Extended Abstracts of the 1994 International Conference on Solid State Devices and Materials, Yokohama, 1994, pp. 1-3

Invited

Growth Dynamics of III-V Semiconductor Films

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This paper reviews our present understanding of particular aspects of the surface processes involved in the growth of epitaxial semiconductor films by molecular beam epitaxy (MBE). Emphasis is placed on adatom migration and incorporation on GaAs (001) substrates during the growth of GaAs, a comparison with equivalent growth effects on (110) and (111)A oriented substrates and the influence of mismatch and substrate orientation on growth mode and strain relaxation in the InAs/GaAs system.

1. Introduction

The last ten years have seen major advances in the evaluation of surface dynamics of epitaxial film growth at the atomic level. These advances have been made possible by a combination of several different techniques, including film growth and in-situ monitoring of surface processes in real time. The relevant growth technique is molecular beam epitaxy (MBE), not only because of the close control of growth parameters which it permits, but also because of the ultra-high vacuum (UHV) environment involved, which enables a whole range of surface measurement techniques to be applied during growth. The most significant of these have been reflection high energy electron diffraction (RHEED) and scanning tunnelling microscopy (STM). The latter is not strictly real-time but has generated 'snapshot' images of surfaces at various stages of film growth, with atomic resolution. Where chemical reactions are involved in growth (the most common situation with semiconductors), modulated beam relaxation spectroscopy (MBRS) has produced some useful input in a limited number of cases. The final ingredient, without which any progress would have been much more limited, has been the development of theoretical models which can be related directly to experimental results. By far the most successful of these has been Monte Carlo simulation based on extensions of the solid-on-solid (SOS) model first reported by Weeks and Gilmer in 1979 [1].

In this lecture I will review the present status by reference to adatom migration and incorporation on GaAs (001) substrates during the growth of GaAs, a comparison with equivalent growth effects on (110) and (111)A oriented substrates and the influence of strain and orientation in the growth of InAs on GaAs.

2. Adatom Migration and Incorporation

Neave et al[2] first demonstrated that it was possible to extend the RHEED oscillation technique to include the kinetics of adatom migration and incorporation by using a vicinal plane substrate. This provides a template of exact low index orientation terraces having a width defined by the angle of misorientation, separated by monoatomic (or monomolecular) steps, whose structure depends on the direction of misorientation. Growth on such a surface can occur either by two-dimensional (2D) nucleation on the terraces, or by step propagation, depending on the incident flux and substrate temperature. RHEED enables this transition to be monitored. The determination of adatom migration parameters requires a suitable theoretical framework within which the RHEED results can be modelled. The most successful is based on Monte Carlo simulation of the growth process[3], using the solid-on-solid model[1]. The simulation

effectively calculates the temporal variation of step density and surface steps are the dominant morphological feature responsible for the variation of RHEED intensity during growth.

The rate of step propagation, or adatom incorporation rate at a step (R_I), can be determined directly from the increase of oscillation period with temperature on a vicinal surface, since:

$$R_I = \frac{\delta\tau}{\tau+\delta\tau} \quad \frac{J_{Ga}}{N_s} \qquad (1)$$

where τ is the period of the RHEED oscillation on a singular surface for the same Ga flux J_{Ga} and $\delta\tau$ is the change in period on the vicinal plane. N_s is the step site density on an (assumed) ideal unreconstructed surface with straight steps.

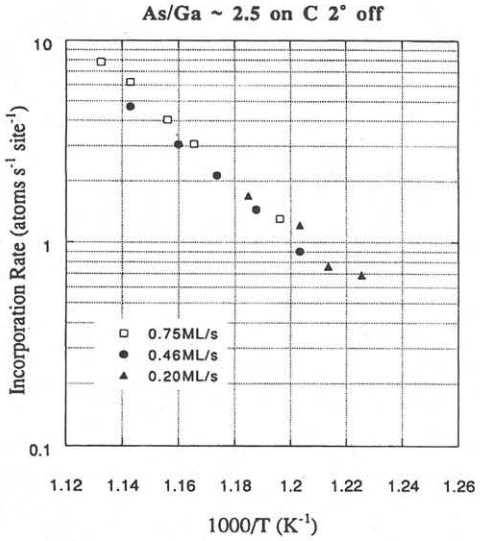

Figure 1. Maximum incorporation rate at steps on a vicinal GaAs (001) surface as a function of substrate temperature and Ga flux.

Several important results have been obtained from a systematic study of this effect[4]. Figure 1 shows the incorporation rate for a specific direction and extent of misorientation as a function of temperature for a range of Ga fluxes. Despite an almost fourfold change, the incorporation rate is independent of the flux. Nor is there any significant dependence on the extent of misorientation (between 1° and 3°). This means that steps cannot act a perfect sinks for adatoms, since even if the temperature is too low for all arriving atoms to reach the steps, the adatom density close to the steps must be proportional to the incident flux. Further, the observation of zeroth order kinetics is a direct indication that if all adatoms were to reach the steps by diffusion, a number would detach and migrate back on to the terraces, where some would form nuclei. These measurements therefore apply exclusively to the incorporation rate and are independent of diffusion.

The energy barrier to incorporation (E_I) can be determined from the Arrhenius relationship:

$$R_I = R_o \exp(-E_I / kT) \qquad (2)$$

Figure 2 shows the results for surfaces misoriented from (001) in the [110], [010] and [$\bar{1}$ 10] directions, with activation energies of 1.4, 2.1 and 4.2 eV respectively. They are highly anisotropic, since an As terminated [$\bar{1}$ 10] misoriented step is "stickier" to Ga adatoms than a Ga-terminated [110] misoriented step.

