yields

$$\frac{\mathrm{d}x}{\mathrm{d}t}\;\frac{g^*_{\mathrm{AlN}} + \left(g^*_{\mathrm{GaN}} - g^*_{\mathrm{AlN}}\right)x}{g^*_{\mathrm{GaN}}g^*_{\mathrm{AlN}}\,\Phi_{\mathrm{V,total}}} = C \;. \tag{8}$$

By using variable separation and integration, the Al molar fraction x can be obtained as a function of growth time t

$$x = \frac{-g^*_{\mathrm{AlN}} + \sqrt{g^{*\,2}_{\mathrm{AlN}} + 2\left(C\,t\,g^*_{\mathrm{GaN}}g^*_{\mathrm{AlN}}\,\Phi_{\mathrm{V,total}} + C_0\right)\left(g^*_{\mathrm{GaN}} - g^*_{\mathrm{AlN}}\right)}}{g^*_{\mathrm{GaN}} - g^*_{\mathrm{AlN}}} \;, \tag{9}$$

where C_0 is a constant expressed as

$$C_0 = g^*_{\mathrm{AlN}}\,x_1 + \frac{g^*_{\mathrm{GaN}} - g^*_{\mathrm{AlN}}}{2}\,x_1^2 \;. \tag{10}$$

Example of designing a linearly graded $Al_xGa_{1-x}N$ layer

Suppose the total MO volume flow rate $\Phi_{\mathrm{V,\,total}}$ is kept at 24 sccm, the growth rate of GaN at 24 sccm TMGa is 3.3 μm/h, and the growth rate of AlN at 24 sccm TMAl is 0.5 μm/h. If a 50 nm thick $Al_xGa_{1-x}N$ grading layer is needed, whose Al molar fraction x linearly changes from 0 to 1 with the thickness (linearly graded from GaN to AlN), what is the growth time of this grading layer?

Since the growth rate of GaN and AlN at 24 sccm MO volume flow rate is known, the value of g^*_{GaN} and g^*_{AlN} can be calculated. The initial Al molar fraction x_1 is 0, the final Al molar fraction x_2 is 1.0, and the thickness D_0 is 50 nm. Thus the constants C and C_0 are known from Eq. (6) and (10). By using Eq. (9), the relation between Al molar fraction x and the growth time t is obtained, which is shown in Fig. 1. The growth time for the grading layer varying from GaN to AlN is 3.46 minutes. (All the calculations are done by Mathcad program.)

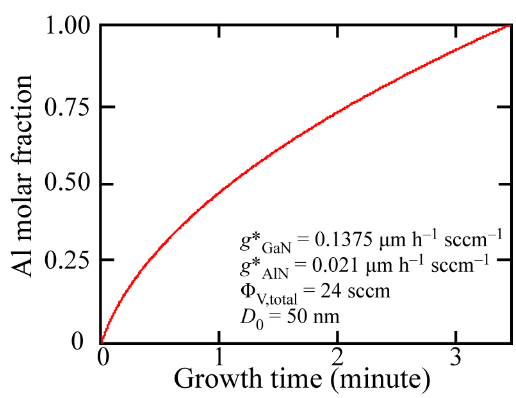

Fig. 1: Al molar fraction versus growth time

Fig. 2 and Fig. 3 show the TMAl volume flow rate and the growth rate versus growth time, respectively. The TMAl volume flow rate increases dramatically at the beginning of the grading layer growth, then gradually saturates. That is because the growth rate decreases rapidly at the beginning of the growth. In order to keep the Al molar fraction x changing linearly with the thickness D, the TMAl volume flow rate has to increase rapidly so as to compensate the rapidly decreasing growth rate. Fig. 2 also shows a strong bowing for the TMAl volume flow rate versus time. However, in practice, the TMAl volume flow rate is controlled by a Mass Flow Controller (MFC) which can only change the flow linearly with time. In order to obtain a curve as shown in Fig. 2, it is necessary to divide the curve into several linear operating regions. Thus the MFC can linearly control the TMAl volume flow rate within each linear operating region.

