Journal of the Physical Society of Japan
Vol. 76, No. 11, November, 2007, 114801

Crack-Tip Stress Concentration and Mesh Size in Networks

Satoko NAKAGAWA and Ko OKUMURA*

Department of Physics, Graduate School of Humanities and Sciences, Ochanomizu University, 2-1-1 Otsuka, Bunkyo-ku, Tokyo 112-8610

(Received May 15, 2007; accepted August 27, 2007; published October 25, 2007)

We consider two-dimensional networks with different mesh sizes but with the same bulk elasticity. We introduce a small (pseudo-) line crack in each network and numerically calculate the force distribution when the networks are (strongly) stretched in the direction perpendicular to the line crack. Even in highly deformed networks, we find that there exist strain-dependent scaling relations between the maximum stress (appearing at the crack tip) and the mesh size: the larger the mesh size, the smaller the stress concentration, and, thus, the stronger the network. Our finding might suggest a way of reinforcement of materials with voids under a given amount of solid.

KEYWORDS: gels, fracture
DOI: 10.1143/JPSJ.76.114801

When there is a crack in materials, the stress is enhanced near the crack tip,[1] which is one of the principal factors governing the strength; to appreciate this, just take a piece of paper and apply a tensile force with hands: the paper hardly breaks unless you are very strong; it easily breaks, however, after you introduce a short line crack, ideally by a sharp knife, in the middle of the paper in the direction perpendicular to the tensile force: the crack expands from the tip because of the enhanced crack tip stress. Accordingly, control over the tip stress concentration[2] is among other ideas to seek strong composites or structured materials,[3–6] often, by mimicking natural materials such as nacre[7–11] or double network gels.[12,13] Here we demonstrate an important feature of stress concentration, implying a guideline to create tough structured materials: in materials with voids the stress concentration could be reduced by making the void size larger. This strategy also leads to make the materials light and economical in the sense that from a given amount of solid we could produce more amount of the bulk material with voids as the void size is increased for toughening.[14]

To model a structure with voids, we consider *a coarse-grained model*: $N \times N$ points, initially arranged in a two-dimensional square lattice, with each point connected to the four nearest neighbors with a spring of length l [Fig. 1(a)]. The energy of the system is given by

$$U = \frac{1}{2}\sum_{i,j=1}^{N}\sum_{s=1}^{4}\frac{k(i,j,s)}{2}(|\mathbf{X}_{ij}^{(s)} - \mathbf{X}_{ij}| - l)^2, \qquad (1)$$

where $\mathbf{X}_{ij}$ represents the coordinate of each points and $\mathbf{X}_{ij}^{(s)}$ is that of the nearest neighbor points of $\mathbf{X}_{ij}$:

$$\mathbf{X}_{ij}^{(s)} = \begin{cases} \mathbf{X}_{i+1\,j} & (s=1) \\ \mathbf{X}_{i\,j+1} & (s=2) \\ \mathbf{X}_{i-1\,j} & (s=3) \\ \mathbf{X}_{i\,j-1} & (s=4) \end{cases} \qquad (2)$$

Here, the spring constant $k(i,j,s)$ is set to a constant k everywhere except at the boundary (i.e., i or/and j are either 1 or N).

*E-mail: okumura@phys.ocha.ac.jp

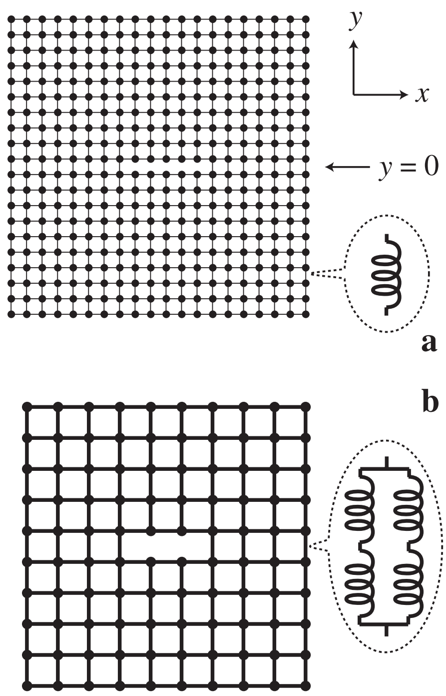

Fig. 1. Illustration of the present models for materials with voids for a small N and m ($N = 20$, $m = 2$): (a) the original network system and (b) another system with the double mesh size. In (b), a bundle of two serial connections of two original springs in (a) are used to connect the points, to obtain the identical bulk elasticity. Crack size ($a = 6l$) is the same in the two systems.

