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Surface effects in the failure probability of heterogeneous materials with tough-to-brittle crossover

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The surface effects on heterogeneous material breakdown are studied using a stochastic transfer-matrix approach on systems with one-dimensional cracks. By computing and comparing the failure probabilities $F_L^{(p)}(\sigma)$ and $F_L^{(o)}(\sigma)$, for systems with periodic and the open boundary conditions respectively, we find that, over a very large range of the sample sizes L and applied stress σ, $F_L^{(o)}(\sigma)$ is significantly larger than $F_L^{(p)}(\sigma)$. Their ratio $F_L^{(p)}(\sigma)/F_L^{(o)}(\sigma)$ is smallest near the minimum of $F_L^{(p)}(\sigma)$, where the ratio decreases exponentially as the stress reduces. This implies that overwhelmingly most of the cracks that result in the failure of an entire sample are those nucleated from the surfaces. The previously discovered optimum sample size itself $L_{\min}$, where the failure probability reaches a deep minimum and the material undergoes a tough-to-brittle transition, decreases slightly with the introduction of surfaces. [S0163-1829(98)02215-2]

I. INTRODUCTION

In a heterogeneous or composite material with a distribution of local breaking strengths, many small cracks can be nucleated in weak regions of the sample under applied stresses. These cracks may be stopped from cleaving the sample by strong regions or pins and the material is then considered to be toughened against fracture. The only toughened samples that fracture or fail at low stress are those having such randomly distributed bonds that allow the weak or crackable regions to percolate or merge (due to local load sharing and the stress enhancement at the tips of cracks) into cracks larger than that of a critical size M, beyond which, due to the stress enhancement, even the strongest bonds or pins cannot stop growing cracks. Such a tough system crosses over to being brittle whenever the applied stress σ is increased sufficiently or, less obviously, whenever the sample size L is increased such that there is a more substantial probability of finding a cracked region of at least size M somewhere in the sample.

This crossover, from tough to brittle, was suggested by Khang *et al.*[1] and actually seen numerically by Duxbury and Leath[2] in their evaluation of the exact recursion for a simple model of linear cracks (the one-dimensional, fiber-bundle model) with local load sharing. They discovered a dramatically deep minimum that occurs in the sample failure probability $F_L(\sigma)$, when the applied stress σ is small. This minimum occurs near $L_{\min}\sim 0.75M$ and its depth $F_{L_{\min}}$ decreases exponentially with σ. But also they saw a reduction of this minimum in their numerical simulation of $L\times L$ samples with open boundary conditions, which raised, for us, the questions of the effect of the boundaries.

Furthermore, as a function of σ, $F_L(\sigma)$ changes from being a Weibull distribution for sample size $L<M$ (with the Weibull parameter proportional to L) to the double-exponential (modified Gumbel) distribution for $L>M$. We see this crossover from Weibull to double-exponential distribution as a characteristic signature of the crossover from tough-to-brittle behavior.[3] There have now been many numerical and experimental confirmations of the double-exponential (modified Gumbel) distribution for brittle systems.[4–6] And although there seem to have been fewer careful analyses of the failure of tough systems, nevertheless, one of the examples studied by Sahimi and Arbabi is striking. In this example,[4] they considered a ''superelastic'' triangular lattice, 90% occupied by identical breakable Hookian springs and 10% occupied by unbreakable Hookian springs. The resulting system was very tough as nucleated cracks generally stopped when they hit the randomly located unbreakable springs. So cracks were able to transverse the system only by a kind of percolation process of avoiding the unbreakable springs, and the result was a Weibull failure probability distribution. So, it seems, perhaps, that the Weibull failure distribution may be characteristic of tough systems.

Strictly speaking, the boundary conditions of the sample failure probability $F_L(\sigma)$ calculated by Duxbury and Leath[2,3] for the one-dimensional fiber-bundle model were actually those for a sample of size L embedded in a larger sample, i.e., they calculated the *interior* failure probability, due to the fact that all the sample configurations included in the recursion calculation satisfy the interior boundary conditions. A section of sample is considered to have *interior* boundary conditions when it is surrounded on each end by intact fibers. In this paper, we shall use a stochastic matrix method to examine exactly the effects of various boundary conditions, especially the importance of the surfaces in two-dimensional samples. It turns out that the presence of open surfaces (edges) substantially increases the sample failure probability over a large range of sample sizes, including the most interesting region where the deep minimum appears and the tough-to-brittle crossover takes place. These results provide an explanation of why most cracks start from the surface in real materials and a starting point for more detailed calculations of surface effects in material breakdown.

In the next section we define the model by specifying the breaking-strength distribution and the local-load-sharing rule (with the generalization to include the cases of the bonds that

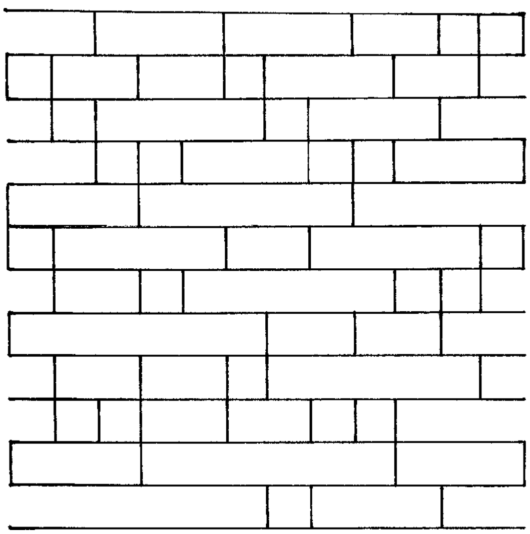

FIG. 1. A square lattice sample with some random vertical bonds broken. All the cracks are one dimensional.

are open to the surfaces). The stochastic transfer matrix (STM) approach and the no-lone-bond approximation will then be introduced. In Secs. III–VI, analytical forms of different STM's will be constructed for arrays obeying the interior, periodic, mixed, and open boundary conditions, respectively. The open surface effects on the sample's failure probability can then be conveniently studied and clearly understood. The last two sections are devoted to the numerical results and some further discussions.

II. THE MODEL AND THE STOCHASTIC TRANSFER MATRIX

We consider an $L\times L$ square lattice in which each bond of the lattice is randomly assigned a breaking strength (such as tensile strength or critical current) chosen from a uniform, local-failure probability distribution $f(\sigma)$ with a maximum bond-breaking strength σ_M, as follows:

$$f(\sigma)=\begin{cases}1/\sigma_M, & 0\leqslant\sigma\leqslant\sigma_M\\ 0, & \text{otherwise.}\end{cases} \tag{1}$$

We also assume, for simplicity, that there are only linear cracks perpendicular to the direction of the stress, which is applied perpendicular to the horizontal rows of the lattice (see Fig. 1). This restriction to linear cracks means that each row (array) is statistically independent of the others and the fracture probability for the square lattice $F_{L\times L}(\sigma)$ can be written as

$$F_{L\times L}(\sigma)=1-[1-F_L(\sigma)]^L. \tag{2}$$

So the problem is reduced to that of finding $F_L(\sigma)$, the failure probability of a one-dimensional array (or fiber bundle) of size L.

