Dynamical Percolation Model of Conductance Fluctuations in Hydrogenated Amorphous Silicon

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Conductance fluctuations in hydrogenated amorphous silicon (a-Si:H) are simulated using a dynamical model of resistor diffusion on a lattice held at the percolation threshold. A fraction of lattice sites is designated as a trap, such that when a resistor diffuses onto that site it remains localized for a finite period of time. When a distribution of traps based on the defect density of a-Si:H is employed, the conductance fluctuations of the resistor network exhibit $1/f$ noise interspersed with random telegraph switching noise, as observed in experimental measurements of a-Si:H.

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Random resistor networks such as a lattice where bonds are randomly removed have proven to be successful models of electronic transport through static disordered media [1–8]. However conduction processes in many disordered materials often occur through a dynamic host environment where transport processes are subject to localized time dependent fluctuations. The influence of these fluctuations may be modeled by allowing the occupancy of the bonds to vary in time through mechanisms such as hopping processes. Dynamical percolation is relevant to a broad range of disordered systems which exhibit complex kinetic interactions, where structural or electronic rearrangements alter the properties of the material [9,10]. Examples include biological systems such as molecular gas diffusion through tissue and physical systems of electronic transport in polymeric ionic conductors, amorphous and crystalline semiconductors, diffusion processes in gelation phenomena, microemulsion systems, and vortex flow through type II superconductors. Despite the wide potential applicability to a diverse range of disordered systems, dynamical percolation techniques remain a relatively unexplored computational method for modeling disordered systems.

In this Letter dynamical percolation has been implemented to model random telegraph switching noise (RTSN) observed in coplanar conductance measurements of a-Si:H. The RTSN in a-Si:H is characterized by sharp jumps of the resistance between two or more discrete resistance values and is observed only for finite time intervals interspersed with the $1/f$ noise that is usually present. While the microscopic origin of RTSN in a-Si:H is unknown, it has been suggested that the switching noise results from time dependent changes in the conductance of inhomogeneous current paths networking the film that are sensitive to hydrogen motion. These filaments are modeled on a two-dimensional lattice for which only half of the bonds are occupied by resistors, corresponding to the percolation threshold. A certain fraction of resistors and adjacent empty sites are allowed to exchange places, which can alter the connectivity and conductance of network spanning filaments, leading to fluctuations in the bulk conductivity of the network. The key result of this paper is that when a distribution of traps based on the known defect distribution in a-Si:H is added to the dynamical percolation model then the conductance fluctuations of the network randomly exhibit RTSN between nonswitching fluctuations which have a $1/f$ spectral density, as observed in a-Si:H. In order to motivate the computer simulation results we begin by briefly reviewing the RTSN data in amorphous silicon.

Figure 1 illustrates the experimental switching noise at a temperature of 300 K for an n-type doped a-Si:H film

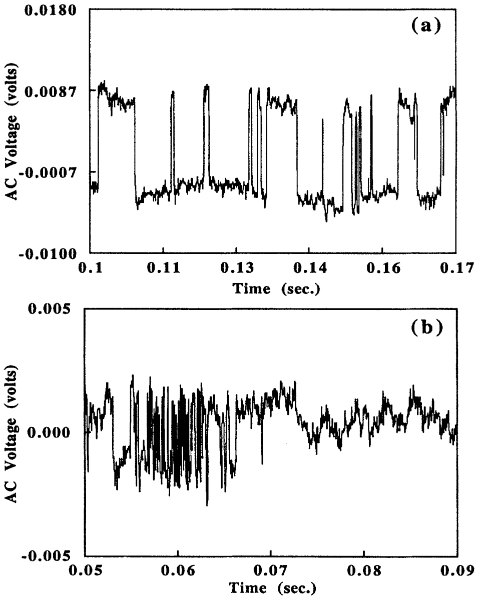

FIG. 1. (a) Time trace of the coplanar conductance as shown by the voltage fluctuations on the digital storage oscilloscope of n-type doped a-Si:H film at room temperature exhibiting RTSN. (b) RTSN is observed only intermittently over random time intervals ranging from seconds to hours. The voltage time trace in (b) was taken under identical experimental conditions as in (a) less than 1 h later. The nonswitching fluctuations (for times >0.7 sec) have a $1/f$ spectral density, as typically observed in a-Si:H.

