Universality in Fragmentation

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Fragmentation of a two-dimensional brittle solid by impact and "explosion," and a fluid by "explosion" are all shown to become critical. The critical points appear at a nonzero impact velocity, and at infinite explosion duration, respectively. Within the critical regimes, the fragment-size distributions satisfy a scaling form qualitatively similar to that of the cluster-size distribution of percolation, but they belong to another universality class. Energy balance arguments give a correlation length exponent that is exactly one-half of its percolation value. A single crack dominates fragmentation in the slow-fracture limit, as expected.

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Mechanical fragmentation of brittle solids is a complicated irreversible and nonlinear problem that has concerned scientists for a long time. Fragmentation can be divided into two classes: continuous and instantaneous fragmentation. In this Letter, we are dealing with only the latter. Instantaneous fragmentation encompasses rapid events such as explosions and collisions. Physical processes in this class of events are abundant in nature. On a very large scale there are fragmentation processes like the formation of asteroids. Industrial fragmentation processes can be found on intermediate scales, and on the microscopic scale one can encounter processes such as fragmentation of atomic nuclei. All these processes have attracted scientific interest for a considerable time.

Based on statistical arguments, two plausible forms for the fragment-size distribution in instantaneous fragmentation were initially proposed [1,2]: one assuming fragmentation to be a Poissonian process, which results in an exponential distribution of the fragment diameter (or of the square root of the mass in 2D) [1–3], and the other arising from maximization of the number of ways fragmentation can occur (maximum entropy), which gives an exponential distribution of the fragment mass [2].

A wide variety of experiments and simulations of instantaneous fracture revealed, however, a distribution which is a power law in the small-size range followed by a large-size residual, or a crossover to a more or less exponential decay in the large-size limit [1,3–8]. This lead to the suggestion by Oddershede *et al.* [5] that impact fragmentation displays self-organized criticality. Since scaling appeared in their experiments up to a size range close to the size of the smallest dimension of the objects crushed in the experiments, they suggested that the exponential large-size decay is a finite-size effect.

In contrast to the latter suggestion, it has recently been shown [3,6] for numerical models that in impact fragmentation the crossover mass and the large-size residual depend on the impact energy, which indicates they are not finite-size effects but inherent parts of the size distribution, as also suggested by the statistical arguments.

As an alternative resolution to the problem, it has very recently been suggested that in fragmentation, criticality appears at a single nonzero value of the impact energy [6]. This seems to be the case for low-energy collisions of objects as demonstrated by Kun and Herrmann [6].

To resolve the true nature of the possible criticality of fragmentation processes and to rule between the competing pictures, it is therefore important to analyze in detail instantaneous fragmentation. To this end we consider in this Letter two completely different physical systems, a disordered 2D lattice of elastic beams, which can be used to model granular materials [3], and a 2D Lennard-Jones (LJ) liquid. The disordered lattice of beams is fragmented by a rapid impact and by applying an isotropic velocity gradient that models an explosion. The latter mechanism is also applied to "fragment" the LJ liquid. We will demonstrate that the impact fragmentation of the disordered lattice of beams becomes critical at a nonzero impact energy at which point the fragment-size distribution becomes a pure power law. Away from this critical energy the size distribution satisfies a scaling form such that the scaling function is very similar to that of percolation clusters below the percolation threshold [9]. The explosive fragmentation of the disordered lattice of beams and the LJ liquid both become critical only in the limit of zero expansion velocity. Also in these cases the fragment-size distributions seem to satisfy the same scaling form. For the LJ liquid we did not, however, reach the true equilibrium distribution. Despite the similar scaling, in fragmentation the correlation length exponent and the Fisher exponent are not those of percolation. Both fragmentation processes seem, however, to have the same exponents, and the correlation length exponent can be understood by an energy-balance argument.

As described above, we use in this Letter two numerical models: (I) a 2D fluid described by molecular-dynamics simulation of atoms interacting via a LJ pair potential [10, 11], and (II) a randomly distorted square lattice of breakable elastic beams [3]. In model I, N particles under periodic boundary conditions are equilibrated in the liquid state (at a supercritical temperature and triple-point density)

