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UNIVERSALITY CLASS OF THE FRAGMENTATION OF PLASTIC MATERIALS

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Abstract. We carry out an experimental and theoretical study of the fragmentation of polymeric materials by impacting polypropylene (PP) particles of spherical shape against a hard wall. Our experiments revealed that the mass distribution of fragments has a power law behavior with an exponent close to 1.2, which is significantly different from the known exponents of three-dimensional bulk materials. To understand the fragmentation of plastic materials we developed a three-dimensional discrete element model where the sample is represented as a random packing of spherical particles connected by elastic beams. The model reproduces both the large permanent deformation of the polymer during impact, and the novel value of the mass distribution exponent. Computer simulations revealed that the dominance of shear in the crack formation and the healing of compressed crack surfaces are the key features which give rise to the emergence of the novel universality class of fragmentation phenomena.

1 INTRODUCTION

Fragmentation of heterogeneous materials is a very complex scientific problem with an enormous technological importance [1, 2]. From the usage of explosives in mining through the comminution of minerals to the liberation of grains in particle composites fragmentation processes play a crucial role which calls for a thorough understanding. During the last decade research efforts have been concentrated on the breakup of heterogeneous brittle materials which is by now fairly understood [1, 2, 3, 4, 5, 6, 7, 8]. Experimental and theoretical investigations have revealed that the energy imparted to the solid has to surpass a threshold value (critical energy) to achieve complete breakup [4, 5, 6]. In this fragmented state the mass (size) distribution of pieces follows a power law functional form with universal exponent depending mainly on the effective dimensionality of the system [1, 3, 4, 5, 6, 7, 8]. The branching-merging scenario of dynamically propagating cracks provided a qualitative physical picture underlying the universality [1].

Industrial processes require also the fragmentation of polymeric materials which exhibit ductile fracture. For polymers a complex deformation state may arise before breakup which leads to a more complicated crack initiation and propagation compared to brittle materials. In spite of its industrial relevance and scientific importance, the breakup of polymeric materials is still poorly understood. In the present project we carried out a detailed experimental and theoretical investigation of the impact fragmentation of polymers which revealed a broad spectrum of novel features. Our experiments showed that the mass distribution of plastic fragments exhibits a power law behavior with an exponent close to 1.2, which is substantially different from the one of bulk brittle materials in three-dimensions [9]. In order to understand the physical origin of the low exponent, a three-dimensional discrete element model is developed where the sample is discretized in terms of spherical particles connected by elastic beams. To capture the fracture mechanisms of plastic materials, in the model broken particle contacts are able to reconnect when compressed against each other leading eventually to the healing of cracks. Computer simulations revealed that the healing mechanism together with the dominance of shear stresses in the crack formation are responsible for the emergence of the novel universality class of fragmentation phenomena [9].

2 EXPERIMENTS

In the fragmentation experiments we used spherical particles made of polypropylene as a test material. The most important physical properties of PP are summarized in Table 1. Mechanical properties of PP can easily be controlled by the temperature, providing excellent possibilities to test the effect of mechanical properties on fragmentation processes.

Table 1: Physical properties of polypropylene used in the experiments.

Young modulus	1300	MPa
Glass transition temperature	-10	^oC
Melting point	160	^oC
Density	0.9	g/cm^3

For the purpose of the experiments a single particle comminution device was constructed which accelerates particles one-by-one by the centrifugal force in a rotor up to the desired velocity. The rotor ensures that the particles hit the hard wall at a rectangular angle in an evacuated environment eliminating the disturbing effect of inclined impact and of turbulent air flow. Experiments were carried out using Spherical PP particles of diameter $d = 5$ mm which were impacted at different impact velocities v_0 in the range 30 m/s-180

