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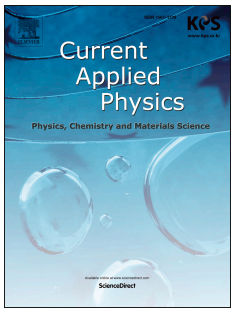

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PII: S1567-1739(17)30300-0

DOI: 10.1016/j.cap.2017.10.019

Reference: CAP 4615

To appear in: *Current Applied Physics*

Received Date: 27 July 2017

Revised Date: 25 October 2017

Accepted Date: 30 October 2017

Please cite this article as: K.C. Kim, S.S. Jang, Molecular dynamics simulation study on the structural properties of poly (ethylene terephthalate) under uniaxial extension and thermal shrinkage processes, *Current Applied Physics* (2017), doi: 10.1016/j.cap.2017.10.019.

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ACCEPTED MANUSCRIPT

Molecular Dynamics Simulation Study on the Structural Properties of Poly (Ethylene Terephthalate) under Uniaxial Extension and Thermal Shrinkage Processes

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Abstract

In thermal shrinkage process for polyethylene terephthalate (PET) films, PET film is uniaxially stretched and then thermally relaxed. We investigate the effect of heat relaxation temperature on the thermal shrinkage of uniaxially stretched PET film using molecular dynamics simulation method. Through our investigation, we find that the thermal shrinkage ratio of the amorphous PET film is reduced as a function of heat relaxation temperature, whereas the skirt ratio is weakly correlated with the heat relaxation temperature, exhibiting the most negative skirt ratio in the case of the highest thermal shrinkage ratio. Our analysis on the PET film at molecular level further verifies that the trans-gauche transformation observed in ethylene glycol units during the simulated process is a driving force for the thermal shrinkage of uniaxially stretched PET systems.

Keywords: PET film; uniaxial stretching; thermal shrinkage; molecular dynamics simulations; conformation.

1. Introduction

Polyethylene terephthalate (PET), the condensation product of ethylene glycol and terephthalic acid, has been widely utilized in the form of fibers and films.[1] Approximately forty percent of the synthetic fiber produced in the world is based on PET polymers.[1] Either uniaxially or biaxially stretched PET films are widely used for tape applications such as magnetic tape and

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