When this system of size $L = (N-1)l$ is extended in the y direction by the amount ΔL, each spring of length l is extended by $\Delta L/(N-1) \equiv l\varepsilon$ with the strain ε defined as $\Delta L/L$. The force F acting on springs in parallel with the y axis (corresponding $s = 2$ and 4) is homogeneous ($F = kl\varepsilon$), while that in perpendicular to the y axis (corresponding $s = 1$ and 3) is zero. The "stress" σ defined as force "per spring", i.e., F/l, satisfies the Hooke's relation $\sigma = k\varepsilon$. Note here that our two-dimensional model can be viewed as a two-dimensional section of a three-dimensional body like a plain strain problem in the theory of elasticity.

The force distribution under stretch is no longer as simple as above when a line crack is introduced. Here, we introduce a pseudo line crack by cutting n bonds in the middle ($y = 0$), i.e., by setting $k(i, j, s)$ to zero at corresponding points ($j = N/2$ for $s = 2$ and $j = N/2 + 1$ for $s = 4$ for even N). Here, the crack length a and the void size d are identified with $(n + 1)l$ and l, respectively. We stretch the network in the y direction so that the strains at upper and lower ends, initially located at $y = \pm L/2$, are $\pm\varepsilon$, and obtain the equilibrium force distribution via numerical calculations: we solve the coupled $N \times N$ equations of motions,

$$\eta \frac{dX_{ij\,\alpha}}{dt} = -\frac{\partial U}{\partial X_{ij\,\alpha}}, \tag{3}$$

where α is the x or y component of the $\mathbf{X}_{ij}$ vector; after a sufficient time t with an appropriate damping constant η, the dynamics can be relaxed to a unique state, which is identified with the minimum energy state of the system under the constraints. We confirmed that η changes only the dynamical process to reach the equilibrium state: our results given in this paper are essentially insensitive to the parameter η.

Typical equilibrium positions of points are shown in Fig. 2. Note that this network model is nonlinear when $\varepsilon \sim 1$. A typical distribution of forces F working on each spring at mechanical equilibrium under stretch is shown in Fig. 3: the distribution shows the maximum F_M at the crack tip as expected. We note here that strains in our calculations below are rather large as in Fig. 2 because (1) large strain calculations probe the nontrivial (nonlinear) region of the model and (2) smaller strain calculations with high precision become difficult.

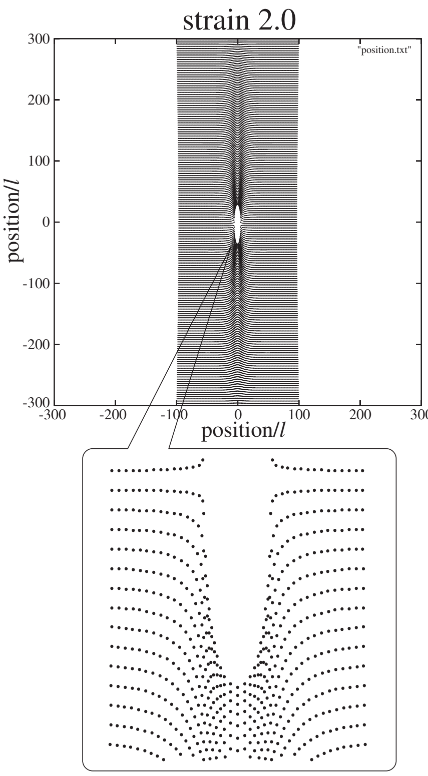

Fig. 2. Equilibrium positions of 200×200-point network with a crack ($a = 20l$) when stretched to $3L$ in the y direction. Positions are represented by small dots. A magnified view around the crack is shown at the bottom.

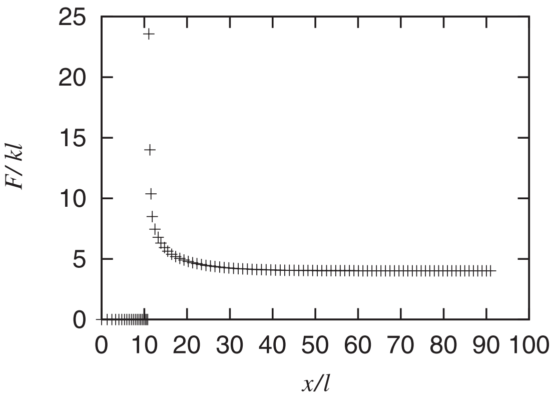

Fig. 3. Force concentration around the crack tip: forces acting on the spring located at $y = 0$ are plotted as a function of x with $x = 0$ being the center of the sample. In this case, the remote force (at $x/l \simeq N/2 = 100$) is enhanced nearly six times near the crack tip; the tip force (the cross located at $x/l \sim 10$ and $F/kl \sim 25$) defines the maximum force F_M. Here, the crack size a, strain ε, and system size N are $40l$, 4.0, and 200, respectively.

