Kertész line of thermally activated breakdown phenomena

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Based on a fiber bundle model we substantially extend the phase-transition analogy of thermally activated breakdown of homogeneous materials. We show that the competition of breaking due to stress enhancement and due to thermal fluctuations leads to an astonishing complexity of the phase space of the system: varying the load and the temperature a phase boundary emerges, separating a Griffith-type regime of abrupt failure analogous to first-order phase transitions from disorder dominated fracture where a spanning cluster of cracks emerges. We demonstrate that the phase boundary is the Kertész line of the system along which thermally activated fracture appears as a continuous phase transition analogous to percolation. The Kertész line has technological relevance setting the boundary of safe operation for construction components under high thermal loads.

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The fracture of homogeneous and heterogeneous materials addresses several fundamental problems for statistical physics among which the analogy of fracture with phase transitions and critical phenomena is of outstanding interest. Since the pioneering work of Griffith in 1920 [1] it is generally accepted that the fracture of homogeneous media is analogous to first-order phase transitions; i.e., fracture occurs abruptly without any precursors as soon as a crack of critical size nucleates due to thermal fluctuations. In heterogeneous materials with quenched structural disorder a different scenario arises. Fracture progressively develops through the accumulation of damage providing also precursors of imminent failure. On the microlevel fracture proceeds in bursts which are characterized by power-law distributions and exhibit scaling behavior typical for continuous phase transitions [2–6]; however, on the macroscale, characteristic quantities such as the Young modulus have a finite jump reminiscent of first-order transitions. To resolve the problem the idea emerged that fracture is a first-order phase transition close to the spinodal point [7]. Later on the first-order scenario was questioned by showing that the disorder is a relevant field in fracture; i.e., varying the amount of quenched disorder one can tune the system from first-order type abrupt failure with discontinuity of the macroscopic quantities to second-order phase transitions where even the Young modulus has power-law behavior [8–10]. In the limit of infinitely strong disorder fracture can exactly be mapped to a percolation problem [11].

The phase-transition nature of fracture phenomena is much less understood in the presence of annealed disorder due to thermal noise. To overcome this problem, in the present Rapid Communication we investigate the thermally activated breakdown of homogeneous materials under a constant external load using a fiber bundle model (FBM) with localized load sharing. Analyzing the microstructure of damage in the last stable configuration, we show that the Griffith-type abrupt rupture is complemented by a disorder dominated regime, characterized by a high amount of diffuse damage and the formation of a spanning cluster of cracks.

We introduce the concept of the Kertész line for fracture; i.e., we show that the phase boundary is the Kertész line of the system along which thermally activated breakdown becomes analogous to the continuous transition of percolation [12]. Besides its theoretical importance, the Kertész line in fracture phenomena has also technological relevance.

To investigate the role of thermal activation, several modeling approaches have been introduced, which provided a detailed understanding of the time dependence of breakdown phenomena [13–20]. To study the analogy of thermally activated fracture to phase transitions we follow the approach of Guarino et al. [18,19]: we consider $N$ parallel fibers on a square lattice of size $L$. The bundle is subject to a constant external load $\sigma$ under which the fibers have a linearly elastic behavior characterized by an identical Young modulus $E$. To take into account the effect of thermal noise in the fracture process, we assume that the local load on fibers $\sigma_i, i=1,\ldots,N$ has time dependent fluctuations $\xi(t)$ so that the load of fiber $i$ at time $t$ reads as $\sigma_i=\sigma^0+i(\xi(t)$, where $\sigma^0_i$ denotes the deterministic part arising from the external load and from the load transferred from broken fibers. The fibers break when the local load on them exceeds a threshold value $\sigma_i>\sigma_{th}$. It is a crucial feature of the model that the system is completely homogeneous; i.e., all the fibers have the same breaking strength $\sigma_{th}=1$ so that the only source of fluctuations is the thermal noise arising due to the finite temperature $T$. Stress fluctuations $\xi$ of thermal origin are characterized by a Gaussian distribution with zero mean and a temperature dependent standard deviation $p(\xi,T)=(1/\sqrt{2\pi T})\exp(-\xi^2/2T)$. The system evolves in discrete time steps sampling new values of $\xi$ independently of each other. Another important element of the model is that after breaking events a localized load sharing is assumed; i.e., the load of a broken fiber is equally distributed over its intact nearest neighbors resulting in a high stress concentration in the vicinity of failed regions.