before time $t = 0$. To model an explosion, at $t = 0$, a constant, isotropic, expanding velocity gradient is applied to all particles, with periodic boundaries moving at constant velocity. The simulation stops only well after distinct clusters of particles (i.e., fragments) have formed and are expanding in a quasisteady (ballistic) manner. In model II, we use a square lattice whose bonds have the elastic properties of beams with a square cross section w^2, Young's modulus E, and length l. Masses m are located on the lattice sites, and the entire lattice is at static equilibrium at $t = 0$. Periodic boundary conditions are applied in the vertical direction, and two alternative boundary conditions are used for the horizontal direction: (1) To model an explosion a constant, uniaxial, expanding velocity gradient is applied to all masses at $t = 0$, and the sites at the left and the right boundaries are forced to move with a constant velocity. (2) To model an impact a displacement $A \sin^2 \omega t$ is applied to the left-boundary masses, over the time duration of $0 \leq t \leq \pi/\omega$. For numerical reasons we do not take into account collisions between fragments. This would be quite a serious omission for example in simulating two colliding objects. If the experimental setup instead leads to a fragmentation pulse propagating in a horizontal thin plate, and fragments can fall down freely, it would be more realistic. If the impact appears as an expansion wave instead of compression, this assumption does not pose any problem. In a qualitative study of universality in fragmentation, we thus find that neglecting collisions between fragments is a reasonable approximation. Furthermore, in a related recent study [6] where collisions between fragments were included, indication of a critical impact energy was also found.

Before discussing the results of the simulations, we present an energy-balance argument [10–12], showing how the typical fragment mass at the initial moments of fragmentation should change as a function of loading. At $t = 0$, a region that will ultimately become a fragment is given expansion energy, related to the homogeneously applied (explosion) velocity of strain increase η. As the fragment and its immediate surroundings expand, the local elastic energy per unit mass increases with the square of the strain. At the critical moment of fragmentation, given by the time of sound traversal across the fragment L/c (with L the diameter of the fragment), free surface opens up around the fragment. In this process the loading energy is balanced by the energy required to form the surface [10–12]. The elastic strain is proportional to $L\eta$. Regardless of dimensionality, the surface energy per unit mass is proportional to $1/L$. Thus, at the moment of fragmentation, when the elastic loading and surface energies are equal, the fragment diameter L is proportional to $\eta^{-2/3}$. The typical fragment mass M_0 is then, in d dimensions, expected to scale as

$$M_0 \propto L^d \propto \eta^{-2d/3}, \tag{1}$$

at the beginning of fragmentation. Excessive elastic energy will later in the process break the large fragments into smaller pieces (with the excessive elastic energy we mean the elastic energy stored in the fragments which is not being dissipated at the formation of the first fragment surfaces). Since fragments can only become smaller, we expect that Eq. (1) also determines the scaling of the large-size limit of the final fragment-size distribution.

If fragmentation really becomes critical, then Eq. (1) determines the *only* length scale in the system. Since the fragments are simple two-dimensional objects (Fig. 1) and not fractals as, e.g., in percolation, the correlation length should scale in two dimensions as $\sqrt{M_0} \propto \eta^{-2/3}$. The exponent $2/3$ is exactly one-half of the correlation length exponent of percolation. One should also expect that within the critical regime the fragment-size distribution satisfies a scaling form. As in percolation we try to express the fragment-size distribution $n(m)$ as

$$n(m) \propto m^{-(\alpha+1)} f(m/M_0), \tag{2}$$

where f is a scaling function.

This form for the fragment-size distribution is also supported by experimental observations. There are two recent investigations of brittle fragmentation [5,8], where the cumulative fragment-size distributions $[N(m) = \int_m^\infty n(m')\, dm']$ were fitted by the empirical form

$$N(m) \propto m^{-\alpha} \exp(-m/M_0), \tag{3}$$

with α and M_0 the fitting parameters. Equations (2) and (3) are equivalent if $f(z) = (\alpha + z)\exp(-z)$. Notice that this form for $f(z)$ assumes the cumulative distribution Eq. (3) to be exact. As it turns out below, we can only deduce that $f(z)$ approaches a constant for $z \to 0$ and that it approaches an exponential decay for $z \to \infty$. This is [9] also the behavior of the scaling function of the cluster-size distribution in percolation.

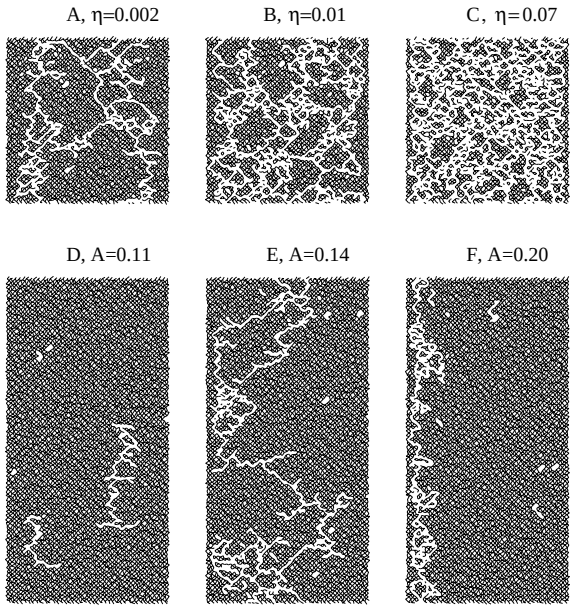

FIG. 1. Fragment patterns for model II: (A–C) uniaxial, homogeneous expansion (explosion), and (D–F) high-speed impact.

