



# Mechanical behaviors and molecular deformation mechanisms of polymers under high speed shock compression: A molecular dynamics simulation study



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## ABSTRACT

Molecular dynamics (MD) simulations based on a united atom (UA) approach are performed to analyze the mechanical behaviors of polyethylene (PE) under high speed shock compression. With shock loads in a wide range from 0.3 km/s to 2 km/s, the behaviors of shock wave propagations in the polymer are presented. It is found that shock front thickness decreases as the shock load increases and even approaches to zero when the shock load reaches 2 km/s. Hugoniot curves in  $u_s$ - $u_p$  and  $P$ - $u_p$  are presented, which agree qualitatively with the experimental results. In addition, the molecular morphological evolution is analyzed by the statistical method, which indicates that the major molecular deformation mechanism is bending instead of torsion. More evidences show that how internal mechanism associated with distributions of bond lengths, bond angles, dihedral angles and normalized mean-square radii of gyration.

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## 1. Introduction

Polymeric materials have a wide range of engineering applications [1,2], which stimulate huge interests in academics due to their fantastic mechanical, thermal and electrical properties [3–6]. The material properties of polymers are determined not only by their chemical composition but also by the mutual arrangement of their macromolecule [7,8]. Shock wave is normally caused by a strong impact into a solid surface and propagates through the solid at a high speed. Significant and abrupt changes in the material state variables (e.g., pressure, mass density, temperature, etc.) are always caused by a shock wave, accompanied with permanent and irreversible changes of molecular configuration [9,10]. Recently, polymers are applied as a kind of impact-resisting materials in industry, which can absorb a large amount of shock energy and retain structural integrity [11–14].

However, it is also a challenge to study the mechanical properties of polymers for their complicated and changeable molecular structures. Rauls and Ravichandran [15] carried out an experimental study of shock wave profiles in polymer/particle composites

to determine how shock width and rise times depend on the particulate size. A linear change in shock wave rise time was observed as a function of mean particulate diameter. Dlott et al. [16] combined two measurement techniques to study the high strain rate mechanical dynamics of polymethyl methacrylate (PMMA) under shock compression. Wood et al. [17] used the plate impact technique to investigate the shock response of PMMA between particle velocities of 0.13 and 0.77 mm/ $\mu$ s. A linear Hugoniot in the  $u_s$ - $u_p$  plane was obtained, with the equation  $u_s = 2.99 + 0.92u_p$  based on the experimental data. There are many other experimental studies of polymeric materials subjected to shock wave excitation [18–22]. Generally speaking, the kinetic performance could be obtained via experimental tests. However, the transformation of molecular structures in the polymer under shock load can hardly be investigated directly through these experimental methods.

Molecular simulations have been widely used to analyze the shock wave propagation and interaction phenomena in crystalline solid [23–29]. Yao et al. [27] studied on high-velocity shock compression of cubic SiC using a Tersoff potential based on MD simulation. Soulard et al. [28] analyzed the propagation of an incident shock and compression waves in a porous media from a set of large scale MD simulation. Seif et al. [29] examined the shock deformation of copper nano-films and nano-rods with MD

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simulation. In addition, MD simulation was also successfully applied for the investigation on polymer and polymer based composites. Fu et al. [30] investigated the shock response of PE polymer modified by nanoparticles (NP) using a coarse-grained MD method. They concluded that  $u_s$ - $u_p$  Hugoniot analysis yielded a linear relationship under the range of particle velocity investigated. Sewell et al. [31,32] studied the shock-induced structural changes and post-shock relaxation in monodisperse melts of *cis*-1, 4-polybutadiene. They investigated the effects of the repulsive wall of the non-bonded potential by comparing simulation results for two potentials. The Rankine-Hugoniot shock pressure and the shock temperature depended on chain length and non-bonded interaction potential. Mattsson et al. [33,34] performed both density functional theory (DFT) MD simulation and classical MD simulation of shock impacted PE and poly (4-methyl-1-pentene) (PMP). It was concluded that both polymers were well characterized by the exp-6 and ReaxFF while only DFT was suitable for the situation of shocks pressure above 50 GPa. Lane et al. [35] extended those results to include low-density polymer foams using non-equilibrium MD techniques and good quantitative agreement with experiment was achieved. Consequently, the computational technique of classical MD simulation has been proved to be an important tool for modeling the mechanical response of solids under ultra-high speed shock compression. Previous work mainly focused on three aspects, namely the shock response, the influence of fillers and the post shock kinetic properties. However, the molecular morphological evolution of pure polymer matrix under high speed shock compression has been barely studied, which is the motivation of this work.