When a stress σ is applied to a one-dimensional array, either some of the bonds break until a stable structure with cracks is reached, or bond failure continues until the entire array is completely fractured. We use a modified local-load-sharing rule of Harlow and Phoenix,[6] which is to assume that the stress experienced by any surviving bond is given by

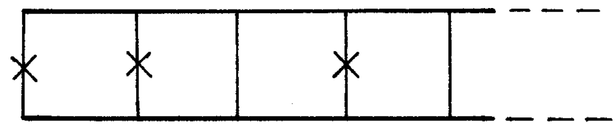

FIG. 2. A row of the sample with the first, second, and fourth bonds broken.

$$\sigma_k=\left(1+\frac{k}{2}\right)\sigma \quad \text{with} \quad k=k_i+2k_s, \tag{3}$$

where k_i is the number of adjacent broken bonds situated in the interior of the sample, and k_s is the number of adjacent broken bonds open to the surface. The term $2k_s$ indicates that all the stress on the surface crack is borne by the first intact bond, i.e., the surface crack has only one intact end to carry its stress. The term k can then be considered as an *effective* total number of broken bonds adjacent to the surviving bond. As an example, we label the bonds in an array from one of its ends. Suppose that the first, second, and fourth are broken while the third and fifth are intact as shown in Fig. 2, the effective k for the third bond (or the first unbroken one counted from the surface) is $1+2\times2=5$. This local-load-sharing rule (introduced by Harlow and Phoenix[6] without the consideration of the surface), though idealized, catches much of the basic and important physical features of the fracture process in composites and random materials. It could also be easily modified to account for chemical changes in the bonds at the surface, but we have not considered that here.

With σ_k and $f(\sigma)$ given by these simple models, we can now write the survival probability $W_k(\sigma)$ of a single bond with k effective broken neighboring bonds as

$$W_k=1-\int_0^{\sigma_k} f(\sigma')d\sigma'=\begin{cases}1-(1+k/2)\sigma/\sigma_M & \text{for} \quad k\leqslant M\\ 0 & \text{for} \quad k>M.\end{cases} \tag{4}$$

From the above expression of W_k, we can see immediately that for a given ratio σ/σ_M, there is always a critical crack size $M\equiv2[\sigma_M/\sigma-1]$, the integer part of $2(\sigma_M/\sigma-1)$, such that any crack of an effective size bigger than M must cause the entire array to fail. In other words, under the given applied stress σ the strongest bond (with breaking strength σ_M) can only withstand the enhanced total stress at one tip of cracks of size M or smaller.

The main purpose of this paper is to calculate the surface and other boundary effects in the failure probability $F_L(\sigma)$ and hence $F_{L\times L}(\sigma)$, and also to discuss the analytical form of $F_{L\times L}(\sigma)$. Since the problem under consideration is one where the result is dominated, especially in brittle region, by the "worst" situation (or the weakest configurations), we need to consider all the possible configurations the array may have. In terms of the survival probabilities of each configuration, the array's failure probability can be written as

$$F_L(\sigma)=1-\sum_{C_L} \times\{\text{survival probability of configuration } C_L\}, \tag{5}$$

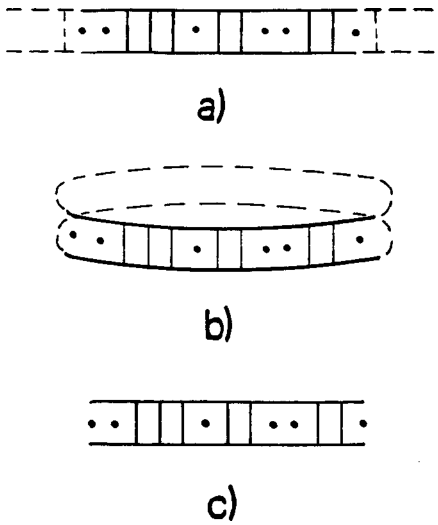

FIG. 3. A partially broken row in the interior (a) of a larger sample, with periodic boundary conditions (b), and with open boundary conditions (c). The vertical lines represent intact bonds, and the dots represent broken bonds.

where C_L runs over all possible array configurations of length L subject to the required boundary condition.

The total number of configurations increases factorially with the array length L as expected. However, those of small L can be easily written down term by term for each possible array configuration. Our notation will be to use a total of L ''0'' 's and ''1'' 's to represent the broken and the intact bonds at specific positions in an array configuration C_L. For example, a short array of $L=5$ with its first and fourth bonds broken will be represented by 01101, and its survival probability will depend upon its boundary conditions, or how it is connected to the rest of the array. There are several different boundary conditions we shall consider, namely, interior, open, periodic, and mixed. Their survival probabilities are denoted by the configuration in the appropriate brackets as illustrated in Figs. 3(a)–3(c). It is easy to see that each of these probabilities can be written as a product of W_k's and various sample failure probabilities F_k's with shorter lengths $k<L$. We therefore need to establish the recursion relation relating F's with different sample lengths, and this is achieved by the construction of stochastic transfer matrices (STM) for different boundary conditions.

The stochastic transfer matrix approach was introduced earlier to study the fracture of brittle composites.[7] It turns out that it is also useful in dealing with our present tough-to-brittle problems, especially when different boundary conditions are introduced. We first group all possible array configurations with given size L according to their endings, namely, their last clusters of broken bonds on one end. As an example, $\langle *{*}{*}100\rangle$ represents the total probability of all interior array configurations of length 6 with their fourth bond intact, while the fifth and the sixth are broken, summed over all possible states of the first three bonds. The advantage of this grouping based on their endings is to make the construction of the STM much easier to understand physically and, at the same time, to drastically reduce the sizes of the matrices. The STM is defined as the matrix that transfers the probability column vector P_L for an array of length L into P_{L+1} for a longer array of length $L+1$:

$$\mathbf{T}_L(\sigma)P_L=P_{L+1}, \tag{6}$$

where the elements in each column vector P_L are the configuration probabilities for all possible distinct and stable endings. For a given ratio σ/σ_M (or equivalently M), there are only a limited number of possible endings with nonvanishing probability. Therefore the dimensions of $\mathbf{T}_L(\sigma)$ are restricted to be equal to or smaller than that number.

