SHOCK WAVE PROPAGATION IN POLYETHYLENE VIA MOLECULAR DYNAMIC SIMULATION

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Introduction

Shock wave is usually propagated through solid when the explosion or high speed shock occurs. Polymer can absorb a large amount of shock energy and retain structural integrity as a kind of shielding materials. Their kinetic performance could be traced via experimental tests. However, the dispersive wave mechanism has been barely studied before.

In this paper, we study the shock wave propagation in amorphous polyethylene (PE) via molecular dynamic simulation (MDs). In order to eliminate the "end effect", a semi-infinite model is established to trace the shock wave propagation and investigate the molecular morphological evolution in PE under high velocity shock compression. This paper focuses on the variation of wave propagation under different shock velocities and analyzes the dispersive wave mechanism. The influences of chain number and chain length on the dispersive wave are also discussed.

Model and simulation

The initial configuration of amorphous PE is generated using a Monte Carlo self-avoiding random walk algorithm. To enhance computational efficiency, the united atom (UA) approach is adopted to model the PE system, in which each group of -CH_2- monomer is considered as a single monomer particle. The interatomic force field is described by the Dreiding potential. In order to eliminate the "end effect", all simulations are performed with periodic boundary conditions in x and y directions and free surfaces along z direction (shock direction). Moreover, three models are built with different chain lengths and chain numbers to discuss their influences on the dispersive wave.
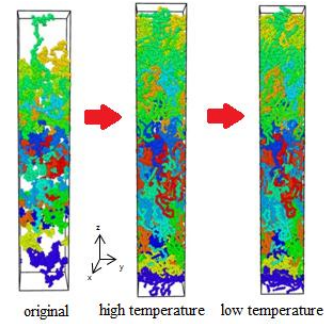

Fig. 1 Illustration of relaxation process for PE system

The isochoric-isothermal (NVT) ensemble is performed using the Nosé-Hoover thermostat for system relaxation. The system experiences high temperature and low temperature environment sequentially to reach equilibrium states, as shown in Fig. 1. When the local density near the two free surfaces approaches the bulk density and the global density becomes stable, the system is accepted as an equilibrium state. Fig. 2 (a) and (b) illustrate that the shock waves are generated by slamming the samples with a rigid piston at different velocities. Since shock propagation is an instantaneous process, all the simulations are carried out in the microcanonical (NVE) ensemble.
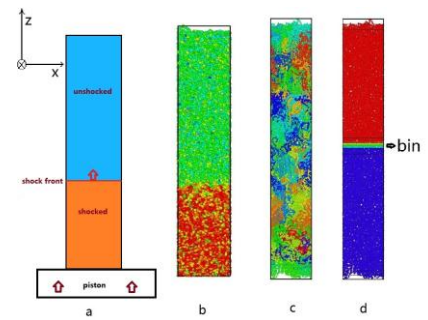

Fig. 2 (a) Schematic diagram of the approach of shock wave generation and (b) (c) (d) molecular models colored with velocity, molecule and position

Analysis

We analyze the local properties of PE by the binning analysis method, in which the sample is divided into several bins with equal widths along z direction, as shown in Fig. 2 (c) colored with molecule and Fig. 2 (d) colored with position. We discuss the influences of chain length and chain number. It is concluded that the former has a major effect on the kinetic performance of PE.

