



A reactive molecular dynamics simulation study to the disintegration of PVDF and its composite under the impact of a single silicon-oxygen cluster

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ABSTRACT

With the applications of polymers and their composites in aerospace industries becoming more and more common, it is of great significance to investigate their ultrahigh-speed particle erosion behaviors. Taking poly (vinylidene fluoride) (PVDF) and its composites containing polyhedral oligomeric silsesquioxanes compound (3,3,3-trifluoropropyl)₈Si₈O₁₂ (FP-POSS) as the research objectives, this paper analyzed the failure process under the impact of a single silicon-oxygen cluster using reactive molecular dynamics simulations. Firstly, in terms of erosion surface morphologies and erosion rates, the influence of FP-POSS on the erosion resistance of PVDF matrix was analyzed. The results indicated that the erosion resistance of neat PVDF is poor, but the addition of FP-POSS can significantly enhance its erosion resistance performance and reduce its impact crater size and erosion rate. Then in order to understand these results, the movement and fracture processes of molecular chains in neat PVDF were investigated. The effect of constraints on the movement of molecular chains was analyzed, and two stages during the chain fracture process derived respectively from the cluster impact and the thermal degradation were also obtained. Finally, by calculating the gyration radii of molecular chains and the strain field distributions, the influence and the inner mechanism of FP-POSS on the erosion resistance of PVDF were further analyzed.

1. Introduction

In space, the influence of ultrahigh-speed cosmic dust particles and atomic clusters on a spacecraft cannot be ignored. In 2002–2004, the international space station (ISS) detected the existence of cosmic dust smaller than 10 nm [1]. Cassini-Huygens Cosmic Dust Analyzer (CDA) also detected the particle which velocity is more than 200 km/s and diameter is smaller than 10 nm [2]. If the intelligent structural materials in a spacecraft were subject to ultrahigh-speed dust or dusty plasma erosion, the normal physical and mechanical properties of the materials will change, which will then deteriorate the spacecraft operation performance, accuracy and service life.

Many studies using molecular dynamics (MD) simulations to model the particle-surface interaction have begun since 1960s [3]. As the computing performance develops, these studies are focused on not only the properties of inorganic materials [4–9], such as erosion yield, crater size, surface morphology, phase transition, plastic deformation, nucleation and initiation of micro-cracks and so on, but also those of polymers and organic molecular solids [10–12]. At present, many

research articles about kiloelectronvolt (keV) particle impact have been published. Delcorte et al. [10,13–15] studied the mechanisms of energy transfer and material sputtering of polyethylene induced by keV projectiles using MD simulations. Smiley et al. [16] simulated the bombardment of benzene molecular solid by a series of 5-keV carbon projectiles from C₆H₆ to C₁₈₀. In order to enable chemical reactions, Garrison et al. [17] performed the similar simulations using the AIREBO potential and obtained the amount of energy going into reactions, and the number of free and reacted H atoms. Some other articles have studied the atomic oxygen (AO) erosion using the ReaxFF force field. Rahnamoun et al. [18] studied the effects of AO impact on different materials and verified that adding silicon to Kapton can enhance the stability of the Kapton against AO impact. Rahmani et al. [19] showed that the mass loss, erosion yield, surface damage, AO penetration depth, and temperature evolution are lower for the polyimide (PI) systems with randomly oriented carbon nanotubes (CNTs) and graphene (Gr) or PI-grafted polyhedral oligomeric silsesquioxane (POSS) compared to those of the pristine POSS or aligned CNT and Gr systems at the same nanoparticle concentration. However, the impact mechanisms between

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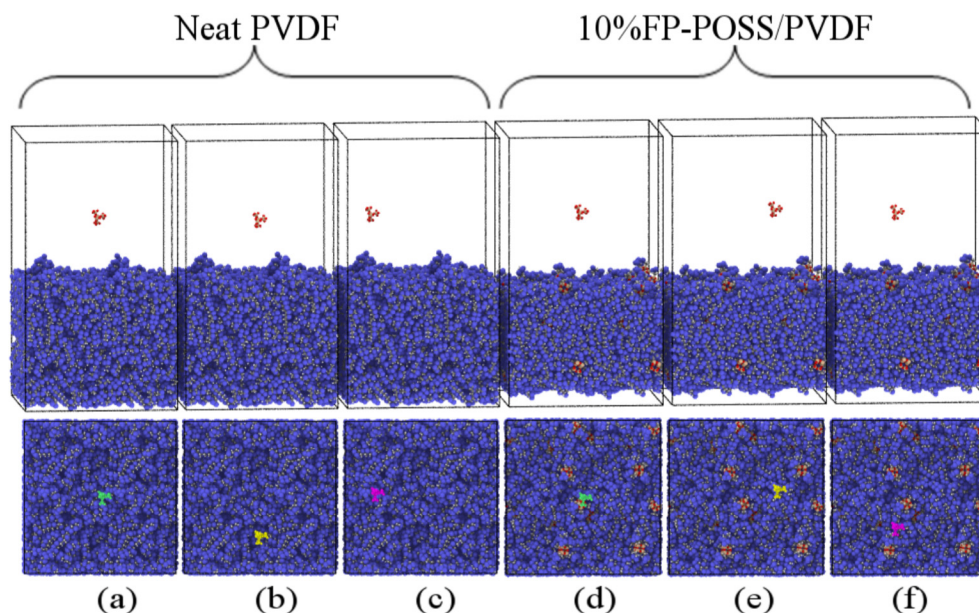


