

Epitaxial Growth of $\text{ZrB}_2(0001)$ on $\text{Si}(111)$ for III-nitride Applications: A Review

J. Tolle,¹ J. Kouvetakis,¹ D.-W. Kim,² S. Mahajan,² A. V. G. Chizmeshya,³
C.-W. Hu,⁴ A. Bell,⁴ F. A. Ponce,⁴ and I. S. T. Tsong⁴

¹*Department of Chemistry and Biochemistry,
Arizona State University, Tempe, AZ 85287-1604*

²*Department of Chemical & Materials Engineering,
Arizona State University, Tempe, AZ 85287-6006*

³*Center for Solid State Science, Arizona State University, Tempe, AZ 85287-1704*

⁴*Department of Physics and Astronomy,
Arizona State University, Tempe, AZ 85287-1504*

We review the growth behavior of epitaxial $\text{ZrB}_2(0001)$ films on $\text{Si}(111)$ via the thermal decomposition of the unimolecular precursor $\text{Zr}(\text{BH}_4)_4$ studied *in situ* by low-energy electron diffraction and low-energy electron microscopy, and *ex situ* by cross-sectional transmission electron microscopy and atomic force microscopy. Under appropriate kinetic conditions, epitaxy was achieved in spite of the very large lattice mismatch between $\text{ZrB}_2(0001)$ and $\text{Si}(111)$. The growth was followed from the initial nucleation stage to the final epitaxial film at various growth temperatures. At 900°C , the growth of $\text{ZrB}_2(0001)$ proceeded by the nucleation of two-dimensional islands. These islands eventually coalesced to form a continuous atomically smooth film. The interface between $\text{ZrB}_2(0001)$ and $\text{Si}(111)$ was modeled theoretically and the most favorable interface consisted of the $\text{ZrB}_2(0001)$ growing on a $\text{Si}(111)-(\sqrt{3} \times \sqrt{3})\text{B}$ surface with the Zr layer nearest to the interface and the B layer on the top surface. The in-plane a lattice parameter of the $\text{ZrB}_2(0001)$ surface has a perfect match with that of $\text{Al}_x\text{Ga}_{1-x}\text{N}$ where $x = 0.26$. Epitaxial layers of $\text{Al}_{0.2}\text{Ga}_{0.8}\text{N}$ grown on a $\text{ZrB}_2/\text{Si}(111)$ substrate by metalorganic chemical vapor deposition (MOCVD) exhibit luminescence properties comparable to or better than those from layers of identical composition grown on sapphire substrates.

PACS numbers: 81.15.Hi, 68.55.-a, 68.35.-p

I. INTRODUCTION

Over the past decade, group III nitride semiconductors with direct band gaps have made tremendous advances in optoelectronic and microelectronic applications. The nitride-based light-emitting diodes (LEDs) cover a spectrum ranging from orange to ultraviolet (UV). With the use of a suitable phosphor, the emitted blue-UV light can be converted to white light for the purpose of general illumination. The long lifetime of nitride LEDs, $\sim 10^5$ hours, makes them very attractive as replacements for conventional lighting systems. However, in order for nitride LEDs to gain widespread acceptance, the cost of the LEDs must be greatly reduced while the luminous efficiency must be increased. The most effective area in cost-reduction lies in the choice of substrates. Currently, the nitride technology is