A set of simulation results for model II is shown in Fig. 1. For explosive expansion (Figs. 1A–1C), the fragments are distributed evenly over the entire system, regardless of η. The typical size of the fragments increases visibly when η is decreased, and indeed seems to diverge when η approaches zero in the way predicted by Eq. (1). In impact fragmentation, for a sufficiently low impact velocity $v = A\omega$, no fragmentation appears (Fig. 1D), and the compressive impact wave only travels back and forth in the lattice. When v is increased above a threshold, fragments begin to appear (Fig. 1E), and eventually begin to localize at the impact boundary (Fig. 1F). This effect is easy to understand. For v well above the fracture threshold, severe fragmentation at the impact boundary appears almost instantly, and a boundary region is separated from the rest of the lattice. Because of inertial effects very little of the impact energy will penetrate into the interior of the system, which will largely remain undamaged. If collisions between fragments were included, we expect fragmentation would extend farther in the material, but would still be localized close to the impact boundary for not very high impact energies. For two colliding objects of fairly similar masses the situation will be different.

To quantify the phenomena described above, we analyzed the total mass of the fragmented part of the sample in the impact fragmentation as a function of the impact amplitude A (with a constant impact frequency ω). We also analyzed the ratio of the total fragment surface to the impact energy [i.e., $S_{\text{tot}} \equiv N_f/(L_s A^2)$ with L_s the system size and N_f the total number of broken beams]. In the case of explosive fragmentation we analyzed the largest fragment mass as a function of η (for explosions the total fragment mass cannot be distinguished from the mass of the system), and the ratio of the total fragment surface to the induced kinetic energy [i.e., $S_{\text{tot}} \equiv N_f/(L_s^2\eta^2)$]. The results are shown in Fig. 2. This figure displays maxima in both the total fragment mass and the relative fragment surface for the impact fragmentation at $A = A_c \approx 0.14$. The maximum in the total fragment mass gets higher and the peak becomes narrower for increasing system size, which is typical of a critical point. It therefore appears that there is a nonzero impact energy $\propto A_c^2$ for which fragmentation becomes critical. We should then also expect that the fragment-size distribution becomes a pure power law at $A = A_c$. In the case of explosive expansion, the largest fragment mass and the relative fragment surface continuously increase for decreasing η, which indicates that there is a critical point close to $\eta = 0$ in agreement with Eq. (1).

The value $A_c \approx 0.14$ is quite reasonable. A simple elasticity-theory estimation of the maximum local strain gives $A = 0.12$ for the amplitude at which the first beams break (i.e., the ones most liable to fracture due to disorder), and $A = 0.19$ for breaking of a typical beam.

The fragment-size distributions are shown in Fig. 3 for both explosion (Fig. 3A) and impact (Fig. 3B). In the first case we try "data collapse" suggested by Eqs. (2) and (3), i.e., we plot $N(m)m^{\alpha}$ as a function of m/M_0 using α and M_0 as the fitting parameters such that all points should fall on a single curve. We find good collapse for $\alpha \approx 0.5$. For impact fragmentation a similar collapse works well for the same value of α. We show in Fig. 3B that an excellent fit to the data is also given by the "empirical" form of $n(m)$ [i.e., $f(z) = (\alpha + z)\exp(-z)$] with similar values for α and M_0. The empirical scaling function is also shown in Fig. 3A for comparison.

The scaling of the correlation length is now determined by the fitted M_0 for the different $A - A_c$ and η. Figure 4A demonstrates that the agreement with the scaling relation Eq. (1) is excellent for all systems. Notice that $\alpha \approx 0.5$ is so small that the average fragment mass is infinite at the critical point, and that fragmentation is reduced to cleaving of the sample [13].

As already noticed before [10], fragmentation under homogeneous expansion of the LJ liquid is a slow process, and it is difficult to reach thermal equilibrium in molecular simulations. We would therefore expect that the results for model I correspond to those at early stages for the disordered lattice of beams under similar homogeneous expansion. The results for these two models are compared in Fig. 4B. This figure shows $N(m)/m^{-\alpha}$ as a function of m/M_o for the expansion fragmentation of both models.

