

ADVANCED COMPUTATIONAL MODELING FOR VAPOR DEPOSITION REACTORS

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ABSTRACT

Computational models are becoming an indispensable complementary tool for experiments that are difficult to perform, costly, or cannot be performed repeatedly. In particular, experiments in space fall under these categories. Much research is being geared to the development of new or better materials under microgravity conditions. For example, the group III nitrides are candidate compounds for light-emitting diodes and semiconductor lasers operating into the blue and ultraviolet regions. However, materials such as indium nitride (InN), exhibit large thermal decomposition at their optimum OMCVD (organometallic chemical vapor deposition) growth temperature. To overcome decomposition of the deposited InN film, the reaction could be conducted at high pressures. Currently, OMCVD is performed at sub-atmospheric pressures in the viscous flow regime, to avoid problems of uniformity associated with large Reynolds number flows. Epitaxial growth of InN at higher temperatures has been attempted, but at pressures below one atmosphere it results in the incorporation of indium metal droplets into the InN films. Nevertheless, surface stabilization data seem to indicate that InN could probably be grown at substrate temperatures up to 900 K in molecular nitrogen, at high pressures. If that is the case, microgravity could provide the venue for maintaining conditions of laminar flow under high pressure. In the past, computational models have been restricted to the simulation of the flow subject to some gas kinetics for the deposition or etching of the materials. In the present work, models for chemical vapor deposition were developed coupling complex chemical kinetics with fluid dynamic properties. This investigation has been performed in collaboration with researchers from various institutions, as shown in the following references:

1. "Development of an advanced computational models for OMCVD of Indium Nitride"; C. A. Cardelino^a, C. E. Moore^b, B. H. Cardelino^c, N. Zhou^d, S. Lowry^d, A. Krishnan^d, D. O. Frazier^b, K. J. Bachmann^e; SPIE-Int. Soc. Opt. Eng. Vol. 3625, pp.447-458 (1999)
2. "Modeling and real-time process monitoring of organometallic chemical vapor deposition of III-V phosphides and nitrides at low and high pressures"; K. J. Bachmann^e, B. H. Cardelino^c, C. E. Moore^b, C. A. Cardelino^a, N. Sukidi^c, S. McCall^e; Materials Research Society Symp. Proc. "In Situ Process Diagnostics and Modeling"; Eds. A. Ochello, A. R. Krauss, E. A. Irene, J. A. Schultz; Vol. 569, pp. 59-70 (1999)
3. "Theoretical study of indium compounds of interest for organometallic chemical vapor deposition"; B. H. Cardelino^c, C. E. Moore^b, C. A. Cardelino^a, D. O. Frazier^b, K. J. Bachmann^e; Journal of Physical Chemistry A, Vol. 105, pp.849-868 (2001)
4. "Semiclassical calculation of reaction rate constants for homolytical dissociation reactions of interest in OMCVD"; B. H. Cardelino^c, C. E. Moore^b, C. A. Cardelino^a, S. D. McCall^c, D. O. Frazier^b, K. J. Bachmann^e; J. Physical Chemistry A, Vol. 107, pp.3708-3718 (2003).
5. "Kinetics of epitaxy"; K. J. Bachmann^e, B. H. Cardelino^c, C.E. Moore^b; in Encyclopedia of Materials: Science and Technology; Update 2004; K.H.J. Buschow, R.W. Cahn, M.C. Flemings, B. Ilschner, E.J Kramer and S. Mahajan, editors; Elsevier Science, Amsterdam, The Netherlands, to be published 2004.

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