

Tensile deformation of semi-crystalline polymers by molecular dynamics simulation

Shengwei Deng¹

Received: 5 May 2017 / Accepted: 25 October 2017 / Published online: 1 November 2017
© Iran Polymer and Petrochemical Institute 2017

Abstract In this work, the microstructure evolution of semi-crystalline polymers during tensile deformation is analyzed by molecular dynamics simulation. A perfect semi-crystalline lamellar structure with crystalline/amorphous interface perpendicular to tensile direction is created with the help of coarse-grained (CG) model of poly(vinyl alcohol) (PVA). During the tensile test, two kinds of strain rates are applied to the lamellar stack to determine the stress–strain curves, yield stresses, and crystallinities. Consistent with experimental findings, two yield points were observed in the semi-crystalline sample which was corresponded to the fine and coarse crystallographic slips in the lamellar structure, where the crystal stems gradually rotated into the direction of applied stress during chain slips. After the second yielding point when the crystal stems had been rotated fully into the direction of applied stress, the lamellar structure was destroyed and it resulted in a decrease of crystallinity. In addition, the increase of the strain rate led to the acceleration of destruction of crystal structures. It is worth noting that the stress induced crystallization was observed in the interfacial region, and newly crystallized beads were belonged to the same microcrystalline domain as crystalline region due to memory effects. This work provides direct comparison of structure evolution between crystalline and amorphous region in semi-crystalline polymers during tensile deformation, and it is helpful for the design and mechanical property analysis of semi-crystalline polymers.

Keywords Molecular dynamics · Crystallization · Deformation · Yielding · Semi-crystalline

Introduction

Semi-crystalline polymers constitute a large group of commercially useful polymers. These polymers generally cannot crystallize completely in the bulk and result in a stable semi-crystalline state [1]. The relation between the structure and mechanical behavior of semi-crystalline polymers is difficult to track due to the complex microstructure [2]. Aside from the amorphous region which is mainly characterized by entanglements [3], the crystalline/amorphous interphase [4] and mechanical anisotropic crystalline lamellae [5, 6] also play important roles in the final mechanical response. The morphology of semi-crystalline polymers in the undeformed state has been extensively studied for decades by models [7, 8], simulations [9] and experiments [10, 11]. To reveal the intrinsic mechanism of mechanical behavior, it is necessary to capture the microstructure evolution during deformation, e.g., various modes of crystallographic slips [12]. However, there have not been many studies [13] that deal specifically with the deformation process of semi-crystalline polymers at a molecular level, especially the direct measurement by experiments.

Computer simulation could be an efficient tool to uncover underlying mechanisms for the observed mechanical properties of semi-crystalline polymers [14]. Various simulation methods are employed to investigate this problem at different length or time scales [15–17]. Generally, the deformation of semi-crystalline polymers is expected that first the amorphous phase is deformed [18] and then crystallographic mechanisms (e.g., slip) [19, 20] are activated. Hence, to show the mechanical contribution of crystalline domains,

✉ Shengwei Deng
dengshengwei@gmail.com

¹ College of Chemical Engineering, Zhejiang University of Technology, Hangzhou 310014, China