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Case ID:M21-097P^
Published: 10/4/2021

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Kinetic Model for Molecular Beam Epitaxy Growth of III-V Bismide Alloys

Background Bismuth-containing III-V semiconductor alloys have received considerable attention as materials for optoelectronic devices operating in the mid- and long-wave infrared spectrum. The infrared spectrum finds important applications in both commerce and government, including medical imaging and diagnostics, autonomous vehicle sensors, telecommunications, and gas sensing among others. The quaternary alloy InAsSbBi grown on readily available large-area GaSb substrates is particularly attractive for these applications as it offers highly-tunable bandgaps. Moreover, bismuth is the largest stable element and is relatively nontoxic and abundant compared to other nearby heavy elements such as lead, thallium, or mercury.

InAsSbBi is a highly mismatched alloy with isoelectronic group V elements of different sizes, ionicities, and electronegativities. Highly mismatched alloys can have miscibility gaps over certain composition ranges that make them challenging to grow. Molecular beam epitaxy is a non-equilibrium technique well-suited to growth of bismide alloys, which exhibit a strong tendency for surface segregation and composition modulation due to the very low solid solubility of Bi in host materials such as GaSb or InAs. Despite its wide use throughout research and production, the impact of molecular beam epitaxy growth conditions on chemical composition is not well understood. A comprehensive model for molecular beam epitaxy growth of bismide alloys is therefore valuable for predicting the outcome of growth experiments and guide the selection of growth temperatures and group V element: Indium flux ratios (V/In flux ratios) to maximize Bi incorporation. Invention Description The growth of Bi-containing III-V alloys requires careful control over temperature and group V fluxes due to the low equilibrium solubility of Bi and its tendency to surface segregate into Bi-rich droplet features. Researchers at Arizona State University have developed a model for molecular beam epitaxy growth based on the kinetics of atomic desorption, incorporation, surface accumulation, and droplet formation for bismide alloy InAsSbBi grown on GaSb substrates. A steady state solution is derived for the Bi, Sb, and As mole fractions and surface layer coverages based on the Bi, Sb, and As fluxes. A nonlinear least-squares algorithm is used to fit the growth model parameters to experimentally measured Bi mole fractions in bulk and quantum well InAsSbBi samples grown at 400 °C and 420 °C. The Bi mole fraction ranges from 0.12% to 1.86% among 17 samples examined. The results indicate that as the growth temperature increases, the rate of Bi incorporation decreases and the rate of Bi self-desorption increases. A strong interaction is observed between Bi and As that plays a role in the desorption of excess Bi from the growth surface, thus reducing the likelihood of Bi-rich droplet formation when an excess As flux is present. Significantly, the model predicts that the incorporation of Bi is limited to mole fractions of 1.43% at 400 °C and 0.30% at 420 °C in lattice-matched bulk InAsSbBi grown on GaSb substrates. Potential Applications • Bismuth-containing III-V semiconductor alloys • Molecular beam epitaxy growth modeling • Semiconductor devices for optoelectronics, medical imaging, sensors, and communications Benefits and Advantages • Predicts outcome of growth experiments without reliance on resource-intensive "guess and check" methodologies • Readily extendable to growth of other bismide III-V ternary alloys such as GaAsBi and InAsBi and to quaternary alloys such as GaAsSbBi Related Publication: Kinetic model for molecular beam epitaxy growth of InAsSbBi alloysASU Profile of Dr. Shane Johnson