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1 μm thick, synthesized in a rf glow discharge deposition system with a gas phase doping level of 10^{-3} PH_3/SiH_3. The coplanar electrodes are $\sim$0.5 mm wide with a separation of 1 mm and exhibit linear current-voltage characteristics. Four probe measurements confirm that the current noise does not arise from contact effects. Typically conduction fluctuations that are characterized by a $1/f$ power spectra are observed in these samples with RTSN appearing only intermittently as illustrated in Fig. 1(b). When RTSN is observed a wide distribution of switching times is often present, with individual switching events extending 20–30 msec in duration. The traditional model for RTSN, that is, single electron capture and emission, is unable to account for the large fractional resistance changes $\Delta R/R \sim (0.1-1)\%$ which occur over macroscopic volumes and at high temperatures in *a*-Si:H [11]. It has, therefore, been proposed that RTSN arises from current filaments, similar to percolation filaments in random resistor lattices, networking through the film [11]. As bottlenecks or narrow pathways of this otherwise macroscopic filamentary structure are altered by local electronic or atomic hopping processes, the bulk conductivity over macroscopic volumes of the film may be dramatically affected, just as a few critical bonds on a percolation network can influence the connectivity of the entire lattice [1,2]. It is known that hydrogen plays a central role in improving the electronic properties of *a*-Si:H by defect passivation; it has been suggested that hydrogen is also closely related to the observed RTSN [11]. One possible origin of the inhomogeneous current filaments in *a*-Si:H could be the known hydrogen microstructure [12]. As hydrogen diffuses throughout the film the resulting atomic reconfigurations may lead to the creation or elimination of pathways favorable for conduction. In one model for hydrogen diffusion [13] hydrogen is thermally excited out of a Si-H bond into an interstitial position, where is can then move freely until it is retrapped into a weak strained Si-Si bond or by a dangling bond. As the Si-Si traps are relatively shallow in energy, their trapping times will be short in comparison to the deep defect states. To investigate the plausibility of this model simulations of dynamical percolation were conducted on random resistor networks.

Simulations of a two-dimensional Cartesian lattice of resistors containing a Gaussian distribution of resistances were performed. Across the top and bottom of the lattice metal electrodes (infinitely conducting ends) are created and held at a fixed potential difference. Since half of the resistors are removed at random, corresponding to the percolation threshold $p_c = 0.5$, a series of filamentary structures between the infinitely conducting ends are generated, such as the one shown in Fig. 2(a). A transfer matrix method [4] is used to calculate the dc conductivity of a lattice over strips of length $L = 100\,000$ units and width $W = 20$ units; this lattice size is chosen to obtain convergence of the conductivity. At each time step a portion of the bonds are allowed to flip to unoccupied nearest neighbor positions and the conductivity is recalculated. As the bonds diffuse the connectivity of the filaments is altered with corresponding conductance changes as indicated in Fig. 2(b), where the diffusion rate corresponds to approximately 4% of the resistors flipping during any given time step.

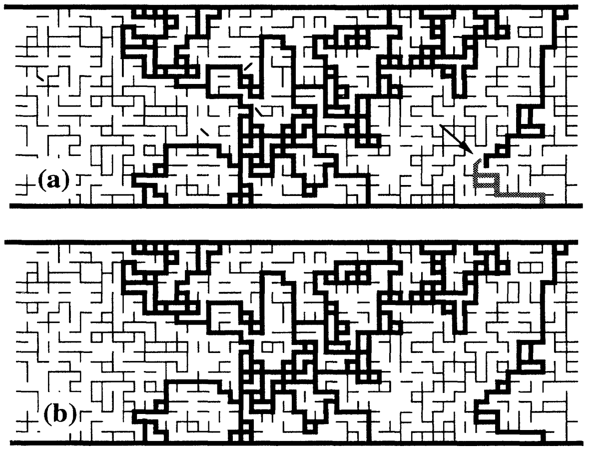

FIG. 2. A small portion of the random resistor lattice with half of the resistors removed for two consecutive time steps. (a) Initially this section contains one large filament spanning the width of the lattice. Only 4% of the resistors adjacent to an empty site are allowed to diffuse in this simulation. Those resistors which will move in the next time step are drawn as a diagonal line. (b) One time step later a new filament which spans the width of the lattice and hence contributes to the dc conductivity has been connected.