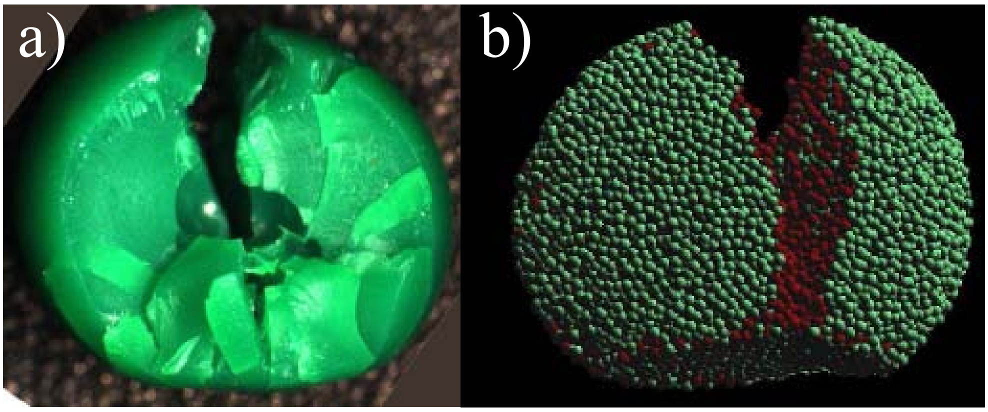

Figure 1: Final states of the impact process at low impact velocities in the experiment (a) and in the simulation (b). Large permanent deformation occurs in the contact area with the hard wall due to compression, while above it vertical cracks are formed due to tensile stresses. In this velocity range the specimen gets damaged but it does not fragment. The simulations are in very good agreement with the measurements.

m/s. Figure 1(a) demonstrates that at low enough velocities, the collision does not result in a breakup, instead the particles suffer a large plastic deformation at the impact site. Above the completely flattened contact zone meridional cracks form due to tensile stresses, however, the particle does not fragment. Most of the energy of the system is dissipated by plastic deformation of the particle. To obtain fragmentation the impact velocity v_0 has to exceed a material dependent critical value v_c, which is about 60m/s for our PP particles. For each impact velocity 400 particles were fragmented collecting the fragments in the grinding chamber of the machine. In the data analysis, $99 - 99.5\%$ of the total mass of the samples was recovered. In order to evaluate the mass distribution of the fragments, we scanned the pieces with an open scanner obtaining digital images where fragments appear as white spots on the black background [7, 8] as it is illustrated in the inset of Fig. 2(a). Based on this technique the identification of fragments is reduced to searching of clusters of white pixels. We determined the two-dimensional projected area w of fragments as the number of pixels of the clusters, from which the mass m of fragments can be estimated as $m \sim w^{3/2}$ since the three-dimensional fragment shape is close to isotropic. We carefully checked the shape isotropy by calculating the ratio of the two eigen values of the moment of inertia matrix of the projected area which always falls between 1 and 2.

Fig. 2 presents the mass distribution $F(m)$ of fragments obtained at three different impact velocities. The inset shows an example of scanned fragments for the highest impact velocity. Note that due to the large number of fragments, the full experiment is composed of 4 such pictures comprising approximately 20000 pieces. It can be observed in Fig. 2 that at lower impact velocities a hump appears on the distribution function $F(m)$ at the largest fragments which then gradually disappears as v_0 increases. The state of complete breakup is reached at the highest impact velocity $v_0 = 75$ m/s where the cutoff

