Detailed Models of III-V MOVPE in Commercial Reactors

R.A. Talalaev, A.V. Lobanova, Yu.A. Shpolyanskiy, I.Yu. Evstratov
Soft-Impact Ltd.
P.O. Box 33, St.Petersburg, 194156, Russia
Yu.N. Makarov
STR Inc.
1610 Swinton Lane, Richmond VA, 23233, USA

Global modeling of Metal Organic Vapor Phase Epitaxy is considered now as a powerful tool for understanding and optimization of deposition process as well as for design of a reactor. Despite the significant progress achieved in MOVPE modeling over the last decade, most of the models still remain "reactor-dependent" because of the necessity to fit unknown model parameters to a particular set of experimental data.

In this paper we report on the results of detailed simulation of MOVPE in industrial single and multiwafer reactors of various configurations. The simulations cover almost the whole range of III-V materials used for fabrication of semiconductor devices, i.e. binary (GaAs and InP), ternary (AlGaAs, InGaAs and InGaP) and quaternary (InGaAlP) layers. Reactor configurations considered include horizontal tube reactors, vertical high-speed rotating disk reactors and planetary reactors.

Complicated reactor design requires the accurate description of gas flow, heat transfer and mass transport of the species in the reactor. It is performed using the commercial general-purpose software CFD-ACE+^{TM}. Depending on reactor configurations, 2D or 3D simulations were made

Chemical models include both gas-phase and surface reactions. Decomposition of metal-organic precursors is taken into account as the principal gas phase reaction mechanism. Surface chemistry models still remain one of the critical issues in III-V MOVPE modeling. To simulate surface chemistry, we used the quasi-thermodynamic approach, described in [1-3] and implemented it as the special software module. The basic advantage of the approach originates from combination of kinetic and thermodynamic considerations of the surface processes. This allows one to reduce significantly the number of model parameters and to avoid a fitting procedure that is frequently used to estimate unknown rate constants. Another advantage of this approach is potential possibility to account for the factors affecting abruptness of heterojunction interface – elastic strain due to lattice mismatch and surface segregation.

All the models have been carefully verified using the experimental data available from the literature. Effects of variation of operating parameters such as deposition temperature, precursor flow rates, reactor pressure etc. on growth rates, layer compositions and uniformities have been studied. Model predictions have been found in good agreement with the experimental data for the wide range of growth conditions and reactor configurations (Figures 1 – 2).

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[3] E.V. Yakovlev, Yu.A. Shpolyanskiy, R.A. Talalaev, S.Yu. Karpov, Yu.N. Makarov, T. Bergunde, and S.A. Lowry, Electrochem. Soc. Proc., 2001-13 (2001) 292.
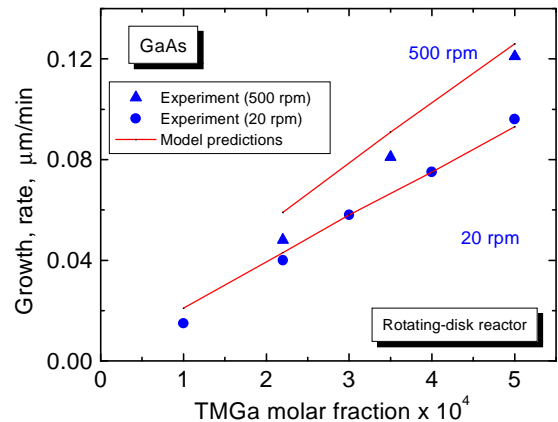
Figure 1. GaAs growth rate in vertical rotating disk reactor versus TMGa supply at different susceptor rotation rates. Lines are model predictions, points are experimental data (C.A. Wang et al., Journal of Crystal Growth 93, 228 (1988)).
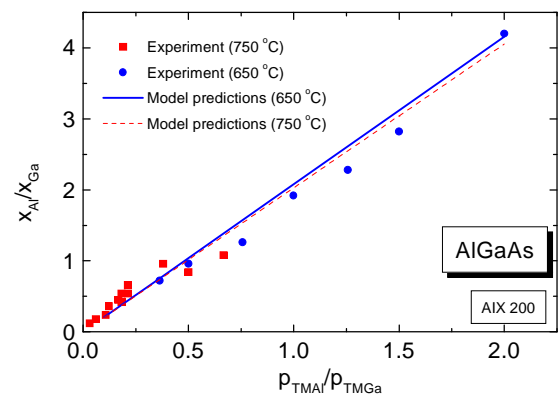

Figure 2. Dependence of Al/Ga ratio in the AlGaAs grown in AIX 200 reactor on ratio of TMAl to TMGa partial pressure at different growth temperatures. Lines are model predictions, points are experimental data (D. Schmitz et al., J. Cryst. Growth 93, 312 (1988)).