The use of a two-dimensional percolation network with this particular geometry held at the percolation threshold to model electronic conduction in three-dimensional *a*-Si:H films requires some justification. Estimates based upon the magnitude of the RTSN [11] along with experimental measurements of amorphous Si/SiN devices using a scanning focused laser beam [14] suggest that the filament diameter is on the order of the *a*-Si:H film thickness, which effectively decreases the dimensionality of the problem. In accord with this filamentary model the experimental presence of RTSN is sensitive to electrode geometry. If the region of *a*-Si:H being experimentally investigated is macroscopically large, multistate fluctuations from many filaments are observed and averaged into $1/f$ noise [15]. Consequently, in order to observe RTSN it is often necessary to reduce the region of *a*-Si:H being probed by etching away a portion of the *a*-Si:H. In these simulations implementing a long narrow lattice produces multiple filamentary structures across the electrodes [16]. The use of a resistor network held at $p_c = 0.5$ does not imply that the entire amorphous silicon film itself is at the percolation threshold. Rather the majority of the current paths in *a*-Si:H will be strongly interconnected and can be considered to be well above the percolation threshold. These filaments carry most of the current (the dc contribution to conductivity) and are relatively quiet in a noise measurement. A few microchannels can be considered to be at the percolation threshold; they carry a fraction of the total current but are very sensitive to small changes in their connectivity and dominate noise measurements. The length of the lattice necessary in order to obtain convergence of the dc conductivity contains many more network spanning filaments at p_c than are estimated to be present in a-Si:H. Consequently, only small sections of the entire lattice are allowed to undergo bond diffusion. In this manner the correct dc static result is obtained while studying the kinetics of smaller lattices which contain the correct number of evolving filaments. Details of the computer calculations are found in Ref. [16].

Initially the resistors were randomly allowed to diffuse throughout the lattice, structurally altering conduction pathways between the electrodes. The results from this preliminary work [16] generated a noise spectrum that had a Lorentzian form where the corner frequency was determined by the bond diffusion rate. As no evidence of RTSN was observed in this initial project, a distribution of traps was incorporated into the lattice where resistors would preferentially fall into traps of lowest energy. In the context of these dynamical percolation simulations a "trap" is defined as a particular lattice site for which a resistor diffusing onto that site remains localized for a fixed number of time steps. When a uniform distribution of trapping times is employed, so that short trapping times and long trapping times are equally likely, the primary effect is to decrease the effective bond diffusion rate with no change in the power spectra or magnitude of the fluctuations. Consequently, a nonuniform distribution of trapping times based on the exponential distribution of band tail energies (believed to arise from strained Si-Si bonds) in a-Si:H was studied, that is, $p(E) = \beta_0 e^{-E\beta_0}$ where $\beta_0^{-1} = kT_0$ is the Urbach energy, determined from subband-gap optical absorption measurements [17]. The average time τ that a resistor spends in a trap can be expressed in terms of the depth of the energy well and is given by $\tau = \tau_0 e^{E/kT}$, where τ_0 is the hopping time. This quantity is estimated from nuclear magnetic resonance measurements [18] to be $\tau_0 \sim 10^{-5}$ sec, which sets the time scale of the simulation. By assuming that trapping is a Poisson process [15] the distribution of trapping times $\tilde{t}$ arising from a single trap of energy E is $p(\tilde{t}\,|\,\tau) = (1/\tau)e^{-\tilde{t}/\tau}$. The resulting distribution of trapping times $p(\tilde{t})$ for the exponential distribution of well depth energies is given by

$$p(\tilde{t}) = \alpha \tau_0^{\alpha} \tilde{t}^{\,-1-\alpha} \gamma(\alpha + 1, \tilde{t}/\tau_0),$$

where $\alpha = T/T_0$ and γ is an incomplete gamma function [19]. This functional form is found to agree with the experimental data of RTSN, as described elsewhere [17].