Analytical [20] and numerical [18,19] solutions of the model have shown that under a constant external load...
σ ≥ 0 the system suffers macroscopic failure at a finite time \( t_f \) at any finite temperatures \( T > 0 \). At high loads \( \sigma > \sigma_c \) even the breaking of a single fiber can trigger the sudden catastrophic collapse of the bundle, where the critical stress is \( \sigma_c = 4 \sigma_{th} / 5 \) on the square lattice [19]. Our simulations show that at lower loads \( \sigma < \sigma_c \) a complex time evolution emerges as a result of the competition of the deterministic dynamics due to stress enhancements around broken clusters (cracks) and of annealed disorder due to thermal noise: fibers primarily break due to the thermal fluctuations of the local load so that broken fibers appear at random locations in the system.

The structure of the bundle right after the first time step is identical to a percolation lattice with occupation probability \( p_c = 1 - P(\sigma_{th} - \sigma, T) \), where \( P = \int_{\sigma_{th}}^{\sigma} p(x, T) \, dx \) denotes the cumulative distribution of stress fluctuations. The load transferred to the intact nearest neighbors of broken fibers may then lead to a correlated growth of cracks with thermally driven bursts. To get an overview of possible breaking scenarios, the microstructure of damage in final stable states of a fiber bundle is presented in Fig. 1. In these configurations a single fiber breaking, which typically occurs along the highly stressed perimeter of the largest cluster, initiates a catastrophic avalanche of breakings, giving rise to macroscopic failure. Under a high external load [Fig. 1(a)] the large amount of local load concentrated at the cluster boundaries makes the system very sensitive to thermal fluctuations. Hence, even at low temperatures macroscopic failure occurs already at cluster sizes much smaller than the system size \( S_{\max} \ll N \), where \( S_{\max} \) denotes the size of the largest cluster.

Lowering the load and increasing the temperature in Fig. 1(b) clusters can reach larger sizes, but the macroscopic fracture of the system is still of the Griffith nature occurring abruptly at a low amount of damage [1]. We emphasize that the microstructure substantially changes in Figs. 1(c) and 1(d) where the high temperature and low load result in a large amount of diffuse damage. The thermally driven growth and merging of clusters lead to the formation of a giant cluster with a size \( S_{\text{max}} \) comparable to the system size \( N \).

The size of the largest cluster proved to be crucial in triggering the final failure of the system and hence for the nature of the fracture transition. For a cluster of size \( S \) all the load of the broken fibers \( S \sigma \) is concentrated on the intact ones along the cluster perimeter. Assuming a compact cluster shape, the number \( n_p \) of highly stressed fibers is \( n_p \sim \sqrt{S} \), which all have the load \( \sigma_p = \sigma + \sigma \sqrt{S} \). A cluster can be stable until \( \sigma_p < \sigma_c \), holds, from which the maximum cluster size \( S_{\text{max}} \), the system can tolerate at load \( \sigma \) reads as

\[
S_{\text{max}} \sim \left( \frac{\sigma_c - \sigma}{\sigma} \right)^2.
\]