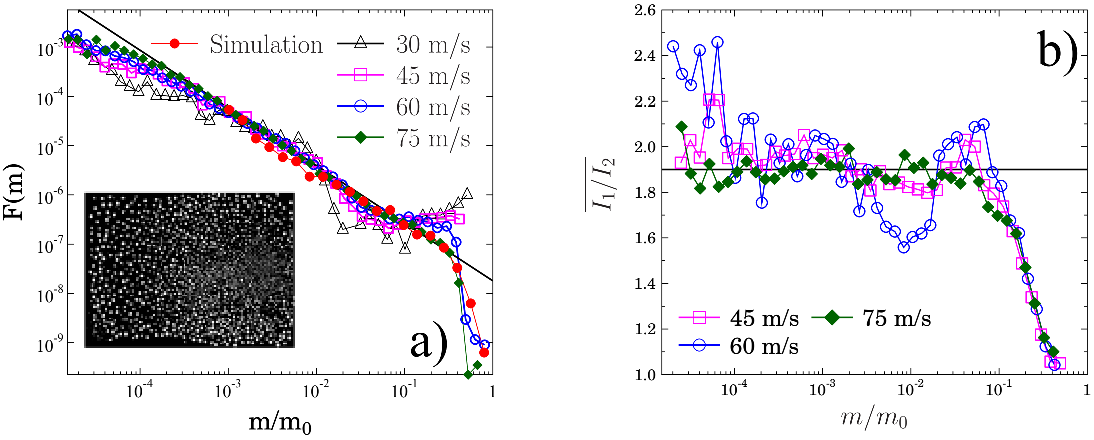

Figure 2: (a) Mass distribution of fragments obtained from experiments at four different impact velocities. m_0 denotes the average mass of PP spheres. At the highest impact velocity $v_0 = 75$ m/s, $F(m)$ shows a power law behavior over 3 orders of magnitude followed by an exponential cutoff for the very large pieces. Simulation results obtained with the parameters $\Theta_{th} = 1$ and $t_h = 0$ are in a very good agreement with the experimental findings. Inset: an example of scanned images of fragments for $v_0 = 75$ m/s. (b) The shape parameter of fragments determined from the scanned images. For most of the fragments the value of $\sqrt{I_1/I_2}$ falls close to 1.9 which implies a high degree of isotropy of fragment shapes.

of the distribution becomes exponential and in the regime of small fragments a power law emerges

$$F(m) \sim m^{-\tau_{pl}} \tag{1}$$

over more than 3 orders of magnitude. It has to emphasized that the exponent $\tau_{pl} = 1.2 \pm 0.06$ is significantly lower than the values $\tau_{br} \approx 1.8-2.1$ obtained in the fragmentation of three-dimensional bulk objects made of disordered brittle materials [1, 2, 3, 4, 5]. The unique value of the exponent demonstrates that the breakup of plastic materials cannot be captured by the usual theoretical approaches.

3 DISCRETE ELEMENT MODEL

In order to obtain a detailed understanding of the physical mechanisms of the fragmentation of plastic materials, we used a Discrete Element Model (DEM) to simulate the fragmentation of a polymeric particles of spherical shape when they impact a hard wall. In the framework of the model the spherical sample is represented as a random packing of polydisperse spheres with a size distribution. Based on the initial particle positions a Delaunay triangulation is carried out in 3D which is used to determine the cohesive interaction of particles: the particles are connected by beam elements along the edges of the Delaunay triangulation such that not only those particles are connected which are initially in contact. The model construction is illustrated in Fig. 3(a) where the packing of spheres and the connecting beam elements can nicely be observed. In the simulations the particles were composed of $N \sim 24000$ spheres.

In three-dimensional space the deformation of a beam is calculated by the superposition of elongation, torsion, as well as bending and shearing in two different planes [10]. In order to capture crucial aspects of the deformation behavior and the fracture of plastic materials, our DEM model has two novel types of components, i.e. the form of the breaking criterion of the beam elements and the reactivation of broken contacts under compression. Crack formation is implemented in the model such that the beams break when they get overstressed according to a physical breaking rule [9, 11]

$$\frac{\varepsilon|\varepsilon|}{\varepsilon_{th}^2} + \frac{\max(|\theta_i|, |\theta_j|)}{\theta_{th}} \geq 1. \tag{2}$$

In the breaking criterion ε denotes the longitudinal strain, furthermore, Θ_i and Θ_j are the generalized bending angles at the two beam ends [10]. Breaking of a beam can be induced by stretching and bending, the two terms of Eq. (2) characterize the contributions of the two failure modes.

Simulations showed that the local shear of the particle contacts provides the main contribution to the bending angles θ_i, θ_j, so that bending dominated beam breaking in Eq. (2) characterizes crack formation due to shear. Varying the values of the breaking thresholds ε_{th} and θ_{th}, the relative importance of stretching and bending can be controlled: increasing the value of a breaking parameter, the effect of the corresponding failure mode diminishes. The extreme case of tension (stretching) dominance is achieved when $\varepsilon/\varepsilon_{th} \ll \theta/\theta_{th}$, while the opposite case is the dominance of bending deformation in local failure events. An important feature of the breaking criterion is that in Eq. (2) the deformation ε is not restricted to positive values. Since the first term of Eq. (2) becomes negative when the beam is compressed, failure is dominated by the bending/shear mode in such a way that increasing compression increases the shear resistance of the beam. This scenario typically occurs for compressed contacts $\varepsilon < 0$ in the impact zone.

In order to represent the plastic behavior of the material in the framework of our DEM, we assume that the beams have a linearly elastic behavior up to fracture, but, whenever two particles are pressed against one-another for time longer than t_h, a new, undeformed beam is inserted between them. This mechanism has the consequence that during the impact process, the particle contacts may undergo a sequence of breaking-healing events which leads to plastic energy dissipation and to the appearance of permanent deformation. Varying the healing time t_h the mechanical response of the model material can be controlled: $t_h = 0$ corresponds to the case of perfect shear plasticity, while $t_h \to \infty$ implies no healing at all, i.e. brittle behavior.