Following the previous study of the size effects of interior arrays embedded in larger systems, we further simplify the calculation by introducing the no-lone-bond approximation, which is to neglect the contributions from all configurations with *lone* bond(s) in the interior of the arrays. It has already been shown numerically by Leath and Duxbury[3] that the quantitative errors due to this approximation are limited and that the qualitative behavior is unchanged. However, this approximation allows us to conveniently write down the survival probability for a configuration of length $L+1$ as that for one of length L multiplied by a relatively simple factor. This factor accounts for the effects of the extension affecting one end of the array less than M-sites deep into the array interior.

III. STM WITH INTERIOR BOUNDARY CONDITIONS

The failure probability for a one-dimensional *interior* array of length L, $F_L(\sigma)$, was obtained previously by Duxbury and Leath using a different numerical method. In this section we first rederive these results through the construction of the corresponding stochastic transfer matrix (STM), $\mathbf{T}_L^{(i)}(\sigma)$, using Eq. (6) and $P_L^{(i)}$ and $P_{L+1}^{(i)}$, whose elements are the probabilities of different endings. The superscript (i) denotes the fact that all configurations involved in the calculation are embedded in the interior of a larger array, namely, they satisfy the interior boundary condition.

For small L, the probability elements for different endings in $P_L^{(i)}$ and $P_{L+1}^{(i)}$ can be written down term by term explicitly. For example, in the no-lone-bond approximation, the five nonvanishing probability elements in the vector $P_3^{(i)}$ are, for general M,

$$\begin{aligned}
\langle *11\rangle &= \langle 111\rangle+\langle 011\rangle+W_0^3+W_0W_1F_1,\\
\langle 110\rangle &= W_0W_1F_1,\\
\langle 101\rangle &= W_1^2F_1,\\
\langle 100\rangle &= W_2F_2,\\
\langle 001\rangle &= W_2F_2,
\end{aligned} \tag{7}$$

and the seven nonvanishing elements in $P_4^{(i)}$ are

$$\begin{aligned}
\langle **11\rangle &= \langle 1111\rangle+\langle 0111\rangle+\langle 1011\rangle+\langle 0011\rangle\\
&= W_0^4+F_1W_1W_0^2+W_1F_1W_1W_0+F_2W_2W_0,\\
\langle *110\rangle &= \langle 1110\rangle+\langle 0110\rangle=W_0^2W_1F_1+F_1W_1^2F_1,\\
\langle 1101\rangle &= W_0W_1F_1W_1,\\
\langle 1100\rangle &= W_0W_2F_2,
\end{aligned} \tag{8}$$

$$\langle 1001\rangle = W_2F_2W_2,$$

$$\langle 1000\rangle = W_3F_3,$$

$$\langle 0001\rangle = W_3F_3,$$

where the angular brackets denote that each end has interior boundary conditions. Basically, the elements correspond to all possible clusters of broken bonds on the right end. The last elements are included since the two bonds immediately adjacent to this array are assumed to be intact with the interior boundary condition. Using Eq. (6), we can easily construct a stochastic transfer matrix for the interior configurations as

$$\mathbf{T}_3^{(i)} = \begin{pmatrix} W_0 & 0 & W_0 & 0 & W_0 & 0 & \cdots & \cdots \\ \frac{W_1}{W_0}F_1 & 0 & 0 & 0 & 0 & 0 & \cdots & \cdots \\ 0 & W_1 & 0 & 0 & 0 & 0 & \cdots & \cdots \\ 0 & \frac{W_2}{W_1}\frac{F_2}{F_1} & 0 & 0 & 0 & 0 & \cdots & \cdots \\ 0 & 0 & 0 & W_2 & 0 & 0 & \cdots & \cdots \\ 0 & 0 & 0 & \frac{W_3}{W_2}\frac{F_3}{F_2} & 0 & 0 & \cdots & \cdots \\ 0 & 0 & 0 & 0 & \frac{W_3}{W_2}\frac{F_3}{F_2} & 0 & \cdots & \cdots \\ . & . & . & . & . & . & \cdots & \cdots \end{pmatrix}. \tag{9}$$

By inspection and induction, we find that it is possible to write $\mathbf{T}_L^{(i)}(\sigma)$ for an arbitrary L in the closed form

$$(\mathbf{T}_L^{(i)})_{1,2n-1} = W_0, \quad n=1,2,3,\ldots,L,$$

$$(\mathbf{T}_L^{(i)})_{2n+1,2n} = W_n, \quad n=1,2,3,\ldots,L-1,$$

$$(\mathbf{T}_L^{(i)})_{2n+2,2n} = W_{n+1}F_{n+1}/(W_nF_n), \quad n=1,2,3,\ldots,L-1, \tag{10}$$

$$(\mathbf{T}_L^{(i)})_{2,1} = W_1F_1/W_0,$$

$$(\mathbf{T}_L^{(i)})_{2L+1,2L-1} = W_LF_L/(W_{L-1}F_{L-1}),$$

$$(\mathbf{T}_L^{(i)})_{n,m} = 0, \quad \text{otherwise}.$$

With the analytical form of $\mathbf{T}_L^{(i)}(\sigma)$, successive multiplications of these matrices will produce $P_L^{(i)}$ for any required L, and $1-F_L(\sigma)$ is simply the sum of all the probability elements in $P_L^{(i)}$. We thus have

$$F_L(\sigma) = 1-(11111\cdots)\mathbf{T}_{L-1}^{(i)}\mathbf{T}_{L-2}^{(i)}\cdots\mathbf{T}_4^{(i)}\mathbf{T}_3^{(i)}\mathbf{T}_2^{(i)}P_2^{(i)}. \tag{11}$$

Since W_k vanishes for any $k>M$ in this model, the nonzero part of $\mathbf{T}_L^{(i)}(\sigma)$ will not be able to grow bigger than $(2M+1)(2M+1)$. Actually, the matrix $\mathbf{T}_L^{(i)}(\sigma) = \mathbf{T}_{M+1}^{(i)}(\sigma)$ for all $L>M$. From the failure probability $F_L(\sigma)$ of an array of length L, we can use Eq. (2) to calculate $F_{L\times L}^{(i)}(\sigma)$, which is the failure probability for a square array completely embedded in a larger two-dimensional sample. It will be seen that the interior array failure probability $F_L(\sigma)$ is indispensable in the calculations of failure probabilities for other more physically interesting systems, e.g., systems satisfying the periodic or open boundary conditions.

IV. STM WITH PERIODIC BOUNDARY CONDITIONS

In this section we consider the failure probability, $F_L^{(p)}(\sigma)$, for a system with the periodic boundary condition—a closed loop of length L as shown in Fig. 3(b). There are several different ways to obtain this failure probability, but we shall discuss the stochastic-transfer-matrix method here. It turns out that this probability is given by the trace of another matrix, $\mathbf{T}^{(p)}(\sigma)$, whose analytical form is similar to $\mathbf{T}^{(i)}(\sigma)$ above and can also be obtained using Eq. (6), the proper choices of $P_L^{(p)}$ and $P_{L+1}^{(p)}$, and the application of the periodic boundary condition.