A time trace of the conductance of the dynamical percolation model which includes the defect structure of a-Si:H is shown in Fig. 3 for trap parameters of $T = 300$ K and $T_0 = 1275$ K. As described earlier it is necessary to work on long ($L \sim 10^5$ bonds) lattices to obtain adequate convergence of the conductivity; however, only a length $L' = 2000$ bonds experience bond diffusion in order to reflect the fact that in a-Si:H the smaller sample geometries exhibit larger RTSN. A typical time trace of over 12 000 time steps which corresponds to 120 msec when $\tau_0 = 10^{-5}$ sec requires ~2 h of CPU time on a Cray X-MP. Occasionally clear evidence of resistance switching is observed, with a wide distribution of switching times, comparable to the duration of the experimental switching. The similarity between the simulated conductance fluctuations and the experimentally observed switching noise (Fig. 1) is striking. Moreover, the average magnitude of the fractional resistance change is $\Delta R/R \sim 1\%$ as in the experimental noise measurements. Consistent with the a-Si:H data, the RTSN in the simulations is observed only intermittently as illustrated in Fig. 3(b). The resistance switching spontaneously changes to nonswitching fluctuations, which have a $1/f$ power spectra, in contrast to the Lorentzian power spectra observed in the computational model without trapping [16]. The observation of RTSN in the simulations is sensitive to the initial lattice con-

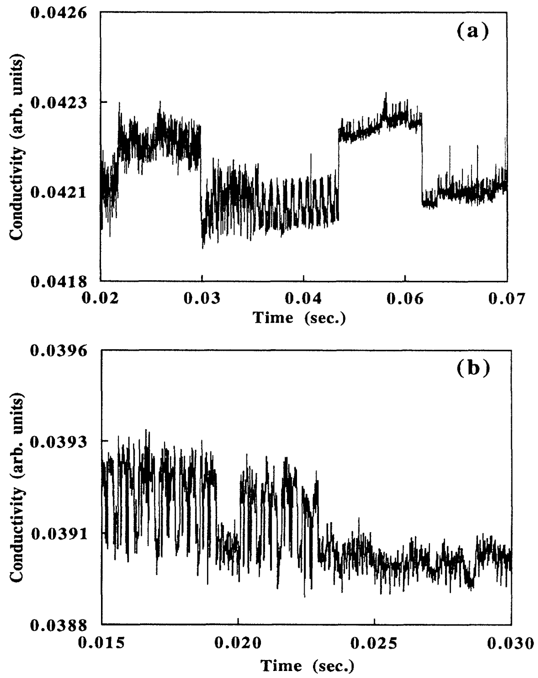

FIG. 3. (a) Time trace of the calculated conductance of the dynamical percolation random resistor simulation with a distribution of trapping sites added to the lattice as described in the text. This short section of the total time trace displays clear evidence of RTSN. (b) Another section of the total time trace displaying RTSN changing to nonswitching fluctuations whose spectral density has a $1/f$ frequency dependence. The time scales and magnitudes of the RTSN in these simulations vary intermittently as in the experimental measurements of a-Si:H.

figurations, just as in a-Si:H the presence of RTSN will vary with changes in the electronic state of the film due to light soaking and thermal annealing [20]. For all cases in which the trapping distribution in question differed significantly from the defect distribution in a-Si:H the resulting fluctuations failed to exhibit RTSN and/or regions of $1/f$ noise consistently. While the observation of $1/f$ noise is not surprising, since a trap distribution $p(\tilde{t}) \sim \tilde{t}^{-1}$ was added to the network, the intermittent presence of RTSN is markedly similar to the experimental observations in a-Si:H and supports the proposal that the switching noise arises from inhomogeneous current filaments subject to localized diffusion processes. Further details of the influence of trapping on the dynamical percolation simulations will be described elsewhere [17].

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