4 COMPUTER SIMULATIONS

We carried out computer simulations of the impact process varying the impact velocity, the breaking parameters of beams, and the healing time over a broad range. Simulations

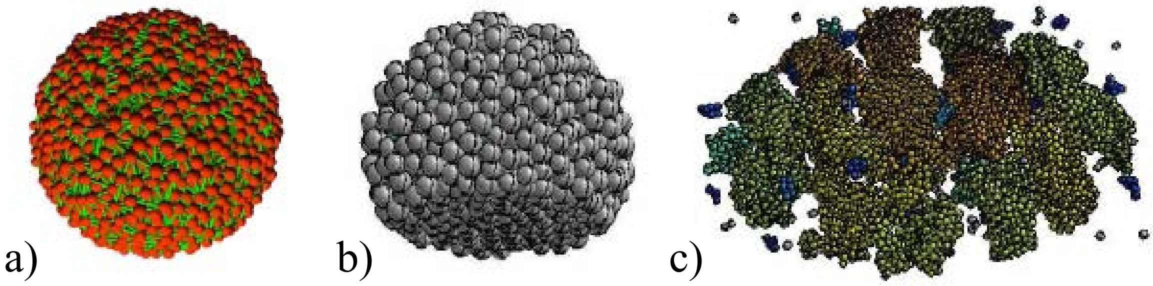

Figure 3: (a) In the framework of DEM the spherical sample is represented as a random packing of spheres which are connected by beam elements along the edges of a Delaunay triangulation in three dimensions. (b) At low enough impact velocities the samples suffers large permanent deformation but it does break. (c) Fragmentation is achieved when the impact velocity v_0 exceeds the critical velocity $v_0 > v_c$. In this regime the sample breaks into a large number of pieces. The simulation results are in a good quality agreement with the experimental findings.

were stopped when the system reached a relaxed state, i.e. when no beam breaking occurred during 1000 consecutive time steps. We control the effect of local failure modes of beams on the fragmentation process by setting the stretching threshold to a fixed value $\varepsilon_{th} = 0.02$ and we vary the bending threshold within a broad range $1.0 \leq \theta_{th} \leq 200$. In this way $\theta_{th} = 200$ implies total tension dominance, while $\theta_{th} = 1.0$ means total bending dominance, and intermediate θ_{th} values interpolate between the two limits.

In Fig. 3(b) and (c) final states of computer simulations are shown at a low and at a high impact velocity. At very low impact velocity the ball does not suffer any apparent damage, most of the impact energy is dissipated by the large permanent deformation at the impact site (Fig. 3(b)). In the limit of high impact velocity complete breakup occurs, the specimen falls apart into a large number of fragments (Fig. 3(c)). Figure 1 presents the comparison of the final state of a low-velocity impact simulation to the experimental finding. It can be observed that the model is able to reproduce both the deformation state and the crack structure of PP, with the parameter values where the beam breaking is dominated by bending $\varepsilon_{th} = 0.02$, $\Theta_{th} = 1.0$, furthermore, compressed contacts easily heal $t_h = 0$. It is interesting to note that the large permanent deformation of the ball in Fig. 1(b) is caused by the breaking-healing sequences of particle contacts. Above this zone tensile stresses arise resulting in opening cracks along the impact direction in agreement with the experiments [9].

Examples of the mass distribution of fragments are presented in Fig. 4 for two limiting parameter sets. In our model heterogeneous brittle materials are realized by the parameter values $\Theta_{th} = 200$, $t_h = \infty$ for which a power law mass distribution is obtained with the usual exponent $\tau_{br} = 1.9 \pm 0.1$ [10]. Computer simulations showed that decreasing the healing time $t_h \to 0$ in the tension limit $\Theta_{th} = 200$ practically does not affect the fragmentation process because fragments are only generated by opening cracks which do