Figure 2(a) presents the average size of the largest cluster \( \langle S_{\text{max}} \rangle \) obtained by computer simulations with the system size \( L = 1024 \). It is important to emphasize that for high load values \( \sigma \rightarrow \sigma_c \), an excellent agreement is obtained with Eq. (1) indicating the Griffith-type abrupt failure of the system triggered by a perimeter site of the largest cluster [see Figs. 1(a) and 1(b)]. The value \( \sigma_c = 0.83 \pm 0.02 \) was obtained by fitting in agreement with the analytic prediction. However, as the load is lowered, at each temperature a threshold load emerges \( \sigma_c(T) \) where strong deviations start from the analytic form of Eq. (1), i.e., for \( \sigma < \sigma_c(T) \) the value of \( \langle S_{\text{max}} \rangle \) rapidly increases approaching the system size \( \langle S_{\text{max}} \rangle \sim N \). This novel behavior of the largest cluster demonstrates the emergence of a new regime of thermally activated fracture at temperature dependent load values \( \sigma_c(T) \) where the abrupt Griffith scenario breaks down and annealed disorder starts to dominate the breaking process [see also Figs. 1(c) and 1(d)]. In the opposite limit, when the external load \( \sigma \) is sufficiently high, the critical cluster size \( S_{\text{max}} \) can be reached immediately in the first step of time evolution giving rise to immediate abrupt failure. Since in this case fiber breaking is a completely uncorrelated process, this scenario occurs if the probability of the formation of a critical size \( S_{\text{max}} \) cluster falls in the order of \( 1/N \),
FIG. 3. (Color online) Phase diagram of thermally activated breakdown of homogeneous FBMNs. The blue (dashed) and red (continuous) curves indicate \( \sigma^*(T) \) and \( \sigma_K(T) \), respectively. The curve of \( \sigma_K(T) \) defines the Kertész line of the system. Black squares indicate the position of the maxima of \( S \) in Fig. 4(b).

\[
1 - P(\sigma_K - \sigma^*, T)^{S_{\text{max}}} P(\sigma_K - \sigma^*, T)^{S_{\text{max}}},
\]

where \( S_{\text{max}} \) has to be inserted from Eq. (1) as a function of \( \sigma \). At a given value of \( T \) Eq. (2) has to be solved for the load as a function of temperature \( \sigma^*(T) \). Based on the above analysis, the phase diagram of thermally activated breakdown of fiber bundles can be set up on the \( \sigma^*-T \) plane. Figure 3 presents that the \( \sigma^*(T) \) line separates the regime of immediate abrupt failure (phase I) from another one, where fracture occurs abruptly but the lower load allows for the gradual growth of cracks (phase II). Phase II of the model corresponds to the classical Griffith type of fracture characterized by the dominance of correlated growth of cracks up to the critical size \( S_{\text{max}} \) of Eq. (1) where abrupt failure occurs analogous to first-order phase transitions. The largest cluster sizes \( \langle S_{\text{max}} \rangle \) deviating from Eq. (1) in Fig. 2 correspond to load and temperature values below the \( \sigma_K(T) \) curve on the \( \sigma^*-T \) plane defining phase III of the system. Phase III is characterized by the dominance of thermally driven random nucleation of cracks and merging of slowly advancing cracks; hence, the microstructure of accumulating damage becomes similar to percolation lattices where even a spanning cluster of broken fibers can emerge [see Figs. 1(c) and 1(d)].

In order to give a quantitative characterization of the competition of the stress dominated failure and thermally driven stable growth and merging of cracks, we introduce the ratio \( \phi \) of the probabilities of new crack nucleation \( P_n=1-P(\sigma_K-\sigma^*, T) \) and of the thermally induced growth of clusters \( P_g=1-P(\sigma_K-\sigma^*, T) \), i.e., \( \phi(\sigma, T)=P_n/P_g \) with \( 0<\phi<1 \). Here \( k=5/4 \) is for the smallest clusters and the analytic value of \( \alpha_r=0.8 \) was used in the formulas. The inset of Fig. 2 presents that plotting the strength of the largest cluster, i.e., the ratio of \( \langle S_{\text{max}} \rangle \) and the average number of broken fibers \( \langle N_b \rangle \) as a function of \( \phi(\sigma, T) \), an excellent data collapse is obtained for parameter values \( (\sigma, T) \) in phase III of the system. The data collapse implies that \( \phi \) is an appropriate control parameter of thermally activated breakdown, the value of which clearly distinguishes regimes dominated by different fracture mechanisms. The collapsed data can be very well fitted by the functional form

