PERGAMON

Solid State Communications 124 (2002) 167–170

solid state communications

www.elsevier.com/locate/ssc

Percolation study of defect tolerance in missing-crossbar networks

Michael P. Zwolak, Richard Zallen, Massimiliano Di Ventra*

Department of Physics, Virginia Polytechnic Institute and State University, Blacksburg, VA 24061-0435, USA

Received 13 August 2002; received in revised form 23 August 2002; accepted 10 September 2002 by M. Cardona

Abstract

We present a percolation study of two-dimensional crossbar networks and investigate their defect tolerance to missing crossbars. We find that the rate at which connectivity degrades in such circuits is nearly constant up to a missing-crossbar fraction f of about 50%, for both site and bond percolation. On the other hand, for $f > 0.5$ the rate of defect tolerance decreases very rapidly. This study provides a measure of the degree of reliability of crossbar networks presently envisioned for nanoelectronics, suggesting that this type of architecture is quite robust with respect to defect concentration. © 2002 Elsevier Science Ltd. All rights reserved.

PACS: 85.35.-p; 85.35.kt; 85.4B.Qx

Keywords: A. Nanostructures; A. Nanoelectronics; D. Percolation

With the expectation of the development of electronics based on circuit elements having nanometer-scale dimensions, a variety of molecular constituents have come under active consideration [1–8]. Theoretical studies of such systems have naturally focussed on the new and subtle quantum-transport issues that arise in such structures [10–16]. However, since the synthesis of nanoscale circuits may involve methods (such as self-assembly and self-ordering [1–8]) which could incorporate a significant concentration of defects (such as missing or non-conducting nanowires or active elements), it may also be useful to consider global issues such as the sensitivity of the long-range connectivity of two-dimensional networks to the defect concentration. Percolation theory [17,18] addresses such issues.

Recently, Heath et al. [19] reported impressive results for a massively parallel custom-configurable computer that operates quite successfully even though 3% of its hardware elements were defective. These authors suggest that their defect-tolerant computer architecture, whose wiring network features 'fat-tree' crossbar structures, could accommodate a defect fraction as high as 50%.[1]

Several interesting examples have been explored that use such network geometry with nanowires as interconnects and/or active elements, such as a set of parallel nanotubes overlayed by a set of nanotube crossbars [20,21]. Even though this type of crossbar network promises to be an ideal candidate for future nanoelectronics circuitry, the question of how sensitive such redundant architecture is to defects is still unsettled.

In this paper we investigate the percolation properties of a family of two-dimensional networks that models aspects of the defect tolerance of a system containing a specific type of defect, missing or inactive crossbars. This family of networks encompasses a wide range of anisotropies and a wide range of average coordination numbers. Both bond and site percolation are considered. The type of line defect we consider in the present paper is far more fatal than the single site or bond defect that will be randomly introduced to study the percolation properties of a given network. Nonetheless, we find that the rate at which connectivity degrades in such networks is nearly constant up to about 50% of the fraction f of missing crossbars for both site and bond percolation. On the other hand, for $f > 0.5$ the rate of defect tolerance decreases very rapidly (faster than exponentially). This study quantifies the degree of reliability of two-dimensional crossbar networks envisioned for nanoscale circuitry,

* Corresponding author. Fax: +1-540-231-7511.
E-mail address: diventra@vt.edu (M. Di Ventra).

[1] See footnote 26 in Ref. [19].

PII: S0038-1098(02)00541-0

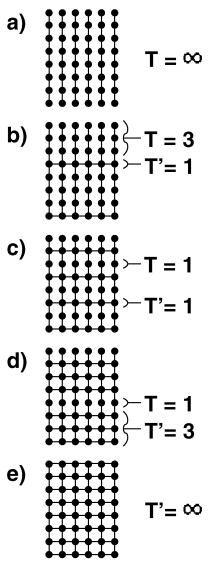

Fig. 1. Schematic of the family of networks considered in the present work. From (a), an array of separate vertical linear chains, horizontal linear chains are introduced to form the network (e). Clusters of T missing crossbars alternate with clusters of T' crossbars.

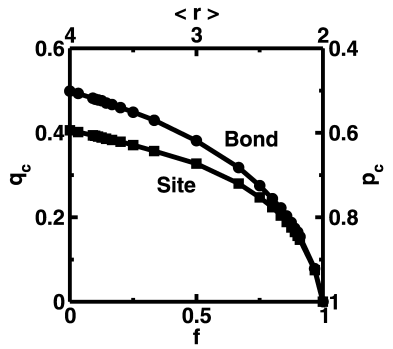

Fig. 2. Percolation results for the missing-crossbar networks of Fig. 1. The quantity q_c is the cutoff threshold $1 - p_c$, complementary to the percolation threshold p_c. The horizontal axes give the missing-crossbar fraction f and the mean coordination number $\langle r \rangle$. The dots and squares are the results of the computer simulations, the continuous curves are polynomial fits to these points.

suggesting that this type of architecture is quite robust with respect to defect concentration.