We next consider a network system consisting of $N/m \times N/m$ points connected by new springs of length ml, each of which is a bundle of m serial connections of m original springs [Fig. 1(b)]: the total number of the original springs in both systems is both $2N(N - 1)$. This implies that the bulk elasticity is identical with each other as explained just below. This preparation of networks corresponds to considering two porous systems made from the same amount of the solid but with different void sizes, $d = l$ and ml.

The bulk elasticity of the network is identified as follows. When the new spring of length ml is extended by δ the original spring is stretched by δ/m (with strain $\varepsilon = \delta/ml$) so that the elastic energy per new spring consisting of m^2 original spring is given by $U_1 = k(\delta/m)^2/2 \cdot m^2$, which leads to the elastic energy per unit volume (or area) $u = U_1/(ml)^2 = k\varepsilon^2/2$, irrespective of m.[15)]

For a given N ($= 200$) and various void sizes $d = ml$ ($m = 2, 5, 10$), we calculate the maximum force F_M among forces acting on a "new spring (a bundle of m serial connections of m original springs)", as a function of the mesh size d. Typical example of change of F_M with d for a given strain ($\varepsilon = 1.0$) and for different crack sizes ($a = 10l$, $20l$, and $40l$) are given in Fig. 4.

When the same plot are made on renormalized axes, σ_M/σ_0 ($\sigma_M \equiv F_M/d$ and $\sigma_0 \equiv k\varepsilon$) and d^*/a, the points are collapsed onto a single master curve when $d^*/a \ll 1$ as in Fig. 5. Here, d^* is a cut-off length, which could be the smallest length scale in the x direction in our simulation; such a length is always found to appear at the tip as the difference between the x-coordinates of the tip and its nearest point, as illustrated in Fig. 6. We confirmed that the cut-off scale d^* thus selected monotonously increases with d and results in a better data collapse than d.

Figure 5 and similar plots for different strains we have calculated all suggest a universal scaling form when $a \gg d^*$,

$$\frac{\sigma_M}{\sigma_0} \cong \left(\frac{d^*}{a}\right)^{\nu} \quad (a \gg d^*) \tag{4}$$

The independence of this relation on the system size L comes from the condition, $L \gg a$, well satisfied in our

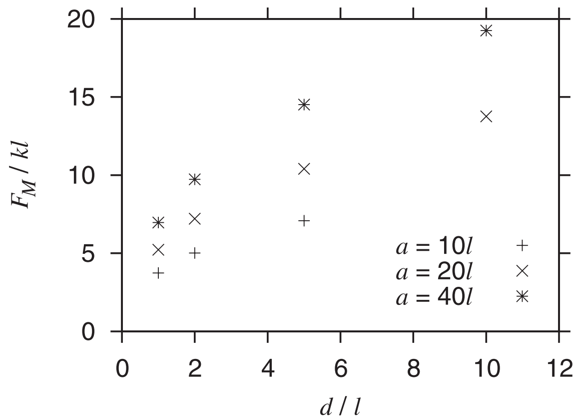

Fig. 4. Change of the maximum force F_M at the tip with void sizes d for a given stress $\varepsilon = 1.0$ and a given system size ($N = 200$). Three crack sizes, $a = 10l$, $20l$, and $40l$, are examined.

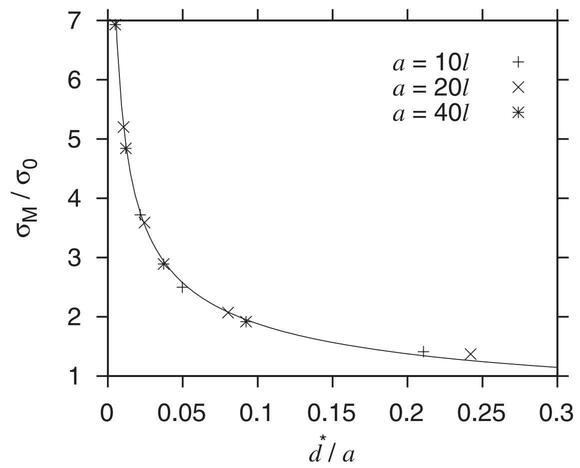

Fig. 5. The same plot with Fig. 4 but with renormalized quantities. The data for $\varepsilon = 1.0$ are collapsed onto a solid curve, or eq. (4) with $\nu = -0.45$ (see Table I), when $d^*/a \ll 1$. The maximum stress in the system becomes smaller as the void size gets larger, following the scaling law indicated in the text.