As a typical representative of polymer, PE has been widely studied before. The methods to simulate polymer systems can be generally classified into two categories, namely full-atom [36] and UA [37]. Compared with UA, full-atom would require approximately three times the number of atoms due to adding hydrogen, which would cost a large amount of computational expense. Therefore UA is widely utilized in the simulations of PE. Rutledge et al. [38–41] studied plastic deformation of the stack of alternating crystal and amorphous layers typical of semi-crystalline PE. Plastic deformation was accompanied by melting and recrystallization at low strain rate. Meanwhile, at high strain rate, yield mechanism apparently occurred with cavitation in the inter-lamellar domain. Tschopp et al. [37] and Rabczuk et al. [42] employed MD simulation to study deformation mechanisms during uniaxial tensile deformation of an amorphous PE polymer. They investigated the influence of chain lengths, number of chains, strain rates and temperatures on mechanical properties of PE polymer. The energy contributions were calculated to help elucidate the inherent deformation mechanisms. The results showed that the elastic and yield regions were mainly dominated by inter-chain non-bonded interactions whereas strain hardening regions were mainly dominated by intra-chain dihedral motion of PE. Jiang et al. [43] established a MD model to simulate the uniaxial deformation of PE and revealed the relationship between strain rate and microstructure evolution at different temperatures. Conformational parameters such as the bond length, bond angle, and radius of gyration were measured quantitatively. Choi et al. [44] studied the conformation and dynamics of precisely branched PE using MD simulation, including PE molecules containing regularly spaced, short chain branches along its linear backbone. Sahputra and Echtermeyer [45] investigated fatigue of amorphous PE under low strain using the UA approach based on MD simulation. They concluded that cyclic loading changed the total potential energies of the system, especially the van der Waals potential. There are plenty of literature dedicated to the mechanical properties of PE, which shows that the UA is an efficient technique to simulate the mechanical behaviors of PE.

In this paper, emphasis is focused on the mechanical behaviors and molecular deformation mechanisms of amorphous PE under high speed shock compression via MD simulation. The organization of this paper is as follows. First, the periodic model is established and simulation details are presented. Next, the shock wave propagations are presented with different shock loads. Afterward, Hugoniot curves in  $u_s$ - $u_p$  are and  $P$ - $u_p$  presented. In the end, the molecular morphological evolution is analyzed by statistical method.

## 2. Models and simulation

### 2.1. Interatomic force field

In order to enhance computational efficiency, the UA approach is adopted to model the PE system, in which each group of  $-\text{CH}_2$ -monomer is considered as a single monomer particle. The interatomic force field is described by the Dreiding potential [46]. The Dreiding potential consists of four contributing terms, which are used to characterize bond stretching, chain bending, chain rotation and van der Waals non-bonded interactions, respectively. The total force field energy can be expressed as

$$E = E_b(r) + E_a(\theta) + E_d(\phi) + E_n(r), \quad (1)$$

where the subscripts  $b$ ,  $a$ ,  $d$ ,  $n$  mean bond, angle, dihedral angle and non-bonded interactions, respectively. Each term can be written as

$$E_b(r) = K_b(r - r_0)^2 \quad (2)$$

$$E_a(\theta) = K_\theta(\theta - \theta_0)^2 \quad (3)$$

$$E_d(\phi) = \sum_{i=0}^3 K_i(\cos \phi)^i \quad (4)$$

$$E_n(r) = 4\varepsilon \left[ (\sigma/r)^{12} - (\sigma/r)^6 \right], r \leq r_c \quad (5)$$

where  $K_b = 175$  kcal/mol and  $K_\theta = 30$  kcal/mol/rad<sup>2</sup> are the stiffness constants for the bond length and bond angle potentials, respectively.  $r_0 = 1.53$  Å and  $\theta_0 = 109.5^\circ$  are the equilibrium bond length and bond angle, respectively. The variable  $K_i$  contains the coefficients of dihedral multi-harmonic ( $K_0 = 1.736$  kcal/mol,  $K_1 = -4.49$  kcal/mol,  $K_2 = 0.776$  kcal/mol,  $K_3 = 6.99$  kcal/mol). The non-bonded or Van der Waals interactions are described with a Lennard-Jones potential (Eq. (5)), where  $r$  is the distance between two atoms,  $\sigma$  is the distance at zero energy, and  $\varepsilon$  is the energy well depth. The cutoff distance  $r_c$  is taken as 10 Å. The values for all of the constants used in the inter-atomic potential are given by Jacob et al. [47] and Rutledge et al. [48].

### 2.2. Initial configuration

The initial configuration of amorphous PE is generated a Monte Carlo self-avoiding random walk algorithm [49], as shown in Fig. 1(a). A face-centered cubic (FCC) lattice superimposed on the specified cell with the nearest neighbor distance of 1.53 Å is used to generate a molecular chain. Molecular chains are put into the lattice in a probabilistic stepwise manner, which based the probability of chain growth in certain directions on the bond angle and the density of unoccupied sites. In order to eliminate the “end effect” and save the computational expense, the simulations are performed with periodic boundary conditions in  $x$  and  $y$  directions. The simulated system consists of 40 chains and each chain consists

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