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Epitaxial Growth
of III-Nitride Compounds
Computational Approach
Preface

Ever since the developments of blue light-emitting diodes and laser diodes using epitaxial GaN thin films, III-nitride compounds such as AlN, GaN, and InN have been paid much attention for the use of light emission over a wide range of wavelengths. To improve the device performance of these materials, strict control over the growth conditions and thorough understanding of surface reconstructions and the growth kinetics are essential. In particular, the surface reconstructions and the growth kinetics are crucial for understanding the physics and the chemistry on various technological stages in III-nitride growth.

In this book, we present a unified treatment for the growth mechanisms of epitaxial growth in III-nitride compounds on the basis of state-of-the-art computational approach using ab initio calculations, empirical interatomic potentials, and Monte Carlo simulations. This book is the first attempt to gather together the information of theoretical/computational aspects of the growth of III-nitrides, which is scattered in the scientific literature, into a single comprehensive work. The most fundamental and basic aspects of the crystal growth of III-nitride compounds are presented, along with the underlying scientific principles. We also provide the readers with important theoretical aspects of surface structures and elemental growth processes during the epitaxial growth of III-nitride compounds. The book features advanced discussion of fundamental structural and electronic properties, surface structures, fundamental growth processes, and novel behavior of thin films in III-nitride compounds.

This book will serve as a great practical use to researchers, engineers, and graduate students seeking advanced knowledge of the crystal growth and the application of III-nitride compounds. We hope that the book provides the readers with valuable insight and perspective into this rapidly developing and important field.

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