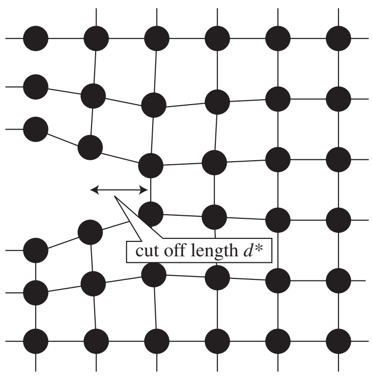

Fig. 6. The cut-off length d^* is identified with the smallest length scale appearing in the numerical calculation: the x-coordinate difference between the tip and its nearest neighbor.

simulation. The exponent ν seems to weakly depend on a given strain, approaching $\nu = -1/2$ as strain gets smaller, as indicated in Fig. 7 and summarized in Table I.

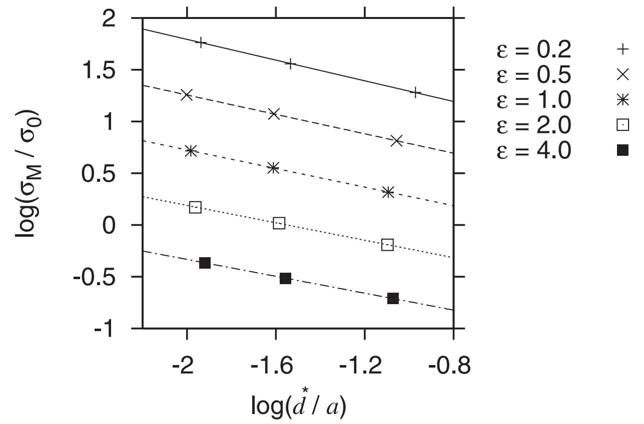

Fig. 7. Relation between σ_M and d^* for three smallest values of d^*/a at different strains from $\varepsilon = 0.2$ to 4.0 for a given crack length $a = 20l$. The points for $\varepsilon = 0.2$, 0.5, 2.0, and 4.0 are shifted by 1.0, 0.5, -0.5, and -1.0 upwards, respectively, to avoid overlap. The slope slightly depends on strain as stipulated in Table I.

Table I. Weak dependence of the exponent ν on strain ϵ, determined from Fig. 7.

ε	0.2	0.5	1.0	2.0	4.0
$-\nu$	0.50	0.47	0.45	0.42	0.41

Equation (4), confirmed in our numerical calculations, indicates that *the larger the void size, the smaller the stress concentration*. How large can be the void size? For example, the maximum mesh size of a net for filtering is determined by the size of particles to be filtered. Similarly, the void size is always restricted from the above, in practical situations.

The above result might be surprising at first sight in the light of the Griffith's conclusion:[16] small flaws should be removed to make materials strong. However, we should remind that the Griffith's flaws imply sharp line cracks, in which case a large crack weakens the material; in our models, the sharpness of the line crack tip is dulled by the void scale; *if we regard the mesh size as an effective radius of curvature of a crack tip (although without strict justification)* the above result is intuitively understandable at least for a linear elastic body because of classic analytical expressions obtained by Inglis.[1] What the above result suggests is that this intuition could remain essentially correct even in a highly deformed regime, which is nontrivial.

In other words, eq. (4) could be expected[13] from the well-known stress field near the fracture tip for a linear-elastic body:

$$\frac{\sigma(r)}{\sigma_0} \cong \left(\frac{a}{r}\right)^{1/2}, \tag{5}$$

where r is the distance from the tip. This stress field, mathematically diverging at the tip, should be cut off in practice at a scale where the continuum view breaks down. Identifying this scale with a cut off length d^*, we obtain eq. (4) with $\nu = -1/2$ [The correctness of this view (at $\nu = -1/2$) is indirectly supported by refs. 17, 18]. In our simulation, the exponents are not exactly one half, because (1) our system is linear-elastic only in the small strain limit and (2) there is a finite size effect, or a/L_m is not exactly zero in our system.[15)] This and preliminary calculations for even strongly nonlinear system (where the exponent in eq. (1) is changed from two) suggest that even in highly nonlinear-elastic region eq. (4) still holds with a negative ν.

