MODELING OF SIGE EPITAXIAL GROWTH IN A WIDE RANGE OF GROWTH CONDITIONS

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Si/SiGe heterostructures has lately attracted much interest in the Si CMOS and bipolar technologies. Benefits of using the commercially available equipment and necessity of rising the structure growth rates draw attention to a higher pressure range compared to the conventional MBE and UHV-CVD techniques. Elaboration of such processes would be facilitated by development of a versatile model of SiGe epitaxial growth, valid in a wide range of operating conditions. In this paper, the previously developed model of CVD of SiGe epilayers from SiH₄-GeH₄-H₂, accounting for surface reactions, elastic strain, Ge surface segregation, and different coverages of Si and Ge surface atoms with hydrogen, is extended to describe the unsteady growth of Si/SiGe heterostructures. The model is based on the quasi-thermodynamic approach, considering adsorption and desorption as the rate-limiting stages of the growth. The model is validated using a wide range of experimental data. Good agreement of the computed Ge concentration profiles in a silicon cap layer with the data of Tok et al (J.Cryst.Growth, 209, 321 2000) is illustrated in Fig.1.

The steady version of the model is applied to analysis of the process in production-scale reactors. Detailed 3D simulation of the SiGe epitaxial growth in a single wafer rotating disk reactor of the Centura type under various growth conditions has been carried out. 3D flow patterns, temperature and species concentration distributions in the reactor, and 2D alloy growth rate and composition distributions over the wafer are computed and analyzed. The two latter distributions are shown to be rather uniform under typical growth conditions (T = 650 °C, P = 100 Torr, and GeH_4 :SiH₄ = 0.06), though the epilayer proves to be somewhat enriched with Ge near the wafer edge (see Fig.2). The unsteady model is used to study the Ge concentration profiles in silicon cap layers grown in the considered reactor. The Ge concentration decay length is shown to decrease considerably in transition from the low-pressure range to a much higher pressure of around 100 Torr (see Fig.3). Combined with a much higher growth rate, this feature suggests an additional benefit of growth of Si/SiGe heterostructures in production-scale reactors at in a higher pressure range.



Fig.1. Computed (lines) and experimental (points) Ge concentration profiles in a silicon cap layer.



Fig.2. Distribution of the Ge concentration in the SiGe epilayer over the wafer in a single wafer rotating disk reactor.



Fig.3. Ge concentration profiles in a silicon cap layer at low and much higher pressures.