Let us first consider a one-dimensional array of length L, satisfying the periodic boundary condition (a closed loop) with its length long enough $(L>M+2)$ to accommodate all possible $(2M+1)$ endings for a given M, the maximum crack size the array can possibly withstand. The largest ending configuration for a given M has M broken bonds plus an unbroken one at each end and takes up $M+2$ total sites. For the case of $M=2$, those $2\times2+1=5$ endings in $P_N^{(p)}$, terminating at an arbitrary site, say site N in the loop, are $(\cdots1)$, $(\cdots10)$, $(\cdots101)$, $(\cdots100)$, $(\cdots1001)$. Here, the regular parentheses are used to denote the fact that the configurations are subject to the periodic boundary condition. The desired STM acting on $P_N^{(p)}$ should then produce $P_{N+1}^{(p)}$ with its $2M+1$ elements being the probabilities of the same set of endings but shifted by one site at $N+1$. Again, using Eq. (6), we can easily construct the stochastic transfer matrix between two column vectors, both with the same set of ending configurations, for the above $M=2$ case as

$$\mathbf{T}_2^{(p)}=\begin{pmatrix} W_0 & 0 & W_0 & 0 & W_0 \\ \dfrac{W_1}{W_0}F_1 & 0 & 0 & 0 & 0 \\ 0 & W_1 & 0 & 0 & 0 \\ 0 & \dfrac{W_2}{W_1}\dfrac{F_2}{F_1} & 0 & 0 & 0 \\ 0 & 0 & 0 & W_2 & 0 \end{pmatrix}. \quad (12)$$

The form of $\mathbf{T}_M^{(p)}$ for arbitrary M and L can be easily deduced to be the following, which has the dimensions of $(2M+1)(2M+1)$,

$$\begin{aligned}
&(\mathbf{T}_M^{(p)})_{1,2n-1}=W_0, && n=1,2,3,\ldots,M,+1,\\
&(\mathbf{T}_M^{(p)})_{2n+1,2n}=W_n, && n=1,2,3,\ldots,M,\\
&(\mathbf{T}_M^{(p)})_{2n+2,2n}=W_{n+1}F_{n+1}/(W_nF_n), && n=1,2,3,\ldots M-1,\\
&(\mathbf{T}_M^{(p)})_{2,1}=W_1F_1/W_0,\\
&(\mathbf{T}_M^{(p)})_{n,m}=0, && \text{otherwise}. \quad (13)
\end{aligned}$$

The relation between $\mathbf{T}_M^{(p)}$ and the sample failure probability turns out to be a very simple one. To find $F_L^{(p)}(\sigma)$, we start with the probability of the ith ending configuration, $\langle E_i\rangle_N=1$ in $P_N^{(p)}$, with all other probability elements being zero. After L times of successive multiplication of $\mathbf{T}_M^{(p)}$, the position of $P_{N+L}^{(p)}$ comes back to the original site at N. The imposed periodic boundary condition only allows the corresponding ith probability element in $P_{N+L}^{(p)}$ to be included, which is

$$\langle E_i\rangle_{N+L}=\sum_{j=1}^{2M+1}[(\mathbf{T}_M^{(p)})^L]_{i,j}\langle E_j\rangle_N=[(\mathbf{T}_M^{(p)})^L]_{i,i}$$

and the total failure probability for the periodic array becomes

$$F_L^{(p)}(\sigma)=1-\sum_{i=1}^{2M+1}\langle E_i\rangle_{N+L}=1-\mathrm{Tr}[(\mathbf{T}_M^{(p)})^L]. \quad (14)$$

One might be tempted to find the lowest eigenvalue for $\mathbf{T}_M^{(p)}$, which is the only relevant quantity in the large L limit. However, failure probabilities of smaller samples are needed in the matrix element and a recursive calculation is inevitable.

As a simple example, we can easily write down the nine surviving configurations of length $L=4$ and $M=2$ under the periodic boundary condition and the no-lone-bond approximation: (1111), $4\times(1110)$, and $4\times(1100)$. The sample failure probability is thus equal to $1-W_0^4-4W_0W_1^2F_1-4W_2^2F_2$, which is identical to what would be obtained using Eqs. (12) and (14) above.

V. STM WITH MIXED BOUNDARY CONDITIONS

To calculate the failure probability of an open array, our main interest of this paper, it is obvious that probability elements such as $\langle1101110]=W_0W_1F_1W_1W_0W_2G_1$ have to be evaluated. Here $G_L(\sigma)$ is the failure probability for an array of length L with one of its ends open to the surface (denoted by the square bracket), and the other in the interior of the sample (the angular brackets as before)—a mixed boundary condition. In this section we calculate $G_L(\sigma)$ first, again using the STM method.

In the no-lone-bond approximation, the sample survival probability $(1-G_4)$ of an array of length $L=4$, satisfying the *mixed* boundary condition, is equal to the sum of the following elements: $\langle**11]$, $\langle*110]$, $\langle1100]$, and $\langle1000]$. In order to construct a matrix with a closed form, which also generates all required probability elements for $G_L(\sigma)$, we have to consider an *augmented* probability column vectors $P_L^{(m)}$ and $P_{L+1}^{(m)}$, which consists of all types of the elements listed above, plus those with a lone bond at the surface end. All the elements in $P_4^{(m)}$ are then

$$\begin{aligned}\langle**11]&=\langle1111]+\langle0111]+\langle1011]+\langle0011]\\&=W_0^4+F_1W_1W_0^2+W_1F_1W_1W_0+F_2W_2W_0,\end{aligned}$$

$$\langle*110]=\langle1110]+\langle0110]=W_0^2W_2G_1+F_1W_1W_2G_1,$$

$$\langle1101]=W_0W_1F_1W_1,$$

$$\langle1100]=W_0W_4G_2,$$

$$\langle1001]=W_2F_2W_2,$$

$$\langle1000]=W_6G_3.$$

From Eq. (6), we finally find, by inspection of the terms in $P_L^{(m)}$, the augmented matrix $\mathbf{T}_L^{(m)}(\sigma)$ is given by

$$\begin{aligned}
&(\mathbf{T}_L^{(m)})_{1,2n-1}=W_0, && n=1,2,3,\dots L-2\\
&(\mathbf{T}_L^{(m)})_{2n+2,2n}=W_{2n+2}G_{n+1}/(W_{2n}G_n), && n=1,2,3,\dots l-1\\
&(\mathbf{T}_L^{(m)})_{2n+3,2n+1}=W_{n+1}^2F_{n+1}/(W_n^2F_n), && n=1,2,3,\dots L-2,\\
&(\mathbf{T}_L^{(m)})_{1,2L-3}=W_0[1+W_{L-1}F_{L-1}/(W_{L-2}^2F_{L-2})],\\
&(\mathbf{T}_L^{(m)})_{2,1}=W_2G_1/W_0,\\
&(\mathbf{T}_L^{(m)})_{3,2}=W_1^2F_1/(W_2G_1),\\
&(\mathbf{T}_L^{(m)})_{i,j}=0, && \text{otherwise.}
\end{aligned} \tag{15}$$

