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種別(和文)	論文要旨
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（博士課程）
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論 文 要 旨

THESIS SUMMARY

系・コース： Department of, Graduate major in	応用化学 系 応用化学 コース	申請学位（専攻分野）： Academic Degree Requested	博士 Doctor of （工学）
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要旨（英文 800 語程度）
Thesis Summary（approx.800 English Words ）

Thermoplastic elastomers (TPEs) retain permanent deformation after elongation, preventing them from replacing rubber as an environmentally friendly material. To address TPE's vulnerability, in this thesis, an in situ atomic force microscopy (AFM) is used to characterize the evolution of TPEs' microstructure and micromechanical properties before, during, and after stretching. A finite element analysis (FEA) is then developed and implemented to visualize the local behavior of TPE at the nanoscale. Experiments and data analysis show that solving the hard-domain splitting problem in TPE's microphase separated structure is crucial to increasing its strength.

Chapter 1, "Introduction A: Thermoplastic Elastomers", gives an overview of the TPEs' microphase-separated structure of the hard domain and soft matrix, as well as their mechanical properties, which combine flexibility and toughness like crosslinked rubber. In TPE materials, however, because the hard domain acts as a physical crosslinking point, the crosslinking point's binding force is weaker than that of chemically crosslinked rubber, and stress relaxation and residual strain are considered inferior. The importance of elucidating the macroscopic and microscopic structure-property relationships for TPE materials under deformation is discussed to provide design guidelines for TPE materials that can replace cross-linked rubbers. It is also discussed that, while molecular dynamics (MD) simulations predict hard domain behavior during deformation, experimental techniques to validate the predictions are lacking.

Chapter 2, "Introduction B: Atomic Force Microscopy for Polymer Science", discusses the principle of simultaneous measurement of structure and properties of polymeric materials by a nano-palpation technique based on AFM, as well as the effect of deformation of the AFM tip on the sample. It also presents a typical Johnson-Kendall-Robert (JKR) contact theoretical model for analyzing the load-deformation curve produced when an AFM probe is deformed into a sample. The in-situ nano-palpation AFM is also developed and described, which allows in-situ observation of nanostructure and physical properties of specimens under deformation, as well as investigation of stress relaxation and residual strain in TPE materials.

Chapter 3, "Dynamic Stress Network in the TPE", investigates the macroscopic stress relaxation phenomenon of TPE materials under constant strain using a block copolymer TPE, styrene-ethylene-butylene-styrene (SEBS). At 50% elongation, in situ AFM is used to investigate the microstructure and properties of SEBS. It has been confirmed that when the soft matrix is elongated, stress chains connecting the hard domains form in the soft matrix, and that the soft matrix modulus decreases while the number of hard domains increases in the early stages of the relaxation process, before stabilizing in the later stages. Furthermore, by focusing on a specific local region, the formation of hard domains, the emergence of new stress chains, and the splitting of hard domains, i.e., the existence of a dynamic stress network, has been clarified. The topology of the polymer is permanently changed by the dynamic stress network, implying that it is caused by stress relaxation phenomena.

Chapter 4, "Nanoscale Strain-Stress Mapping for the TPE", develops an FEA program for AFM images to better understand the relationship between the "dynamic stress network" and the property changes of TPE materials. In this program, the hard domain distributed in the AFM deformation image is extracted as a set of discrete points and divided into each image by Delaunay triangulation. The strain in each triangle region is calculated during the relaxation process and combined with the AFM modulus image, the local strain and local stress can be discussed. In the early stage of the relaxation process, severe contraction occurs inside the material along the tensile direction and stress concentration is observed. In the later stage, unlike the early stage, the average strain in the tensile direction becomes close to zero, the region of stress concentration disappears, and the stress is uniformly distributed over a small area, describing the visualization of the stress relaxation behavior of TPE materials at a microscopic level.

Chapter 5, "Heterogeneously Formation of the Stress Network in the TPE", observes the microstructure and physical properties of the initial elongation process of the TPE material from unelongated to about 45% elongation by in situ nano-palpation AFM. The micro-elastic modulus and macro-stress were measured. Since both micro-elastic modulus and macro-stress show a non-linear correlation with strain, the FEA method will be used to study them in detail. Initially, almost all regions deformed regularly, but at the cost of stress concentration in some regions. As the strain increases, non-uniform deformation due to accumulated stresses begins. Finally, all the domains are simultaneously undergoing negative deformation with stress relaxation. The number of domains decreases and then increases during this process, which establishes consistency with the MD simulation prediction.

Chapter 6, "AFM Characterization of Triptycene-Appended Polymers", investigates triptycene-appended polymers by AFM. The triptycene units in the side chains of the block copolymer and both terminals of the polymer are described as a special aggregation structure that improves the mechanical properties of the original polymer.

Chapter 7, "Summary and Open Questions", summarizes the contents of this thesis and describes the prospects.