From the above argument the exponent ν defined for a discrete system as in eq. (4) can be identified with the singular exponent β of the stress concentration defined, for the corresponding continuum system (the system in the continuum limit), by the equation, $\sigma(r) \sim r^{\beta}$. We should note, however, that it is impossible to extract a meaningful scaling exponent β directly from the quasi-critical behavior in a discrete system, as shown in Fig. 3, because the tip stress is finite: we might select the position of a fictitious tip where the stress is regarded as diverging although the stress is the maximum at a different point, i.e., at the position of the real tip, and, in addition, the exponent depends on the choice. On the contrary, the determination of ν does not depend on such choice and the exponent ν is expected to describe the singularity of the stress field near the tip in the corresponding continuum system, i.e., $\beta = \nu$.

In conclusion, we have demonstrated that in highly deformed two-dimensional networks the stress concentration around a pseudo-line crack is reduced with the increase in the mesh size via numerical calculation: the tip stress and a cut-off scale d^* (which monotonously increases with the mesh size) are found to satisfy the scaling relation eq. (4), with ν close to one-half but weakly depending on the strain, or on the degree of nonlinearity of the network. Note here that *our model is composed of linear springs* as in eq. (1) which is nonlinear in the positions of points because the expression contains the absolute value of the coordinate difference. We have checked that even if we replace d^* with the mesh size d itself a similar scaling relation is *approximately* valid: even if we change the horizontal axis d^*/a of Figs. 5 and 7 into d/a, in Fig. 5 the points collapse on to a single curve fairly well (though the former choice is clearly better) and in Fig. 7 three points at the same strain are well on a straight line (suggesting an approximate power law) but with a little smaller slope. In other words, the larger *the mesh size* (i.e., d itself) the smaller the stress concentration. This issue might be of relevance in some way to many structured materials which posses by definition a cut-off length for a continuum view: for example, in the case of gels, the cross-link density of the network could be a controlling parameter of the strength. On the contrary, in some very soft foams (cellular solids), it is found that the fracture energy is virtually independent of the geometrical parameters such as d.[19)] Bridging the gap between these two seemingly different behaviors, for example, would be an important problem to more closely connect our simple model calculations to real materials.

Acknowledgments

K.O. thanks the Ministry of Education, Culture, Sports, Science and Technology of Japan for a Grant-in-Aid for Scientific Research and Katsumi Hagita for refs. 17 and 18.

1) C. E. Inglis: Trans. Inst. Nav. Archit. **55** (1913) 219.
2) K. Okumura and P.-G. de Gennes: Eur. Phys. J. E **4** (2001) 121.
3) H. J. Gao, B. H. Ji, I. L. Jager, E. Artz, and P. Fratzl: Proc. Natl. Acad. Sci. U.S.A. **100** (2003) 5597.
4) W. J. Clegg: Science **286** (1999) 1097.
5) T. Kelly and B. Clyne: Phys. Today **52** (1999) 37.
6) Ch. Hellmich and F.-J. Ulm: J. Eng. Mech. **128** (2002) 898.
7) J. D. Currey: Proc. R. Soc. London, Ser. B **196** (1977) 443.
8) A. P. Jackson, J. F. V. Vincent, and R. M. Turner: Proc. R. Soc. London, Ser. B **234** (1988) 415.
9) M. Sarikaya and I. A. Aksay: *Biomimetics: Design and Processing of Materials* (AIP, New York, 1995).
10) D. R. Kattii, K. S. Katti, J. Sopp, and M. Sarikaya: J. Comput. Theor. Polym. Sci. **11** (2001) 397.
11) F. Song and Y. L. Bai: J. Mater. Res. **18** (2003) 1741.
12) J. P. Gong, Y. Katsuyama, T. Kurokawa, and Y. Osada: Adv. Mater. **15** (2003) 1155.
13) K. Okumura: Europhys. Lett. **67** (2004) 470.
14) Y. Huang and A. J. Kinloch: Polymer **33** (1992) 1330.
15) Strictly speaking, the system size L_m of the networks with different m are slightly different from $L = l(N-1)$: $L_m = ml(N/m-1)$. In the following, however, we are interested in the case where the system size is much larger than the crack size and study singular behaviors near the crack tip: we expect the properties are rather insensitive to the system size L_m and we call a possible weak dependence on physical quantities on L_m *finite size effect*. In numerical estimations, the system is streched by $\Delta L_m = \varepsilon L_m$ for a given strain ε.
16) A. A. Griffith: Philos. Trans. R. Soc. London, Ser. A **221** (1920) 163.
17) C. Hsieh and R. Thomson: J. Appl. Phys. **44** (1973) 2051.
18) R. Thomson: Solid State Phys. **39** (1986) 1.
19) Y. Shiina, Y. Hamamoto, and K. Okumura: Europhys. Lett. **76** (2006) 588.