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Growth Rate Calculations for Epitaxially Grown Thin Films

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Artificially fabricated semiconductor structures were introduced more than 20 years ago with some spectacular results in both basic physics discoveries and in commercial applications (Maclean 2001). Quantum well lasers, for example, are now found in every compact disc (CD) and digital video disc (DVD) player. The quantum well laser is a prime example of what has been termed a first-generation quantum device that is a device that reproduces the function of its respective conventional bulk device but with higher performance specifications (e.g., more stability over a broader temperature range). Second-generation quantum devices (still in the research stage) are multi-functional; a single structure can accomplish a task that would normally require as many as 10 conventional devices. A factor of 10 reduction in the number of components naturally leads to a significant increase in speed as well as a reduction in power consumption.

These multi-functional devices will require the production of complex structures with very short period superlattices, non-linear graded composition profiles, gross alterations in the lattice constant, etc. The key to accomplishing this goal is to have precise, atomic-scale control of the growth process. Unlike Si-based devices, which are primarily fabricated using implantation techniques, the III-V semiconductors require atomic layer-by-layer growth of the heterostructures (Current 1992). The remarkable advances that have been made over the past decade in a variety of advanced structures involving III-V compound semiconductors has come about primarily due to the advent of, and refinements in, the primary fabrication technique known as molecular beam epitaxy (MBE).

Semiconductor device fabrication via MBE growth occurs in an ultra-high vacuum (UHV) environment ($\sim 10^{-11}$ Torr) where a molecular beam of group III and group V molecules impinges on a single crystalline substrate. In MBE the mean free path for the impinging flux is much greater than the distance from source to sample, consequently the growth kinetics are determined by the relative sticking coefficients of the two species, by the diffusion rate of the two species once they are in contact with the substrate surface, and by the dissociation rate of the molecules.

Although MBE produces the highest quality samples, it has one major drawback; it is a very expensive technique to implement on a production scale. A basic production MBE system can cost upwards of ten million dollars. In addition to the equipment cost, both the consumables associated with running the machine as well as the required manpower create large overhead costs for the manufacturer. Consequently, it is of great interest to make the MBE production process as efficient as possible. One major source of production downtime comes while calibrating the most important aspect of the production, namely, the growth rate. It can take several days for a manufacturer to calibrate the growth rate from a source material in order to get the appropriate atomic ratios. Naturally, a better understanding of the physics governing the growth rate of these materials could enhance the efficiency of the MBE manufacturing process. What is needed is a model that can accurately predict the fraction of atoms that evaporate from the source material and arrive at the sample substrate to contribute to the growth of the structure.

Accurately predicting the growth rate is a difficult problem to solve because it is related to both static (such as the temperature of the material and the residual vacuum chamber pressure) and dynamic variables (such as the source-sample distance and solid angle) (Herman et al. 1989). However, with recent advances in both dynamic computational techniques and microcomputers, solution of this problem is possible. Our approach is to develop a model that describes the growth rate as it relates to the source temperature and geometry (i.e. solid angle and source-sample distance). Ideally, this model will have sub-monolayer accuracy and be computationally efficient.

The growth rate model will describe the molecular beam flux evaporating from the metallic Gallium (Ga) source and impinging on the surface of a GaAs substrate. This is directly related to Ga's vapor pressure. A material's vapor pressure, P, determines the number of atoms that evaporate from a sample's surface as a function of temperature (Tsao 1993). The complete temperature dependence of vapor pressure requires a formula with four adjustable constants. Many formulas have been suggested, but the one found

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to be the most accurate by Nesmeyanov (Nesmeyanov 1963) is

$$\log P = D - \frac{A}{T} + CT + B\log T \,. \qquad (1)$$

In this equation, T is the temperature (in Kelvin) and A, B, C, and D are fitting parameters.

In order to develop an accurate model of the growth rate, it is necessary to determine which terms in the vapor pressure equation are the most dominate. In Figure 1 each individual term is plotted with its appropriate fitting constants for Ga. The log P is also plotted on the graph. From examining Figure 1 we see that the vapor pressure curve is dominated by the A/T term from equation 1. The next dominant term is determined to be the B log T term. In order to