The family of networks we consider is shown in Fig. 1 by five examples, two of which ((a) and (e)) correspond to the end members, and one (c) corresponds to the midpoint of the set. Network (a) is simply an array of separate vertical linear chains. The bonds represent, for example, nanowires or conducting carbon nanotubes or sections of conducting polymer, and may contain active circuit elements [19–21]. The sites represent elements or contact points which are intended, in the ideal or perfect circuit (represented by network (e)), to communicate with a similar array of horizontal linear chains, referred to from now on as crossbars [19–21]. Between (a), with no crossbars present, and (e), with all crossbars present, we consider cases with a fraction f of crossbars missing. This fraction will play the role of a built-in defect concentration. For the perfect defect-free network, Fig. 1(e), $f = 0$; for the opposite limit, Fig. 1(a), $f = 1$.

For the intermediate cases, we look at structures that are periodic (two-dimensional crystals) and also maximally homogeneous. Clusters of T missing crossbars alternate with clusters of T' crossbars (see Fig. 1). The vertical repeat is $T + T'$ bond lengths (except for the endpoint networks, for which it is one bond length). Furthermore, either T or T' (or both, for network (c)) is equal to one. These simplicity conditions restrict the networks considered to an easily-visualized series, while still allowing us to examine enough values of f to map out the trend from $f = 0$ to 1.

The series of networks is two-dimensional (except for endpoint-network (a)) and anisotropic (except for endpoint-network (e)). The anisotropy is reflected in the ratio of the horizontal to the vertical conductivity, which is given by $T'/(T' + 1)$ when $f < 0.5$ and is given by $1/(T + 1)$ when $f > 0.5$. All sites of the perfect (square-lattice) network (e) have coordination number r (number of bonds stemming from a site) equal to 4; all sites in the decoupled-chains network (a) have $r = 2$. All of the other networks contain both coordinations, and the average coordination $\langle r \rangle$ decreases linearly with the missing-crossbar fraction f: $\langle r \rangle = 4 - 2f$. For the midpoint network (c), $T = T' = 1$, $f = 0.5$, and $\langle r \rangle = 3$.

We have carried out computer simulations for bond percolation and for site percolation on 21 networks of this family, using a network size of 3000×3000.[2] For each value adopted for the bond (or site) occupation probability p, the size of the spanning cluster (if present) was used to estimate the percolation probability P (the probability that a randomly chosen element belongs to the unbounded cluster). Results of 10 simulations (for each network and p value) were averaged, and p was then changed using a step size of 0.001. The results for $P(p)$, the percolation probability as a function of p (which were insensitive to the choice of a top-to-bottom or left-to-right spanning-cluster criterion [17]), were then used to determine the percolation thresholds p_c^{bond} and p_c^{site}. For the square-lattice limit of Fig. 1(e), the thresholds agreed well with the known values [17] of 0.5 (bond) and 0.593 (site); we obtained values of 0.501 and 0.594, respectively.

Fig. 2 shows our results for the percolation thresholds of this series of networks, plotted as a function of the missing-crossbar fraction f (the scale at the bottom) and the average coordination $\langle r \rangle$ (the scale at the top). In the context of this

[2] This network size has been chosen to obtain converged results in the case of network (e) (Fig. 1(e)) for both site and bond percolation thresholds.

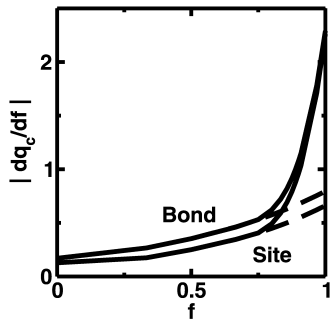

Fig. 3. Absolute value of the derivative of the cutoff threshold ($q_c = 1 - p_c$) with respect to the missing-crossbar fraction f, as a function of f for both site and bond percolation. This quantity represents the sensitivity of the defect tolerance to the missing-crossbar fraction. The dashed lines are high-f extrapolations of the exponential behavior in the $0.50 < f < 0.75$ region.

paper, we have plotted q_c on the vertical axis, where $q_c = 1 - p_c$. The cutoff threshold q_c is the fraction of unoccupied (disconnected or defective) elements which produces the absence of long-range connectivity and prevents transmission of a signal across the circuit. The quantity q_c can be interpreted as a rough measure of the defect tolerance of the network. When q_c is large, the network can accommodate a large concentration of individual defective elements without the loss of long-range connectivity; when q_c is small, a small concentration of defective components can break the circuit. The low-defect region near $f = 0$ (i.e. no crossbars missing) is expected to be the one of main interest. Here the initial slope $\frac{dq_c}{df}|_{f=0}$ represents the sensitivity of the defect tolerance to the missing-crossbar fraction characterizing the network. For bond percolation, the results of Fig. 2 yield a value of -0.18 for the initial slope:[3] for each 1% of crossbars missing, the cutoff threshold drops by 0.18%. For site percolation, the corresponding quantity is 0.13%. Interestingly, the sensitivity of the defect tolerance is nearly independent of the missing-crossbar fraction up to about $f = 0.5$. On the other hand, the same quantity decreases dramatically for $f > 0.5$. This behavior is shown in Fig. 3, where $|dq_c/df|$ is plotted as a function of f. It can be understood intuitively by looking at Fig. 1. For $f < 0.5$ (e.g. Fig. 1(d)) the network consists of highly-connected ($z = 4$) thick stripes separated by occasional (missing-crossbar) strips of single $z = 2$ connections that are readily crossed. It is only when crossbars cluster and extended chains of $z = 2$ sites appear (e.g. Fig. 1(b)) that percolation becomes more difficult and p_c increases dramatically.[3]