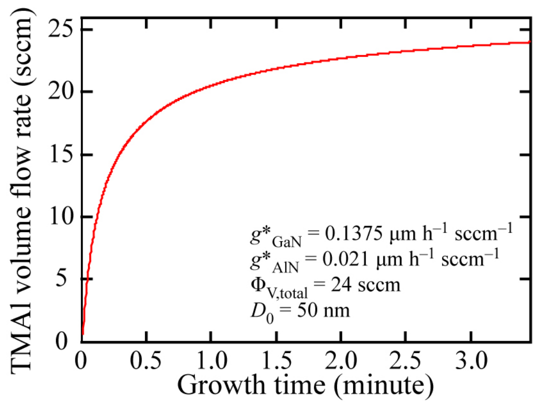

Fig. 2: TMAl volume flow rate versus growth time

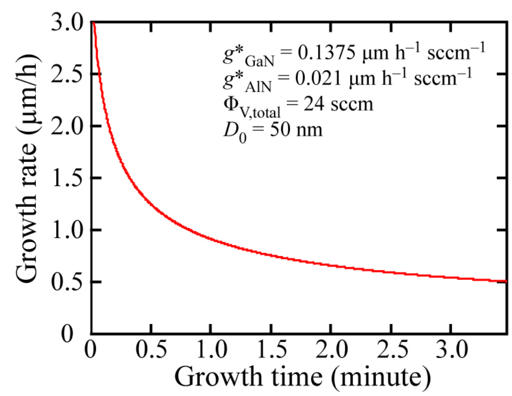

Fig. 3: Growth rate versus growth time

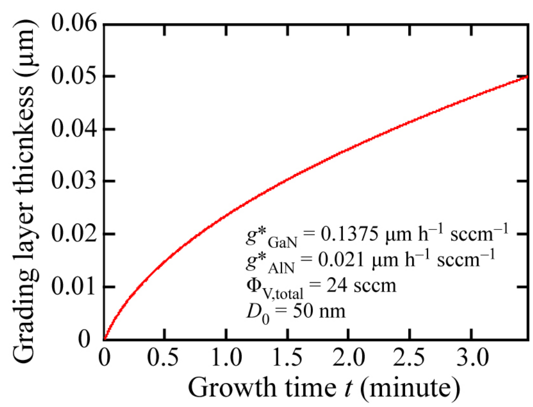

Fig 4: Grading layer thickness versus growth time

Fig. 4 is the dependence of the grading layer thickness versus growth time. The thickness of the grading layer increases sub-linearly rather than linearly with the growth time. The reason is that the growth rate decreases with the growth time, as is shown in Fig. 3.

Fig. 5 shows the relation between the Al molar fraction and the grading layer thickness. The initial Al molar fraction is 0 (GaN). When the thickness is 50 nm, the Al molar fraction is 1.0 (AlN). The Al molar fraction increases linearly with the grading layer thickness, which is consistent with the requirement that the $Al_xGa_{1-x}N$ layer linearly graded from GaN to AlN within 50 nm.

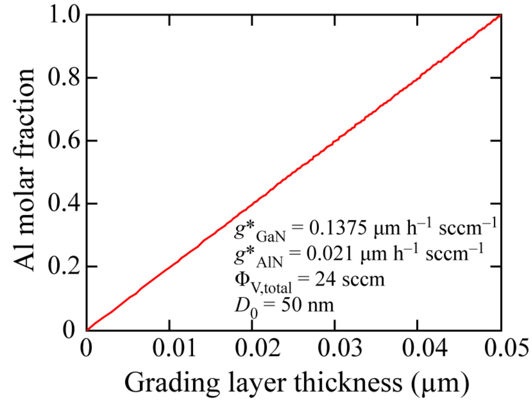

Fig 5: Al molar fraction versus grading layer thickness

Finally, the relation between the growth rate and the TMAl volume flow rate is shown in Fig. 6. As is expected from Eq. (1), the growth rate should change linearly with the TMAl volume flow rate. The experimental result fits this linear relation very well.

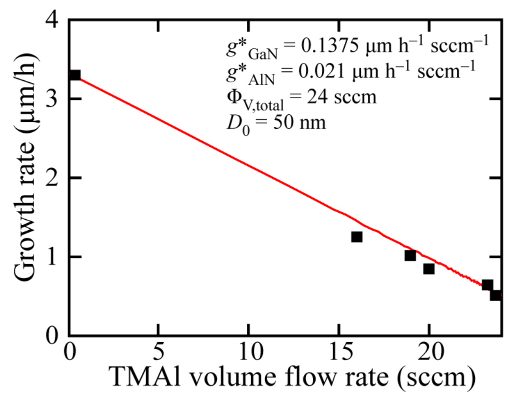

Fig 6: Growth rate versus TMAl volume flow rate