\[
\langle S_{\text{max}} \rangle/(N_b) \sim (\phi-\phi_c)^\beta \text{ for } \phi > \phi_c,
\]

which indicates a continuous phase transition at \( \phi_c=0.9208 \pm 0.0003 \) from the Griffith-type abrupt failure \( \phi<\phi_c \) to the slowly proceeding disorder dominated fracture \( \phi>\phi_c \) as the external load and temperature are varied. The value of the critical exponent \( \beta=0.15 \pm 0.02 \) agrees very well with the order-parameter exponent \( \beta=5/36 \) of percolation in two dimensions [21]. Along the phase boundary between the Griffith and disorder dominated fractures \( \phi=\phi_c \) must hold; hence, the curve of \( \sigma_K(T) \) in Fig. 3 was determined by numerically solving the equation \( \phi(\sigma_K, T)=\phi_c \) for \( \sigma_K \).

The percolation nature of the transition between the two phases at \( \phi_c \) is further supported by Fig. 4(a) which shows that the fraction of broken fibers \( \langle N_b \rangle/N \) is a unique function of \( \phi \) and at \( \phi_c \) its value is \( \langle N_b \rangle/N=0.59 \), in agreement with the critical occupation probability \( p_c=0.5927 \) of two-dimensional percolation [21]. The sharp maximum of the average size of clusters \( \langle S \rangle \) in Fig. 4(b) indicates the formation of a dominating cluster at \( \phi_c \) which spans the entire lattice. Note that the positions of the maxima of \( \langle S \rangle \) fall on the \( \sigma_K(T) \) curve in the phase diagram of Fig. 3, demonstrating the consistency of the results. Figure 4(c) presents that as \( \sigma \) approaches \( \sigma_K(T) \) from either side at a fixed temperature \( T \) (compare to Fig. 3), the size distribution of clusters \( n_S(\sigma, T) \) gradually converges to a power law with an exponent \( \tau=2.05 \pm 0.05 \) agreeing very well with the corresponding exponent of percolation \( \tau=187/91 \) [21]. Our analysis of the microstructure of damage shows that the emergence of the \( \sigma_K(T) \) line in the phase space of thermally activated breakdown phenomena is analogous to what is observed in systems where phase transition can be defined both thermodynamically and topologically such as in the Ising model. In the presence of an external magnetic field \( H \), in the \( T, H \) phase space of the system it is possible to identify a \( T(H) \) line along which the geometrical structure of spin clusters undergoes a percolation transition. This so-called Kertész line has been found in the phase space of various types of systems from solid-state physics to quantum field theory [12]. Our study revealed the existence of the Kertész line for thermally activated breakdown phenomena, where it separates regimes of different fracture mechanisms. Figure 4(d) demonstrates that the microstructure of damage and the time evolution of the system are strongly related: on the Kertész line the average cluster size obeys a time-to-failure power law \( \langle S \rangle \sim (t_f-t)^{-\delta} \) with the exponent \( \delta=3 \). However, away from the Kertész line scaling breaks down: in the Griffith phase \( \phi<\phi_c \) the sudden acceleration of \( \langle S \rangle(t) \) indicates the instability of the system, while in the disorder dominated phase \( \phi>\phi_c \) clusters evolve slowly retaining the stability. The results agree well with the qualitative features of the cluster size distribution in Fig. 4(c).

In conclusion, our investigation revealed the richness of the phase space of thermally activated breakdown of homogeneous systems. Varying the temperature and the external
load, besides the Griffith-type abrupt fracture analogous to first-order phase transition a disorder dominated phase of fracture emerges where a spanning cluster of cracks occurs. The phase boundary is the Kertész line of the system along which thermally activated fracture becomes analogous to the continuous transition of percolation. The ratio of the probabilities of the growth and nucleation of cracks proved to be a crucial parameter which characterizes regimes of different fracture mechanisms. Our study implies that the Kertész line has a high technological relevance in applications where construction components are often exposed to high thermal loads. In practice, the high disorder phase below the Kertész line is the desirable parameter regime of safe operation to avoid sudden unexpected failures.

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