A COMPUTER SIMULATION OF TRANSPORT STRUCTURES IN LIQUID PHASE ELECTROEPITAXY UNDER APPLIED MAGNETIC FIELD

Sadik Dost, Yongcai Liu, Hamdi Sheibani and Brian Lent
Crystal Growth Laboratory, University of Victoria
PO Box 3055, Victoria, BC, Canada V8W 3P6
sdost@me.uvic.ca

Liquid Phase Electroepitaxy (LPEE), being a solution growth, has a number of advantages over other bulk crystal growth techniques [1-15]. Even so, LPEE has thus far suffered from mainly three "shortfalls" towards its commercialization. The first is the achievable crystal thickness that is relatively small, in the order of a few millimeters [1-5]. This is mainly due to the combined effect of Peltier and Joule heating in the system, leading to higher temperature gradients and a relatively strong natural convection in the liquid solution zone that causes unsatisfactory and unstable growth. This puts a limit on the achievable crystal thickness, particularly in the growth of bulk crystals, and providing less useful material for use. The second shortfall of LPEE has been its low growth rate. The growth rate in LPEE is almost linearly proportional with the applied electric current, and is about 0.5 *mm/day* at a 3 A/cm^2 electric current density [6,7]. Of course, for higher electric current density levels, the growth rate will increase, but in growth of thick (bulk) crystals the combined effect of temperature gradients and natural convection will lead to unstable growth, and the growth will stop. The third shortfall is the need for a single crystal seed of the same composition of the crystal to be grown. Small compositional differences, in the order of 4% depending on the crystal lattice parameters, can be tolerated, but higher compositional differences may lead to unsatisfactory growth.

Our experimental work has addressed the first two "shortfalls" of LPEE in [6,7]. By optimizing the growth parameters of LPEE, and also by using a static external applied magnetic field, a number of bulk (thick), flat $GaAs$ crystals and $In_{0.04}Ga_{0.96}As$ single crystals of uniform compositions were grown, and the growth rate of LPEE was increased more than 10 times for a selected electric current density. The grown crystals under magnetic field or no magnetic field were single crystals, and the results were reproducible in terms of crystal thickness, growth rate, and compositional uniformity. The addressing of the third "shortfall" of LPEE is the subject of a future work.

In LPEE, growth is achieved by passing an electric current through the growth cell while the overall furnace temperature is kept constant during the entire growth period (see Fig.1). The applied electric current is the sole driving force for growth, and gives rise to two growth mechanisms that are known as "electromigration' and "Peltier cooling/heating". The electromigration of species in the liquid solution is believed to take place due to electron-momentum exchange and electrostatic field forces, and sustains a controlled-growth. The Peltier heating/cooling, on the other hand, is a thermoelectric effect occurring when an electric current passes through an interface of two materials with different Peltier coefficients. The Peltier cooling at the growth interface supersaturates the solution in the immediate vicinity of the substrate and leads to epitaxial growth. The Peltier heating at the dissolution interface, on the other hand, causes the dissolution of the source material into the solution and provides constantly the needed feed material for growth. The growth rate is proportional to the applied electric current density.

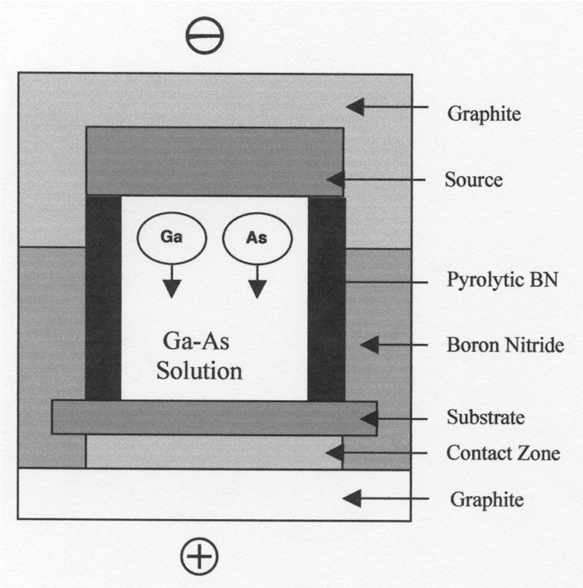

Fig.1. Schematic view of the LPEE growth crucible.