Fig. 3 shows the particle velocity distributions under different shock velocities, 0.3, 0.5, 1, 2 km/s, respectively. It is obvious that speeds of shock waves increase with higher particle velocities. Shock waves diffuse over time at different positions and different wave forms are presented with different shock velocities. The width of shock front is large under low shock speed, yet it decreases as shock speed increases. It can be contributed to the lack of time for wave dispersion as the shock speed increases and the transformation inside the materials as the shock pressure reaches some level with high shock speed.
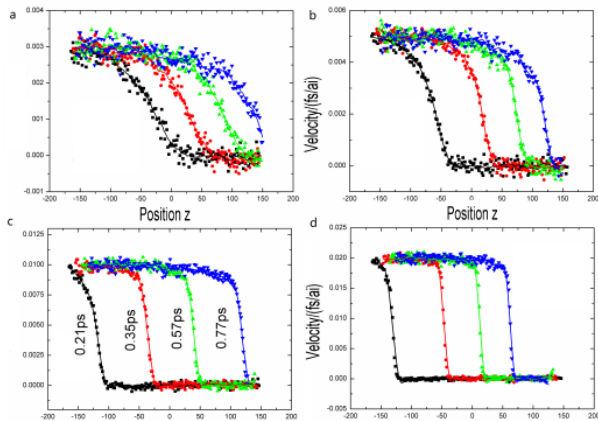

Fig. 3 Distributions of particle velocity along z direction at different time

Fig. 4 shows the distributions of the bond angle, bond length and dihedral angle under shock speed of 1 km/s at different time. As expected, the bond angle distribution is symmetric about $110°$. The crest reduces over time because shock brings large influence on the bond angle and leads to the variation of molecular shape. The curve of bond length shows that the symmetry center moves to the left over time and the crest also reduces. It is because the sample becomes squashed under high speed shock compression and a portion of energy reserves in covalent bonds. The dihedral angle distribution remains almost unchanged, which indicates that the molecular torsion mechanism is a minor factor under high speed shock compression.
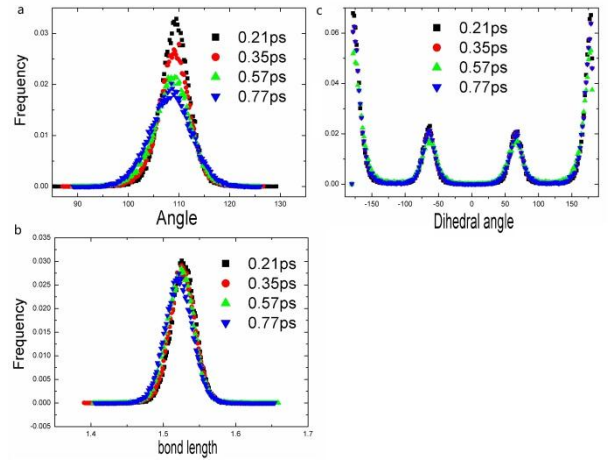

Fig. 4 Distributions of bond angle, bond length and dihedral angle at different time

In Fig. 5, the temperature is calculated after subtracting out the center-of-mass velocity of each bin. It is observed that the pressure and temperature distributions have the similar trend. When the shock wave arrives, the pressure and temperature both rise sharply.

Due to the paper length limitation, some of our work cannot be presented yet. We also monitor the shock front position over time and obtain the wave velocity by calculating the slope of the position-time curve. Afterwards, the Hugoniot curve is fitted, which reveals the kinetic properties of PE. Further discussions about molecular morphological evolution have been proposed by calculating MSD and Rg in each molecule.
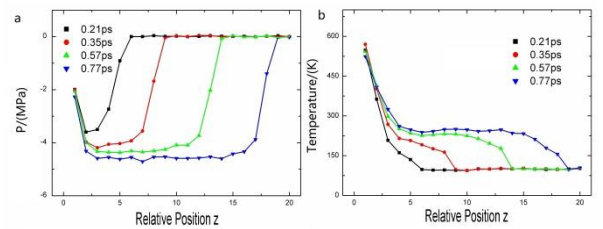

Fig. 5 Distributions of pressure and temperature along z direction at different time

Conclusion

In this paper, the shock wave propagation and the molecular morphological evolution in PE under high velocity shock compression have been presented via MDs. Wave speed, pressure and temperature are affected by shock speed. The major molecular deformation mechanism is bending instead of torsion. We hope that these simulations can provide some guides for material production.