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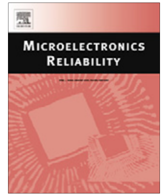

Noise and reliability in simulated thin metal films

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ABSTRACT

Many macroscopic aspects of electromigration damage in thin metal films have been investigated by means of Monte Carlo simulations based on simplified physical model. The employed model, can be described as a *middle-scale model*, in which the physical system is modeled with a high level of abstraction, without a detailed atomic physical model of the system.

Among the many effects of the electromigration phenomenon, the simulator has been used to investigate several statistical properties of electromigration failure and the noise behaviour.

Notwithstanding this simplicity, it is able to generate results in good agreement with many experimental observations: the lognormal distribution of failures, dependence of the mean time to failure from stress current and film geometry, Black exponent, noise statistics.

Furthermore, this simulations confirmed a significant correlation between electromigration noise in the initial phase of stress and time to failure which has been suggested by a few experimentalists. This correlation can be usefully exploited as an early indication of the onset of electromigration damage on a per-sample basis.

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1. Introduction

The recent developments in copper damascene interconnects technology for integrated circuits fostered a renewed interest in many physical phenomena related to interconnects reliability. Among these, a major role is played by electromigration (EM): indeed, the lower vulnerability to electromigration of high melting-point metals (1063 °C for copper vs 658 °C for aluminum) was one of the main reasons for the development of copper interconnects. Electromigration poses many challenges to materials science and technology, as many aspects remain unclear and hence reliability estimations are often made on the basis of a phenomenological approach. The physics of electromigration has been extensively studied, from the atom transport mechanism, to interface and grain boundary aspects, to the mechanical aspects of passivated structures [1–4].

However, we think that the role of the polycrystalline structure of metal interconnection has been frequently underestimated, and that it should be considered a key element for understanding interconnection reliability.

For this reason, we developed a model of polycrystalline thin films with a level of detail which includes the polycrystalline nature of the system, but, on the other hand, makes use of a simple phenomenological physical damage model and ignores the large scale aspects (i.e., stress and strain and other mechanical aspects). Our approach is based on a resistor network, in which the damage is simply modeled removing and restoring resistors from the network. A similar approach has been used in the case of a percolative approach [5], in which all resistors are equivalent and the network simulates a quasi-homogeneous system. Conversely, our model groups resistors into blocks corresponding to grains, and takes into account the interaction between grains. This simulation model is used to generate data that can be compared against electromigration experimental failure statistics and noise, providing additional insight for the comprehension of the relationship between the two.

Typically, experimental studies focused on measurements of mean time to failure (MTF) [6–8], that represents the reference parameter for interconnects reliability. While MTF studies provide information on the reliability of a metalization technique, they are of little use in a production environment, for predicting the reliability of individual wafers or batches of wafers. However, these studies allowed to identify many factors affecting the failure statistics of interconnects, and in particular the role of the grain structure of metal lines. Indeed, since the activation energy of atoms close to grain boundaries is significantly lower than that of bulk atoms, electromigration in Al and Al/Cu interconnections is believed to concentrate along grain boundaries [2,6].

For copper interconnections the details of the electromigration diffusion mechanism are less clearly understood. The current opinion [2,4,9] tend to emphasize the role of surface and interface diffusion, but many questions about the fastest EM pathway remain open. Copper interconnections EM behavior is strongly dependent on deposition technology and conditions, and a transition from "finegrained" to "bamboo" behavior, a feature suggesting grain

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boundary EM, can show up for some deposition technology (CVD see [6]).

In addition to their contribution to EM, grain boundaries have an another important effect in the definition of the current distribution in the stripe, which in turn plays a role in the development of EM damage, whatever be the main diffusion mechanism [10]. In fact, even a small damage at grain boundary level can lead to a current redistribution in the stripe, which in turn influences other EM diffusion locations and processes.

For this reason the grain size and layout have to be carefully taken into account in the model development in order to achieve an effective understanding of the phenomenon. Furthermore, the importance of the polycrystalline structure is enhanced by a positive feedback effect due to current path changes triggered by electromigration. Indeed, the grain boundary damage induces current density redistribution which, by increasing local current densities and creating critical paths, tends to increase the damage rate and speed up further damage evolution.

As a consequence of the leading role of grain boundaries and polycrystalline effects, we propose a model of thin metal films based on a middle-scale description of the structure, leaving aside a detailed description of atomic-level matter transport. Our model is aimed at reproducing the statistical behavior of metal interconnection with a "minimum effort" approach, which minimizes algorithm complexity and hence simulation time.

One of our main goals is to show that many electromigration features (from reliability statistics to the noise behavior) can be reproduced with a very simple model, but which cannot ignore the polycrystalline nature of thin metal films, since the typical dispersion of many experimental results regarding thin film interconnections is rooted into the interactions between the atom transport and the polycrystalline nature of the metal film.

For "deep bamboo" samples, where the stripe width is significantly less than the average grain diameter ($W \ll D$), instead, the behaviour is controlled by surface/interface atom diffusion and mechanical aspects, and the present model has a lower usefulness.

One of the more striking results of this simulation approach is the possibility to explain many experimental observations with the concept of *middle scale effect*. For example, an increase of the well known Black exponent for large stress currents in electromigration experiments can be explained with a Joule self heating effect [6]. However, this increment do happen also with our approach, which does not include explicitly joule self heating and temperature differences. Hence it can be described as a middle scale effect, i.e., a product of the polycrystalline structure of the sample.