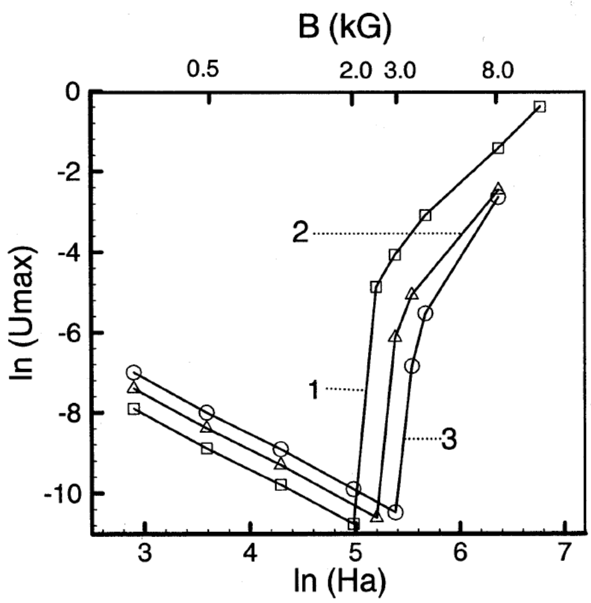

Fig.2 The computed maximum flow velocity values under various magnetic field levels show a similar pattern under all three electric current densities, (1) *J=3 A/cm,* (2) *J=5 A/cm,* and (3) *J=7 A/cm²*.

The objective this article is to extend the 3-D numerical simulations for various levels of applied electric current densities to examine the transport structures under strong magnetic field levels.

RESULTS AND DISCUSSION

Computations were performed under various magnetic field intensity and electric current density levels. The purpose was to determine the effect of the applied magnetic field and also the electric current density levels on the flow structures of the liquid phase. The behaviour of the maximum flow intensity is very similar to that obtained in [15] for only $J=3\ A/cm^2$. The maximum flow intensity, $U_{max} = \sqrt{\left(u^2 + v^2 + w^2\right)}$, is plotted in Fig.2 for all three electric current density levels $J= 3, 5$, and $7\ A/cm^2$ versus various magnetic field intensity levels (in both *kGauss* and the *Hartmann number*). As can be seen the behaviour at each electric current density level is similar to that of [16], that maximum flow intensity decreases with the magnetic field level up to a "critical" value, and then increases significantly with the magnetic field level. This "critical" magnetic field level is somewhere between *2.0* and *3.0 kGauss* in this LPEE set up. Below this level the flow is suppressed, but above this level the flow gets stronger. Such behaviour is not surprising as explained in [15], and is also supported by our experiments [6,7]. This region where is called the "suppressed" region, and the region where the flow gets very strong the "unsuppressed" region.

We have the following interesting observations. In the suppressed region, under the same magnetic field strength the flow intensity gets stronger with the increase in the electric current density level. This is because the temperature gradients in the system become larger due to the increased combined effect of the Peltier and Joule heatings. The relationship between the flow intensity and the Hartmann number (or magnetic field intensity) under different electric current densities also obey the same power law given in [15], $U_{\max} = Ha^{-5/4}$ because the ratios (slopes) of the three lines in the suppressed region are the same. In the transitional region, the flow velocity increases dramatically with increasing magnetic field, but the flow pattern is essentially numerically stable [15]. In the suppressed region, the flow intensity decreases with increasing electric current density (see Fig.2), and the critical magnetic field level, although slightly, also increases with the electric field level. This observation may be explained by considering the fine balance between the competing electromagnetic and gravitational body forces in the liquid solution. At higher electric current densities the convection gets stronger due to increase in thermal gradients, and therefore a higher magnetic body force is needed to balance the buoyancy force. In the unsuppressed region, we observe just the opposite. The flow intensity becomes stronger earlier at lower electric current density levels since the magnetic body force is the dominant in this region. Although we have no numerical results to verify it (due to unstable computations at high magnetic field levels), one may see from Fig. 2 that all three curves (the maximum flow intensity) show the tendency to reach the same value when the magnetic field intensity becomes high enough for which the magnetic body force has the absolute domination over the gravitational body force.

CONCLUSIONS

A three-dimensional numerical simulation for the transport structures, namely fluid flow, and heat and mass transport in the liquid solution in Liquid Phase Electroepitaxial (LPEE) crystal growth of GaAs under the effect an applied magnetic field was performed. Various magnetic field and electric current density levels were considered. The computed flow field in the solution exhibited interesting flow structures. The flow was suppressed up to a critical magnetic field level (about *2.0 kGauss*), and became very strong at higher magnetic field levels. The behaviour of the flow field under magnetic field is in qualitative agreement with experiments. At higher magnetic field levels, the flow patterns show very strong localized structures near the growth interface, that may explain the adverse effect of the natural convection in the solution, leading to uneven growth and holes observed in the grown crystals.

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