Fig. 1. Total six erosion models for neat PVDF and 10%FP-POSS/PVDF. Upper: the side view, lower: the top view. For each model, the clusters are respectively located at different locations and colored differently (green, yellow and pink).

cluster projectiles and polymers haven't been completely explained, especially on the basis of the movement and fracture of molecular chains. It is commonly believed that when the kinetic energy of an incident particle is greater than the threshold energy E_{th} of the substrate material [20], the particle will destroy the surface, otherwise, will deposit or reflect. In other words, by controlling the incident cluster kinetic energy, the cluster-surface interaction can change from soft landing toward implantation [9]. This paper aims at analyzing the failure mechanism of poly(vinylidene fluoride) (PVDF) under ultrahigh-speed cluster erosion and the effect of polyhedral oligomeric silsesquioxanes compound (3,3,3-trifluoropropyl) $_8$ Si $_8$ O $_{12}$ (FP-POSS) on PVDF erosion resistance. Since the composition of cosmic dust is related to the space environment and silicates are the most common minerals in the solar system [21], the Si $_5$ O $_{16}$ cluster is selected as an incident particle. The cluster velocity is assumed to be 20 km/s (823 eV), which is the common cosmic dust velocity and is much greater than the PVDF threshold energy E_{th} .

In our previous work, several properties of binary mixtures of PVDF and POSS compounds have been researched by using MD simulations, such as miscibility, morphology, crystallization, piezoelectricity, mechanical properties and erosion effects of AOs [22–27]. PVDF is prone to be eroded by AOs, but with the incorporation of POSS, the atomic oxygen resistance of PVDF can be effectively improved [27]. Since the erosion effect of clusters cannot be explained by the summation of individual atoms, which is termed as 'nonlinear effect' [28], and the cluster has the properties intermediate between those of individual atoms and bulk material, the study of the cluster erosion is significant.

In this work, firstly the substrates of neat PVDF and 10%FP-POSS/PVDF (mass ratio of FP-POSS is 10%) were constructed, which could be considered as nano-films or coatings. These substrates were eroded once because there was only a single cluster to impact in the periodic boundary condition. Then the erosion results for the two materials were analyzed, and their crater sizes and erosion rates were compared. Finally, by analyzing the movement and fracture behaviors of PVDF molecular chains and the effects of FP-POSS on PVDF, the mechanisms of the erosion results were presented.

2. Simulation methodology

2.1. ReaxFF force field

By numerically solving the Hamilton's equations of motion, molecular dynamics (MD) simulations can calculate the motion parameters of atoms or molecules, such as force, position, velocity and acceleration. In order to simulate the bond cleavage and formation in a molecular system, the ReaxFF force field was used. This force field, proposed by van Duin and coworkers [29–33], can describe the reactions and meet the requirements of large molecular systems. It tends to be faster than Quantum Mechanics (QM) based methods and helps to bridge the gap in simulation scale separating QM and classical methods. It defines the relationships between bond lengths and bond orders, as well as bond energies and bond orders. Generally, it consists of nonbonded terms, covalent terms and specific terms. The nonbonded terms include van der Waals energy (E_{vdW}), and Coulombic energy (E_{Coul}). The covalent terms include bond energy (E_{bond}), overcoordination energy (E_{over}), valence angle energy (E_{angle}) and torsion angle energy (E_{tors}). For the specific terms ($E_{specific}$), different versions of the ReaxFF force field can have different contents, depending on the research systems. That is,

$$E_{system} = E_{bond} + E_{over} + E_{angle} + E_{tors} + E_{vdW} + E_{Coul} + E_{specific}$$

In this work, the 2008 version of the ReaxFF force field [33] was adopted, which is also used in LAMMPS software [34,35]. Its simulation parameters are the same as those in Ref. [27]. The specific terms in the version include lone pair energy (E_{lp}), undercoordination energy (E_{under}), penalty for 'allene'-type molecules (E_{pen}), angle conjugation (E_{coa}), C2 correction (E_{C2}), triple bond energy correction (E_{triple}), torsion conjugation (E_{conj}) and hydrogen bond (E_H). That is,

$$E_{specific} = E_{lp} + E_{under} + E_{pen} + E_{coa} + E_{C2} + E_{triple} + E_{conj} + E_H$$

2.2. Simulation models

In order to study the failure mechanism of PVDF and its composites containing FP-POSS under Si $_5$ O $_{16}$ cluster erosion, a total of six erosion models were constructed, as shown in Fig. 1. They were respectively formed by two types of polymer substrates (neat PVDF and 10%FP-POSS/PVDF) and three Si $_5$ O $_{16}$ clusters at different initial locations. For

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