To summarize, we have studied percolation properties of a family of two-dimensional networks related to each other by the successive removal of extended parallel crossbars. The networks range in average coordination from 4 to 2. Such networks are presently envisioned for nanoscale electronics. We find that such networks are fairly insensitive to the fraction f of missing crossbars for values of f up to about 50%. The results provide a measure of the decrease in network defect tolerance produced by the introduction of missing crossbars, and suggest that this type of architecture is quite robust with respect to defect concentration.

[3] For bond percolation, there exists a useful but approximate dimensional invariant for the percolation threshold. It takes the form $\langle r \rangle p_c = d/(d-1)$, where d is the dimensionality (Ref. [17], p. 170). The two-dimensional version, $p_c = 2/\langle r \rangle$, is right on for our endpoint networks ($\langle r \rangle = 4$ and 2) but it fails for the intermediate networks. In particular, if $p_c = 2/\langle r \rangle$ is used to estimate $|dq_c/df|$ near $f = 0$, the result is too large by about 40%. For the midpoint network ($\langle r \rangle = 3$), $2/\langle r \rangle$ overestimates p_c by 7%. Although it is tempting to attribute this to the mixed-coordination character of the missing-crossbar networks, recent work on the mixed-coordination random lattice ($\langle r \rangle = 6$) shows that p_c in this case is extremely close (0.03%) to $2/\langle r \rangle$ [22]. Thus mixed coordination is not the reason. Since the failure of $2/\langle r \rangle$ to give p_c accurately for our networks is not significantly different from some simple single-coordination networks [17], it probably arises simply from the approximate nature of the empirical invariant.

Acknowledgements

Two of us (M.Z. and M.D.) acknowledge support from the National Science Foundation Grant Nos DMR-01-02277 and DMR-01-33075 and Carilion Biomedical Institute. Acknowledgement is also made to the Donors of The Petroleum Research Fund, administered by the American Chemical Society, for partial support of this research.

References

[1] R.M. Metzger, et al., J. Am. Chem. Soc. 119 (1997) 10455.
[2] C. Zhou, M.R. Deshpande, M.A. Reed, L. Jones, J.M. Tour, Appl. Phys. Lett. 71 (1997) 611.
[3] M.A. Reed, C. Zhou, C.J. Muller, T.P. Burgin, J.M. Tour, Science 278 (1997) 252.
[4] S. Datta, W. Tian, S. Hong, R. Reifenberger, J.I. Henderson, C.P. Kubiak, Phys. Rev. Lett. 79 (1997) 2530.
[5] J.K. Gimzewski, C. Joachim, Science 283 (1999) 1683.
[6] J. Chen, M.A. Reed, A.M. Rawlett, J.M. Tour, Science 286 (1999) 1550.
[7] Z.J. Donhauser, et al., Science 292 (2001) 2303.
[8] M.A. Reed, J. Chen, A.M. Rawlett, D.W. Price, J.M. Tour, Appl. Phys. Lett. 78 (2001) 3735.
[10] S. Datta, W. Tian, S. Hong, R. Reifenberger, J.I. Henderson, C.P. Kubiak, Phys. Rev. Lett. 79 (1997) 2530.
[11] M.P. Samanta, W. Tian, S. Datta, J.I. Henderson, C.P. Kubiak, Phys. Rev. B 53 (1996) R7626.
[12] M. Di Ventra, S.T. Pantelides, N.D. Lang, Phys. Rev. Lett. 84 (2000) 979.
[13] M. Di Ventra, S.T. Pantelides, N.D. Lang, Appl. Phys. Lett. 76 (2000) 3448.
[14] M. Di Ventra, S.-G. Kim, S.T. Pantelides, N.D. Lang, Phys. Rev. Lett. 86 (2001) 288.
[15] Y. Xue, S. Datta, M.A. Ratner, J. Chem. Phys. 115 (2001) 4292.

[16] N.D. Lang, Ph. Avouris, Phys. Rev. B 64 (2001) 125323.
[17] R. Zallen, The Physics of Amorphous Solids, Wiley, New York, 1983.
[18] D. Stauffer, A. Aharony, Introduction to Percolation Theory, 2nd ed., Taylor & Francis, London, 1994.
[19] J.R. Heath, P.J. Kuekes, G.S. Snider, R.S. Williams, Science 280 (1998) 1716.
[20] T. Rueckes, K. Kim, E. Joselevich, G.Y. Tseng, C.-L. Cheung, C.M. Lieber, Science 289 (2000) 94.
[21] Y. Huang, X. Duan, Q. Wei, C.M. Lieber, Science 291 (2001) 630.
[22] H.P. Hsu, M.C. Huang, Phys. Rev. E 60 (1999) 6361.