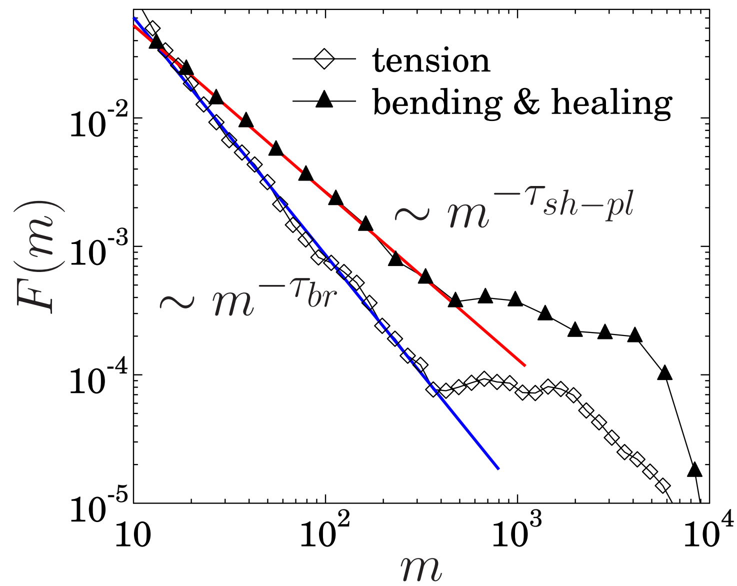

Figure 4: Mass distribution of fragments for two limiting cases of the parameter sets. In the regime of small fragment masses power law distributions are obtained, however, the value of the exponent depends on the dominating cracking mechanism. For tension dominated breakup the exponent $\tau_{br} = 1.9$ is obtained in agreement with the literature, however, for shear dominated breaking in the presence of plasticity a significantly lower exponent $\tau_{sh-pl} = 1.25$ emerges.

not let healing play a role. However, the breakup process substantially changes when shear dominates the crack formation $\Theta_{th} = 1$. At the same time increasing the strength of plasticity $t_h \to 0$ cracks formed at compressed contacts under shear can heal which then results in the merging of fragments. This mechanism has the consequence that the relative frequency of large pieces decreases leading to a faster decay of the distribution with a larger τ. The exponent $\tau_{pl-sh} = 1.25 \pm 0.06$ presented in Fig. 4 is obtained in the plastic limit $t_h = 0$ together with $\Theta_{th} = 1.0$. The results of computer simulations are compared to the measured mass distribution of PP in Fig. 2. A very nice quantitative agreement can be seen which demonstrates that the shear dominated cracking together with the healing mechanism of compressed crack surfaces are responsible for the unique fragmentation of plastic materials. Our simulations indicate that the exponent τ_{pl-sh} is universal, i.e. it does not depend on details of the plastic mechanism or on the materials' micro-structure characterizing a novel universality class of fragmentation phenomena [9].

Since particle contacts are sheared in the compressed zone in the vicinity of the impact site, a large fraction of the imparted energy is dissipated by the formation of small sized fragments and by the plastic deformation. Hence, the shock wave generated by the impact leaves the destroyed zone with a low amplitude which hinders the expansion of the body and the appearance of meridional crack planes typical for the breakup of brittle spheres [10]. Due to the characteristic feature of low shear resistance, we find that the fragmentation of plastic shows similarities to the breakup of liquid droplets colliding with a hard wall. It can be observed in Fig. 3(c) that in the plastic-shear case the fragments escape laterally after impact indicating the "splash" of the entire body similar to liquid droplets [12, 13].

5 CONCLUSIONS

We carried out a detailed experimental and theoretical study of the fragmentation of plastic materials. In the experiments PP particles of spherical shape were impacted against a hard wall. In order to obtain a theoretical understanding of the emerging breakup process a Discrete Element Model was introduced which captured the main mechanisms relevant for fragmenting plastic. Our experimental and theoretical study revealed that the breakup of plastic materials falls into a novel universality class of fragmentation phenomena characterized by a unique value of the mass distribution exponent. Based on DEM simulations we showed that the plastic behavior of the material together with the dominance of shear in crack formation are responsible for the behavior substantially different from brittle fragmentation. It was found that the low shear resistance of the material results in a splashing mechanism similar to the breakup of liquid droplets.

Beyond the industrial importance of the fragmentation of polymeric materials, our results might be applied to obtain a deeper understanding of the fragmentation of highly viscous magma during pyroclastic activity at volcanic eruption [14, 15]. For theoretical investigations our results demonstrate that the breakup of solids cannot be understood as a generic stochastic process since the precise mechanism of crack initiation and growth, i.e. the dominance of tensile or shear stresses govern the process of fragmentation. Further investigations are in progress to determine the value of the critical exponents of the plastic fragmentation universality class.

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