Preface

With outstanding mechanical properties such as high specific stiffness- and strength-to-weight ratio, and excellent material tailorability and designability, carbon fiber-reinforced polymer (CFRP) composites have been increasingly used in different engineering fields, including the structural components in airplane, high-speed train, automobile, and transportation and civil infrastructures. During intended service life, CFRP composite structure is inevitably subjected to changing environmental and loading conditions, and the long-term exposure leads to the degradation of CFRP composite, including the distinct material deteriorations and structural integrity failure, in which fiber/matrix interface is regarded as the critical failure region. Specifically, the degradation of fiber/matrix interface in CFRP composite originates from the variation of interfacial behaviors and interactions at an atomistic level. However, the molecular behaviors and interactions of polymer composite and fiber/matrix interface have not been comprehensively understood. This book reports the investigation of CFRP composite and its fiber/matrix interface under environmental and loading conditions using molecular dynamics (MD) simulation, with a focus on the degradation and failure mechanism of composite and fiber/matrix interface, so as to provide the foundation for predicting the property and performance degradation of CFRP materials during long-term service-life.

Chapter 1 of this book covers the general introduction related to the basic constituents and degradation problems of CFRP composites. Chapter 2 focuses on the experimental observation and molecular modeling of carbon fiber, different types of matrix materials, CFRP composites, and the bonded interface between fiber and matrix in CFRP composites. Chapter 3 describes the basic theories and techniques used in molecular simulations. Chapter 4 introduces the modeling of epoxy and epoxy-based composites, and the investigations of loading and environmental effects on carbon nanofiber-reinforced polymer composite. Chapter 5 presents the investigations of the degradation of fiber/matrix interface under different loading conditions, and Chap. 6 introduces the investigations related to interfacial degradation under environmental conditions. Finally, Chap. 7 contains is the summary and prospects for future investigations. The studies reported in this book include the molecular simulations on the degradations of carbon nanofiber-reinforced polymer composite

under moisture environment and constant velocity loading conditions, as well as of carbon fiber/matrix interface under moisture, salt, and hygrothermal environmental conditions, and constant velocity and constant force loading conditions. This book provides the microscopic insights into degradation of CFRP composite and fiber/matrix interface, as well as the underlying mechanism under the effect of environmental and loading conditions, which contributes to the scientific knowledge in the area of the structural integrity of CFRP composite, and forms the basis for predicting the long-term durability of CFRP structures in engineering field. The reported results are essential for facilitating the structural and property design of CFRP material with optimized performance. This book is useful for the researchers who are interested in investigating FRP materials under environmental and loading conditions, the engineers who would like to obtain more knowledge about FRP materials, and the students who are eager to learn the basics of molecular simulation methods for investigating FRP materials. Overall, this book is helpful for both academic and industrial fields concerning the long-term durability of FRP composites.

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