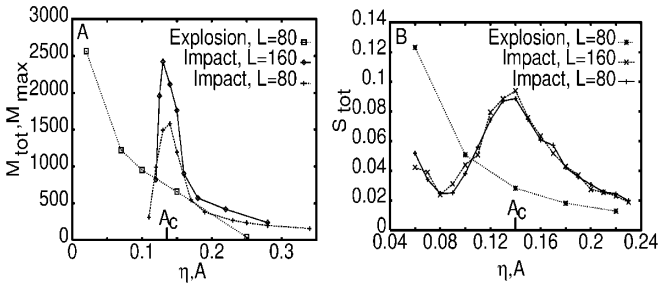

FIG. 2. The total fragment mass (A) and the relative fragment surface (B) as a function of A for two different linear sizes L_s of the system, and the largest fragment mass (A) and the relative fragment surface (B) as a function of η. The location of the critical amplitude A_c is indicated.

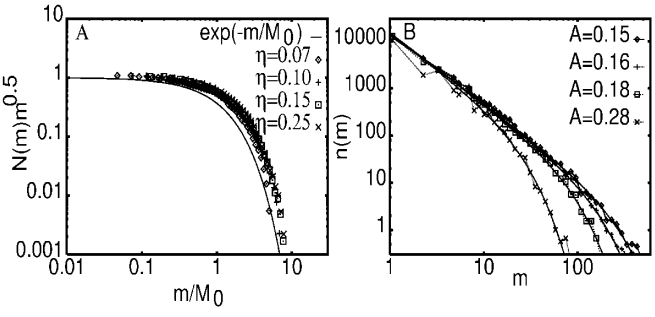

FIG. 3. Fragment-size distributions: (A) $N(m)m^{0.5}$ versus m/M_0 for explosion fragmentation together with the "empirical" form $f(z) = \exp(-z)$, and (B) the spectral distributions $n(m)$ for impact fragmentations fitted with the empirical form for $n(m)$.

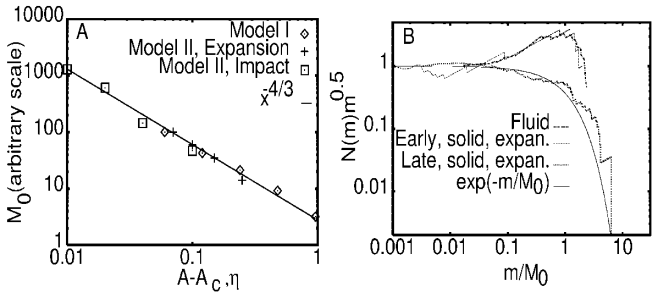

FIG. 4. (A) M_0 as a function of $A - A_c$ and η obtained by fitting the empirical form to $n(m)$ distributions, and comparison with Eq. (1). (B) $N(m)m^{0.5}$ versus m/M_0. The fragment-size distributions for model I and the distributions at an early and late time for explosive expansion in model II.

According to the scaling form, the results should asymptotically approach an exponential function. This is indeed the case for the late-stage distributions for model II. Model I has a fragment-size distribution that is similar to the early-stage distribution for model II. In fact the cumulative fragment-size distribution for model I can well be described by

$$N(m, \eta, A, t) = [a_1 m^{-\alpha} + a_2(\eta, A, t)] \exp\left(-\frac{m}{M_0}\right), \tag{4}$$

where the time-dependent coefficients a_1 and a_2 behave such that $a_1 \to$ const and $a_2/a_1 \to 0$ for increasing simulation time t. It appears that the crossover parameter M_0 as determined by this functional form is quite insensitive to the simulation time, and thus provides a reliable estimate for the correlation length.

Notice also that large fragments are relatively more abundant at the early stages of fragmentation, and that most of the small fragments in the power-law regime are formed as a result of the breakup (or evaporation for the LJ liquid) of large initial fragments. This also is in agreement with the energy-balance principle leading to Eq. (1). The correlation length is set by the impact or explosion energy which determines the typical size of the fragments in the first breakup stage. Thereafter fragmentation continues by breaking the large fragments in a "critical" way, i.e., the resulting fragments form a scale invariant small-size range of the fragment-size distribution.

In conclusion, impact fragmentation becomes critical at a nonzero impact energy. For expansion fragmentation the critical point is at zero strain-increase velocity, in which case a single dominating crack cleaves the sample. In the impact fragmentation only small damage appears below the critical point, cleaving of the sample at the critical point, and fragmentation localized near the point of contact well above the critical point. Fragment-size distributions satisfy in all cases analyzed, i.e., for the two physical systems and for both modes of fragmentation, a scaling form similar to that of the cluster-size distribution in percolation below criticality. Energy-balance arguments explain the observed correlation length divergence at the critical point, $\xi \propto x^{-2/3}$, where $x = A - A_c$ or $x = \eta$ is the distance to the critical point.

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