For example,

$$T_4^{(m)}=\begin{pmatrix}
W_0 & 0 & W_0 & 0 & W_0\left(1+\frac{W_2F_2}{W_1^2F_1}\right) & 0 & \cdots\\
\frac{W_2}{W_0}G_1 & 0 & 0 & 0 & 0 & 0 & \cdots\\
0 & \frac{W_1^2F_1}{W_2G_1} & 0 & 0 & 0 & 0 & \cdots\\
0 & \frac{W_4}{W_2}\frac{G_2}{G_1} & 0 & 0 & 0 & 0 & \cdots\\
0 & 0 & \frac{W_2^2}{W_1^2}\frac{F_2}{F_1} & 0 & 0 & 0 & \cdots\\
0 & 0 & 0 & \frac{W_6}{W_4}\frac{G_3}{G_2} & 0 & 0 & \cdots\\
. & . & . & . & . & . & \cdots
\end{pmatrix}. \tag{16}$$

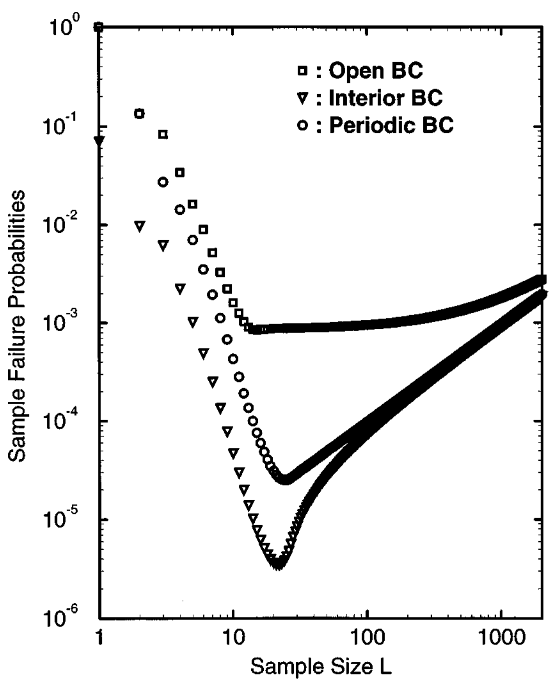

FIG. 4. Log-Log plots of the sample failure probabilities vs sample size for $\sigma_M/\sigma=0.07$, for open, periodic, and interior boundary conditions.

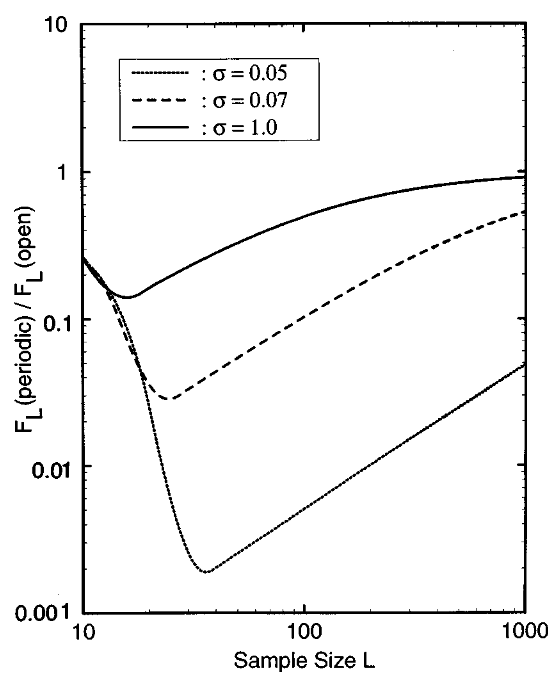

FIG. 5. The ratio $F_L^{(p)}(\sigma)/F_L^{(o)}(\sigma)$ vs L for different external stresses. Since the periodic samples have no surfaces, this ratio is a measure of the fraction of failures that originate in the interior of samples with open boundaries.

Now, to calculate $G_L(\sigma)$ in the no-lone-bond approximation, we only include the probability elements of the first and all even number of endings in the final $P_L^{(m)}$ to obtain

$$G_L(\sigma)=1-(11010\cdots)\mathbf{T}_{L-1}^{(m)}\mathbf{T}_{L-2}^{(m)}\cdots\mathbf{T}_4^{(m)}\mathbf{T}_3^{(m)}\mathbf{T}_2^{(m)}P_2^{(m)}. \tag{17}$$

VI. STM WITH OPEN BOUNDARY CONDITIONS

For the same reason discussed in the previous section, to calculate the failure probability $F_L^{(o)}(\sigma)$ with both ends open to the surfaces, we must construct the enlarged probability columns and the corresponding STM. The probability elements of $P_L^{(o)}$ here consist of all possible open configurations without any lone bonds, plus those with only one lone bond at one end. For example, the elements in $P_5^{(o)}$ are

$$\begin{aligned}[{*}{*}{*}11]&=[11111]+[01111]+[11011]+[00111]\\&\quad+[00011]\\&=W_0^5+G_1W_2W_0^3+W_0W_1F_1W_1W_0+G_2W_4W_0^2\\&\quad+G_3W_6W_0,\end{aligned}$$