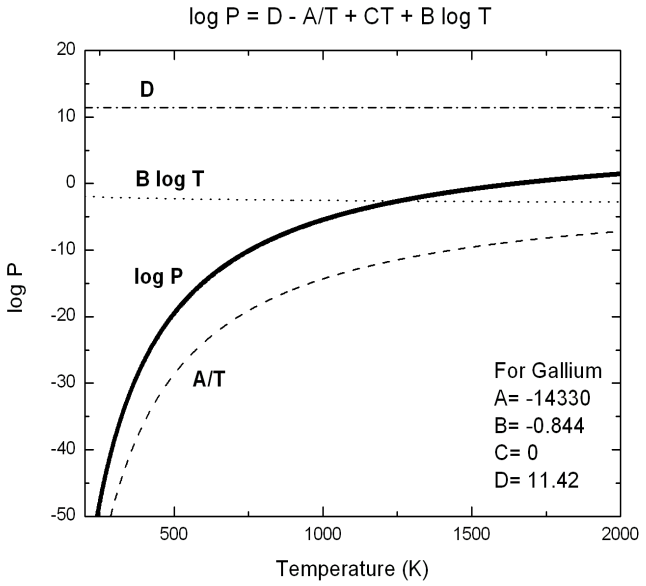

Figure 1. Graph illustrating the dependence of each term in the vapor pressure equation using the appropriate constants for Gallium as a function of absolute temperature. From this the dominating term (A/T) is ascertained.

simultaneously maximize the accuracy of our model but minimized computation time it is necessary to keep only the two most dominant terms from equation (1). Equation (1) then becomes

$$\log P = -\frac{A}{T} + B\log T \,. \qquad (2)$$

From equation (2) the vapor pressure equation is found to be

$$P = 10^{-\frac{A}{T}} T^{B} \,. \qquad (3)$$

Equation (3) assumes a uniform spherical distribution of evaporating material. This assumption will not apply in MBE since it takes advantage of highly directional Knudsen effusion cells (or K-cells) (Herman et al. 1989). To correct for this a new constant, GR_0, is introduced that scales the modified vapor pressure for the geometry of the K-cell and the source-sample distance. Equation (3) becomes the geometry corrected vapor pressure, $P_{GC,}$

$$P_{GC} = GR_0 \times P = GR_0 10^{\frac{-A}{T}} T^{B} \,. \qquad (4)$$

It is important to note that GR_0 will be constant only for a single growth since the source-sample distance and the solid angle between the source and sample will change for each successive production run requiring a new value for GR_0 to be calculated. This can be accomplished by measuring the temperature for a selected growth rate and using this information to solve for GR_0. In equation (4) the constant $A = E_a/k_B$ where E_a is the activation energy and k_B is Boltzmann's constant with a value of 8.617×10^{-5} eV/K. The activation energy is a parameter that describes the amount of energy required to completely remove an atom from the surface of the bulk material, for Gallium metal E_a = -1.457 eV. The fitting parameter B is related to the latent heat of the material and is found to have a value of -9.4101 (Nesmeyanov 1963). The growth rate equation is then expressed as

$$GR(T) = GR_0\, 10^{\frac{-E_a}{k_B T}} T^{B} \,. \qquad (5)$$

Figure 2 shows the derived growth rate equation has excellent agreement with experimentally determined growth rates (LaBella 2000).

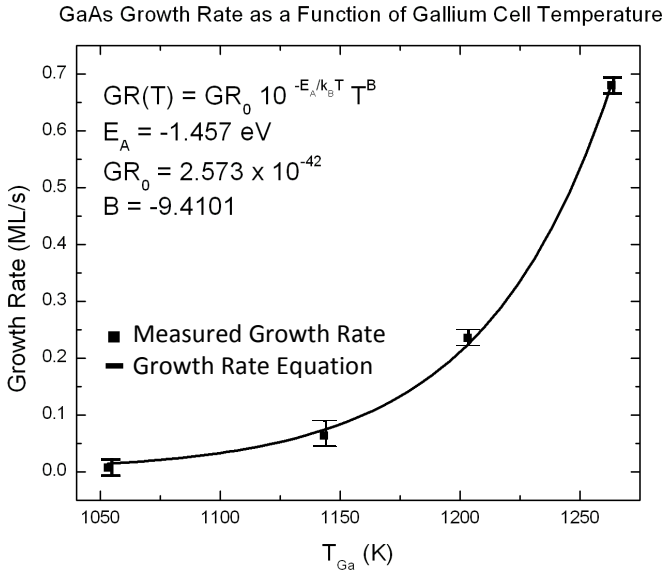

Figure 2. Graph illustrating the GaAs growth rate as a function of Gallium cell temperature. The line represents the developed formula which is graphed with actual growth rate data.

To further enhance the productivity of MBE systems it is necessary to provide immediate growth rate feedback to the user. Using equation (5), it was possible to develop a program to calculate the appropriate K-cell temperature for a desired growth rate. To do this the user inputs values for the current cell temperature, current growth rate, and the desired growth rate. Using this information the computer first calculates GR_0. Next, the calculation of the K-cell temperature is performed unfortunately due to the transcendental nature of equation (5) it is impossible to solve for the temperature algebraically, instead a numerical technique must be utilized that finds the root of the equation given the input parameters (Press et al. 2002). This root corresponds to the K-cell temperature that yields the desired growth rate.

In conclusion we have been successful at developing a model that predicts the growth rate as a function of temperature. This model agrees well with experimentally measured growth rates. Additionally, we have also developed software that can greatly reduce the time needed for growth rate calibrations.

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