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Prediction of Macroscopic Surface Shapes from Adatom Rate Equations in Epitaxial Growth A. BALLESTAD, BAYO LAU, J. H. SCHMID, T. TIEDJE, M. WHITWICK, Physics and Astronomy, University of British Columbia, Vancouver, BC — Epitaxial growth involves adatom diffusion on terraces interrupted by step edge attachment/detachment, and island nucleation. On the other hand macroscale surface morphology is commonly described by continuum growth equations such as the KPZ or MBE equations with coefficients that are expressed in terms of derivatives of thermodynamic quantities. The connection with the microscopic phenomena that occur during growth is typically obscure. For example in experiments the coefficients depend strongly on growth rate, which is not readily apparent in the thermodynamic analysis. Therefore we have developed a perturbation method for low surface slopes, by which the rate equations that describe the adatom dynamics can be converted into continuum growth equations. This method also generates expressions for the coefficients in the growth equations in terms of microscopic parameters. For conditions appropriate for GaAs MBE growth we find a KPZ-like growth equation with a conservative non-linear term $\nabla^2 (\nabla h)^2$. From experimental measurements of the smoothing rate and shape of patterned substrates during GaAs MBE growth, and the theoretical expressions for the growth coefficients, we can determine various interesting microscopic parameters as a function of growth rate and temperature.

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