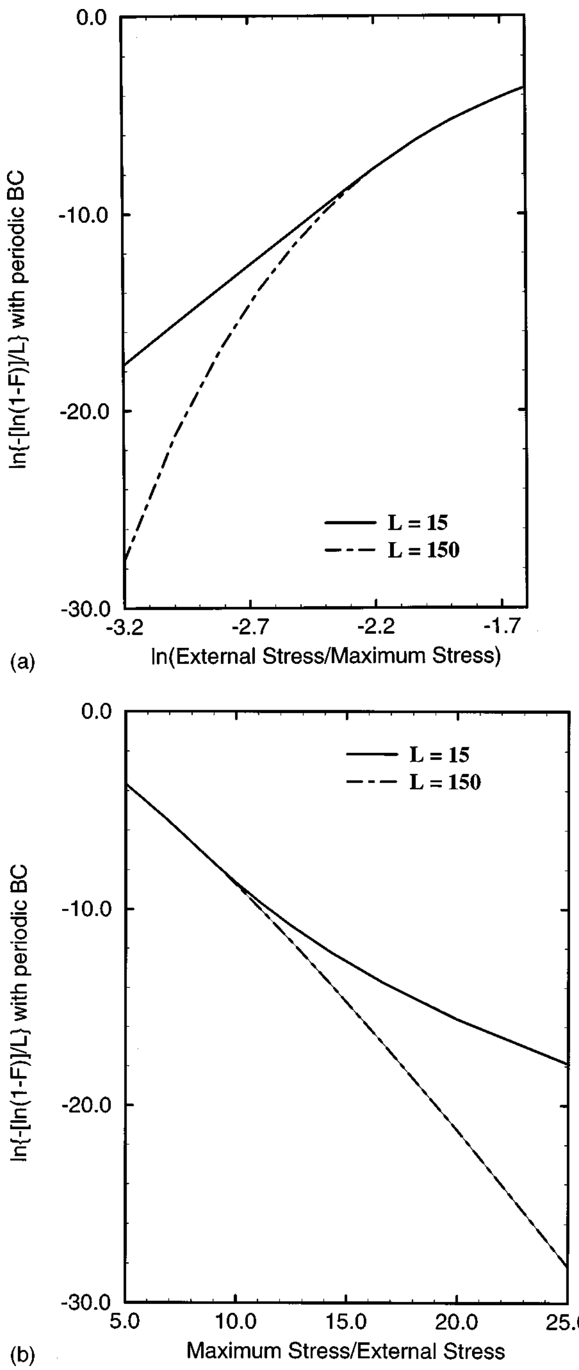

FIG. 6. (a) Weibull plot of $A=\ln[-\ln(1-F_L^{(p)})/L]$ vs $\ln(\sigma/\sigma_M)$ and (b) Gumbel plot of A vs σ_M/σ, for periodic boundary conditions, with $L=15$ and 150.

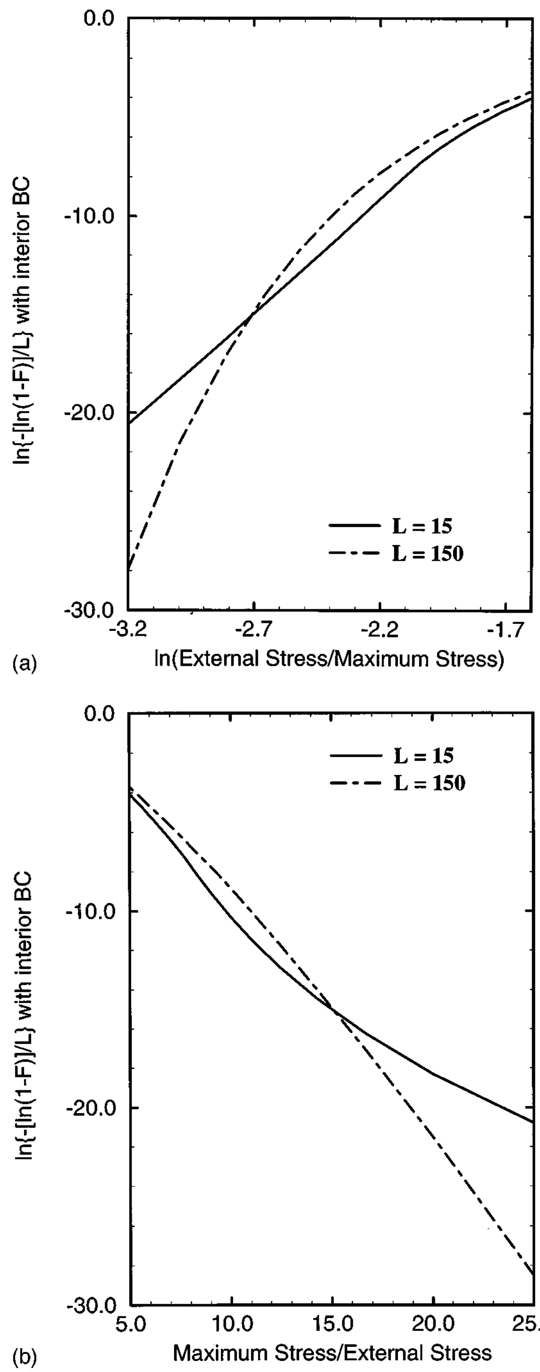

FIG. 7. (a) Weibull plot of $A=\ln[-\ln(1-F_L)/L]$ vs $\ln(\sigma/\sigma_M)$ and (b) Gumbel plot of A vs σ_M/σ, for interior boundary conditions, with $L=15$ and 150.

$$[**110]=[11110]+[01110]+[00110]$$
$$=W_0^3W_2G_1$$
$$+G_1W_2W_0W_2G_1+G_2W_4W_2G_1,$$
$$[*1101]=[11101]+[01101]$$
$$=W_0^2W_1F_1W_1+G_1W_2W_1F_1W_1,$$
$$[*1100]=[11100]+[01100]$$
$$=W_0^2W_4G_2+G_1W_2W_4G_2,$$

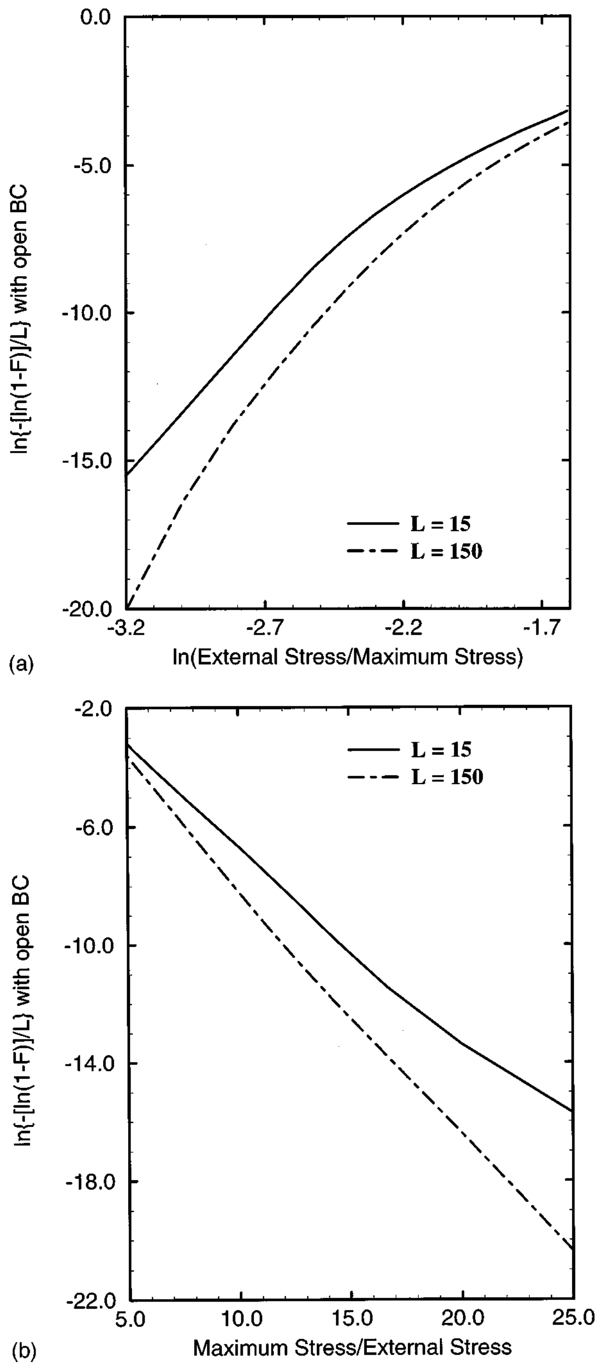

FIG. 8. (a) Weibull plot of $A=\ln[-\ln(1-F_L^{(o)})/L]$ vs $\ln(\sigma/\sigma_M)$ and (b) Gumbel plot of A vs σ_M/σ, for open boundary conditions, with $L=15$ and 150.