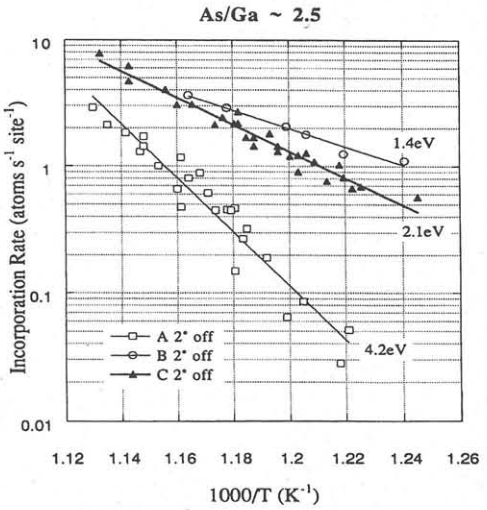

Figure 2. Arrhenius plot of the incorporation rate at steps on vicinal GaAs (001) surfaces misoriented in different directions

3. Growth of GaAs on non -(001) Oriented GaAs Substrates

The extension of RHEED studies to other low index orientations i.e. (110) and {111}, has only occurred comparatively recently and consequently there is not the same body of systematic work as on (001). The incentive to consider other orientations largely derives from the increased activity in growth on patterned substrates in pursuit of the fabrication of various mesoscopic structures with increased degrees of carrier confinement.

The most important point[5,6] is that in general the oscillation period no longer provides a measure of the growth rate (i.e. of the Ga flux). The results for the two surfaces are illustrated in

Figure 3 (i and ii) for (110) and (111) respectively). The (110) surface does not reconstruct, but the (111) surface shows a 2x2 reconstruction. The behaviour in each case is rather similar. There is a substrate temperature - flux ratio regime in which the oscillation period indicates a growth rate less than the actual value. The true value in each case was shown to be constant and the same as for an (001) substrate mounted next to the (111) and (110) substrates in the MBE system. The growth rate is therefore still determined by the Ga flux, but this is not in general measured by RHEED. What then is the origin of RHEED intensity oscillations in this case? We believe it to be closely related to the effect seen on (001) surfaces where an excess of Ga is present, which generates As-induced oscillations. On both (110) and (111) surfaces there is apparently a much lower reactivity between As_x (x = 2 or 4) and Ga than on (001) surfaces, so that unless As is supplied in very large excess, some free Ga is able to form on the surface, at least during the initial stages of growth, and the oscillations are then As-induced. The limiting factor to growth is therefore incorporation into the lattice via a surface reaction, which in a certain sense is rate limiting and represents totally different kinetics from growth on (001) substrates.

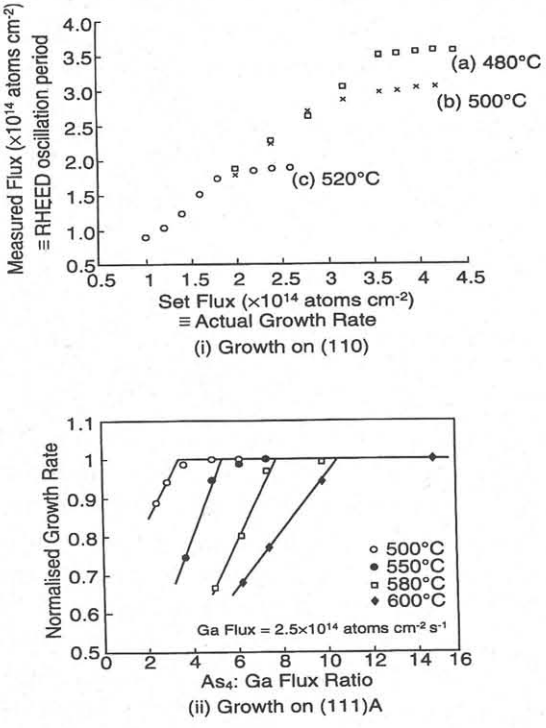

Figure 3. Growth on (110) and (111)A substrates. The RHEED oscillation period does not, in general, indicate the growth rate.

3. Growth of Mismatched Structures

In the GaAs/InAs system the extent of misfit is comparatively large, ≈7%, so the degree of strain rapidly becomes high. If we consider first the growth of InAs on GaAs (001), the behaviour follows a fairly conventional pattern. At most the first ML is formed by a process of 2-D nucleation but after that the growth rapidly becomes 3-D, nominally following the Stranski-Krastanov (SK) mode. There is evidence, however, that even the first ML does not retain its integrity with subsequent growth, but that during that process it breaks up into 3-D clusters of variable thickness [11].

If we now consider growth on (110) oriented substrates, we find the behaviour to be completely different from that on (001), despite there being the same misfit. The first major difference is that growth occurs in a 2-D layer-by-layer mode over a large range of film thicknesses (from 1 to >500MLs) although there is probably no upper limit. RHEED oscillations are sustained during growth and both plan view and cross-section TEM confirm the growth mode to be layer-by-layer[7].

At this stage it is only possible to speculate on the reasons for this difference, or more fundamentally, what physical parameter controls the growth mode. A possible interpretation is that In adatoms are extremely mobile on this surface and it is this mobility which determines the growth mode, not the presence of strain in the system.

References

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