$$[11001]=W_0W_2F_2W_2,$$
$$[11000]=W_0W_6G_3.$$

The desired matrix $\mathbf{T}_L^{(o)}(\sigma)$, which successively generates probability columns $P_L^{(o)}$ for larger and larger L turns out to be the same as $\mathbf{T}_L^{(m)}(\sigma)$ in Eqs. (12), except for some minor modifications,

$$\begin{array}{ll}
(\mathbf{T}_L^{(o)})_{1,2n-1}=W_0, & n=1,2,3,\ldots,l-2\\
(\mathbf{T}_L^{(o)})_{2n+2,2n}=W_{2n+2}G_{n+1}/(W_{2n}G_n), & n=1,2,3,\ldots,L-2\\
(\mathbf{T}_L^{(o)})_{2n+3,2n+1}=W_{n+1}^2F_{n+1}/(W_n^2F_n), & n=1,2,3,\ldots,l-3,\\
(\mathbf{T}_L^{(o)})_{1,2L-4}=W_{2L-2}G_{L-1}/(W_{2L-4}G_{L-2}), & \\
(\mathbf{T}_L^{(o)})_{2,1}=W_2G_1/W_0, & \\
(\mathbf{T}_L^{(o)})_{3,2}=W_1^2F_1/(W_2G_1), & \\
(\mathbf{T}_L^{(o)})_{i,j}=0, & \text{otherwise}.
\end{array} \tag{18}$$

Again as in Eq. (17), within the no-lone-bond approximation, we finally obtain the total failure probability for an open-end array of length L:

$$F_L^{(o)}(\sigma)=1-(11010\cdots)\mathbf{T}_{L-1}^{(o)}\mathbf{T}_{L-2}^{(o)}\cdots\mathbf{T}_4^{(o)}\mathbf{T}_3^{(o)}\mathbf{T}_2^{(o)}P_2^{(o)}, \tag{19}$$

and that for an isolated square sample with open edges

$$F_{L\times L}^{(o)}(\sigma)=1-[1-F_L^{(o)}(\sigma)]^L. \tag{20}$$

VII. THE SURFACE EFFECT

We next evaluated F_L, $F_L^{(p)}$, and $F_L^{(o)}$ numerically by iterating Eqs. (11), (14), and (19) exactly. The most obvious result that appears in our calculations (see Fig. 4) is that the

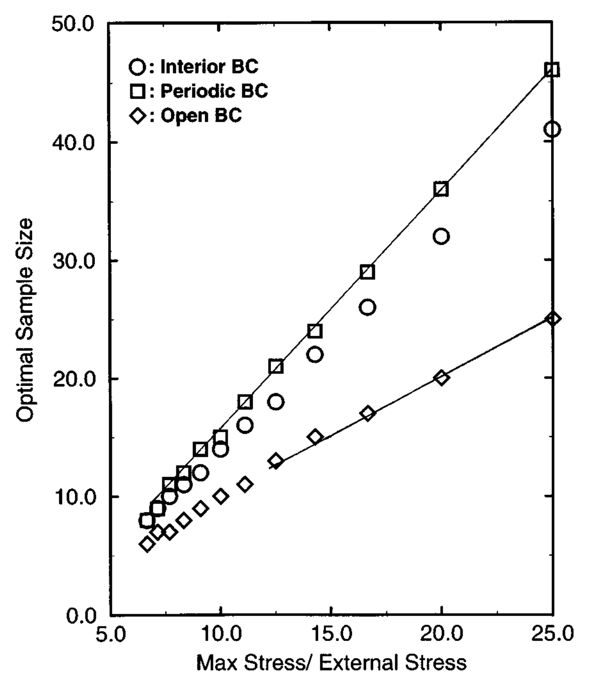

FIG. 9. Plots of $L_{\min}^{(p)}$, $L_{\min}^{(i)}$, and $L_{\min}^{(o)}$, as a test of Eqs. (3) and (4). The slope of one for the open case is just the half of that for the periodic case, as predicted by the model.

introduction of the surfaces *significantly* increases the sample failure probability by *orders of magnitude* over a very large range of sample sizes.

As expected from physical considerations, the numerical results show the following inequalities:

$$F_L^{(o)}(\sigma) > F_L^{(p)}(\sigma) > F_L(\sigma), \tag{21}$$

for a given sample size L and applied stress σ. Of course, all three of these sample failure probabilities merge toward the same thermodynamic limit when the sample size becomes extremely large:

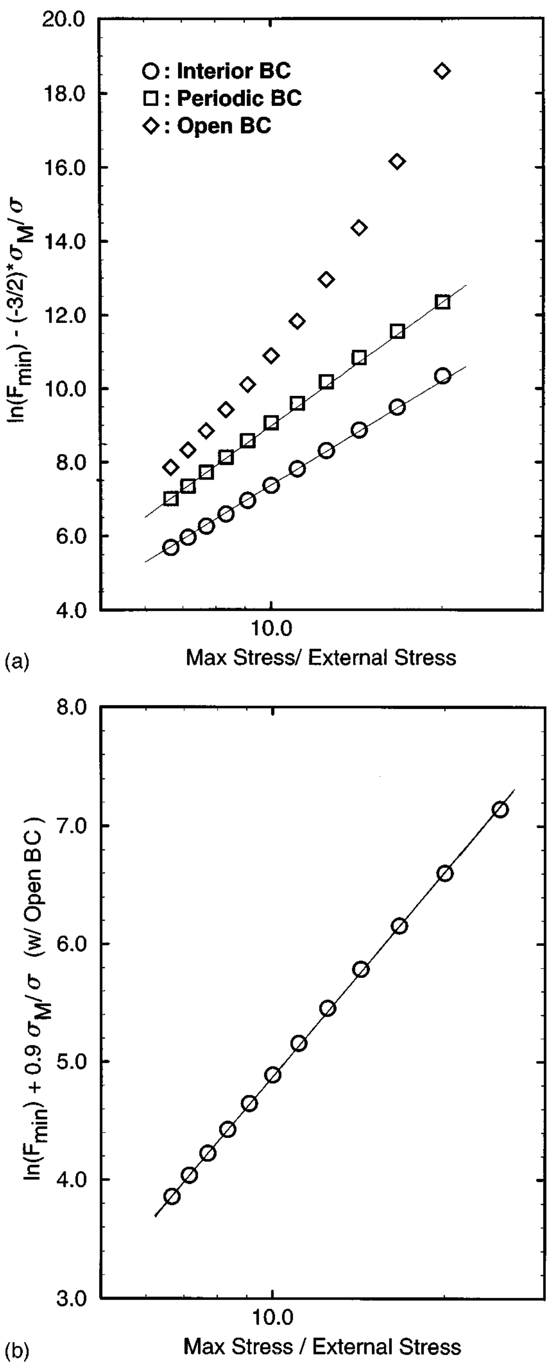

FIG. 10. (a) Plots of $\ln(F_{\min})+1.5(\sigma_M/\sigma)$ vs σ_M/σ for interior, periodic, and open boundary conditions, and (b) plot of $\ln(F_{\min})+0.9(\sigma_M/\sigma)$ vs σ_M/σ for open boundary conditions as fits to Eq. (24).

$$\lim_{L\to\infty} F_L^{(o)}(\sigma) = \lim_{L\to\infty} F_L^{(p)}(\sigma) = \lim_{L\to\infty} F_L(\sigma) = 1. \tag{22}$$

Near the maximum crack size M, we find again a minimum in $F_L^{(p)}(\sigma)$, but it is not as deep as that in $F_L(\sigma)$. And the optimum sample size with periodic boundaries is slightly larger than that for $F_L(\sigma)$. As for the sample failure probability $F_L^{(o)}(\sigma)$ for open systems, we see, from Fig. 4, that the minimum becomes much shallower than that in $F_L^{(p)}(\sigma)$ to the extent that it becomes less obvious that there is an optimum sample size.

Although the only difference we have introduced into the calculation of $F_L^{(o)}(\sigma)$ is to use those modified probabilities at the ends of each sample configurations to model the surfaces, the difference in the total sample failure probabilities between systems with open and periodic boundary conditions turns out to be very significant. In Fig. 5 we plot the ratio of the two probabilities $F_L^{(p)}(\sigma)/F_L^{(o)}(\sigma)$ for different external stresses. At $\sigma/\sigma_M = 0.07$, the ratio has the minimum of about 0.03. This means that only 3% of failures, in two-dimensional samples with open edges, are initiated from the interior of the sample, or that 97% of the failures originate from the surfaces. And this occurs in our calculation because the surface cracks only have one end to hold the stress enhanced. We believe that these results provide a clear explanation of why, in practice, cracks on the surfaces are responsible for most fractures in the real materials.

In order to understand the failure probabilities as a function of the applied stress, we next plot the quantity $\ln[-\ln(1-F_L)/L]$ against $\ln(\sigma/\sigma_M)$ and σ_M/σ. The former is a Weibull plot, and will provide us with a test of the so-called Weibull form.[3,8] The latter is a modified Gumbel plot, which tests the double-exponential modified Gumbel form.[3,8] In Figs. 6(a) and 6(b), we show the two plots for the periodic cases and find that they are rather similar to those obtained earlier for the interior arrays [see Figs. 7(a) and 7(b)]. For an array of a length L smaller than the maximum crack size ($M = [2\sigma_M/\sigma - 2]$), the system follows very closely the Weibull distribution [a straight line at smaller σ/σ_M in Fig. 6(a)]. On the other hand, systems of larger sizes ($L > M$), which are brittle and simply cleave, exhibit clearly the double-exponential modified Gumbel behavior [a straight line in Fig. 6(b) for large L]. Similarly, the corresponding plots for the open arrays in Figs. 8(a) and 8(b) show the same general behavior, however, with the above-mentioned features being significantly distorted by the surface effects. In general, we find that, in all forms of boundary conditions, when the samples are brittle $F_L(\sigma)$ displays a modified Gumbel distribution versus applied stress σ, whereas when they are tough (i.e., have random bonds strong enough to stop simple cracks from cleaving the sample) $F_L(\sigma)$ displays a Weibull distribution versus σ. This is at least suggestive of a general behavior in real samples.

Qualitatively, the optimal sample sizes or minima in F_L, $F_L^{(p)}$, and $F_L^{(o)}$ appear at points $L_{\min}$, which are proportional to M, and in this model is inversely proportional to applied stress

$$L_{\min} \sim A(\sigma_M/\sigma). \tag{23}$$

From Eqs. (3) and (4), it is not difficult to see that, for sufficiently large samples, the constant A is equal to 1 with the open boundary condition where $L_{\min} \sim k_s$, and is equal to 2 with either the periodic or interior boundary conditions where $L_{\min} \sim k_i$. Plots of $L_{\min}$, $L_{\min}^{(p)}$, and $L_{\min}^{(o)}$ versus σ_M/σ are given in Fig. 9, showing the expected behavior.

The qualitative behavior of the minimum failure probability can also be obtained from a simple approximate argument. In the tough region the order of magnitude of $F_L(\sigma)$ is given by

$$F_L(\sigma) \sim (\sigma/\sigma_M)^L L!, \tag{24}$$

since σ^L is the probability that L bonds fail, and $L!$ is the number of ways of ordering these L failures. By Stirling approximation this becomes

$$F_L(\sigma) \sim L^{1/2} \left(\frac{\sigma L}{\sigma_M e} \right)^L. \tag{25}$$

According to Eq. (23), $F_{L_{\min}}$ can be written in the form of

$$F_{L_{\min}} \sim a(\sigma_M/\sigma)^b \exp(-c\sigma_M/\sigma). \tag{26}$$

More careful arguments [involving the analytical solution to a linearized difference equation for the generating function of $F_L(\sigma)$] tend to be of this same form, but with different coefficients (a, b, and c). We therefore tried the three-parameter fits to the above formulas for the three different boundary conditions. The results are shown in Fig. 10, where $c = 1.5 \pm 0.1$ for both the interior and periodic cases [see Fig. 10(a)], and $c = 0.9 \pm 0.06$ for the open boundary conditions [see Fig. 10(b)].

VIII. CONCLUSIONS

We have introduced a simple model with local load sharing and an approach that allows a first-principles calculation of the dramatic effect of surfaces on the failure probability of materials with a heterogeneous microstructure, particularly those undergoing the tough-to-brittle transition. This calculation makes it clear that surface effects should be included in any calculation for the failure distribution of real materials.

We also found that the tough samples displayed a Weibull failure distribution at low stress but the crossover to brittle behavior corresponded also to a crossover to Gumbel-type failure distribution, even with open boundary conditions. It will be interesting to see if experiments on real samples and/or numerical simulations are consistent with these results.

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