Another group of studies has focused on the statistical properties of the typical $1/f^2$ noise [2,3,11,12] associated to electromigration. Since this type of noise is generated during the onset of the damage and of the subsequent current path changes, it is reasonable to conjecture that it could provide useful information even in the early stages of electromigration. In fact many experiments suggest that initial electromigration noise, which is not usually associated with observable damaging effects, can be a reliable leading indicator of subsequent interconnect durability. Hence one of the main goals of our simulation model was to investigate this hypothesis by correlating noise and MTF as extracted from simulation data on a per-run basis.

2. Model

Many simulation approaches have been proposed in the literature, which tackle electromigration from different points of view and with many different *dimensional scales*. In an *atomistic* simulation, electromigration damage is simulated by estimating the force exerted by the electron wind on every lattice atom [13]. At the opposite end of the spectrum we find *mechanical-hydrostatic* simulations, in which the interconnect is modeled as a continuum in which stress, strain and voids develop and migrate [14–16]. Even if these simulation approaches can reproduce the underlying physics quite well, they are often very demanding from the computational point of view, and hence can only be used for the detailed analysis of some particular aspect of the whole phenomenon or the detailed investigation of limited significant aspects. Moreover, applying these approaches to polycrystalline structures would further increase the total computational burden.

In fact, sometimes these simulations are performed without introducing in the description the polycrystalline nature of the systems, limiting the analysis to the study of a homogeneous sample of material [15].

Instead, we propose a low complexity model, only including the necessary physical aspects of the problem, without the burden of a complete and computationally intensive physical description. For this reason, we choose to represent an interconnection metal film with a simple resistor network, composed by a square lattice of interconnected identical resistors, together with a simple phenomenological approach to electromigration damage model. This approach has been used for years in the field of granular materials and percolative conductivity [5,17]. These studies led to impressive results, which showed that even a very simple model can provide useful information about complex phenomena. The proposed approach is similar to [18], but with a much lower model complexity.

As we shall show, it is possible to obtain results with an equivalent or superior significance even with this simplified phenomenological damage model, with a great computational burden reduction.

For such a reason our simulator is based on a two-dimensional model of a polycrystalline metal stripe, consisting of a rectangular resistor network. Such networks are composed of two types of resistors: *internal* resistors, which model bulk material, and *cross-border* resistors, which model the surfaces between adjacent crystals, where electromigration is more likely to occur. The grain structure is provided by a random generator based on a simulated growth algorithm [19]. Starting from a set of random positions (each of them represents a crystal grain), grains (blocks of adjacent nodes) enlarge until they come to contact and fill up all the available space. Resistors connecting nodes in the same grain are *internal*, while resistors connecting nodes of different grains are *cross-border*.

The resistor networks represent the input for the simulator, which computes the time evolution of the damage induced by a given constant current and provides the total electrical resistance of the stripe.

The local electromigration damage is simulated by assuming that only the cross-border resistors, which correspond to grain interfaces, can be initially damaged (i.e., interrupted) by the current flow, and that the probability of failure of each resistor is given by

$$P_f = A[\exp(I/I_0) - 1] \tag{1}$$

where I is the current flowing in the individual resistor and A and I_0 are constant coefficients. Then, the interrupted resistors are subsequently considered and possibly repaired with a fixed probability P_r. In this way, failures are activated by local current stress, while repair is due to atom thermal and stress induced diffusion and considered independent of local currents.

Afterwords, the resistors adjacent to damaged ones are in turn considered subjected to EM damage and this can lead to void development.

Hence the damage starts along grain boundaries and leads to a current increase in the neighborhood. This introduces a positive feedback which leads to an increase of the current flowing in the

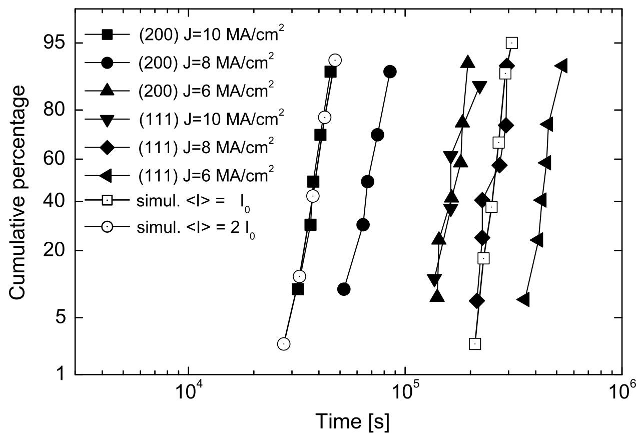

Fig. 1. Simulation results (white symbols) compared with experimental data (solid symbols) from [6] (near the symbols is indicated, with Miller indexes, the crystallographic orientation of the copper samples). Simulations assume $A = 10^{-6}$.

remaining resistors. This increasing current, in turn, increments the rate of failure of the remaining resistors, leading to an accelerated failure process. The damaged region typically grows faster and faster until complete failure of the stripe.

Further details of the damage model can be found in [20].

The simulator output provides, for every time step, the total stripe resistance and the number of failed and repaired resistors. We consider a stripe broken down only after a 20% resistance increase, as is typically assumed in experiments [6].

It is worth noting that I_0 and A in Eq.(1) are simple scale factors for current and time, respectively, and are a function of material and of the fabrication process. For this reason, in this work they will often assume arbitrary values, providing failure times in arbitrary units as a function of a given $\langle I\rangle/I_0$ ratio. Apart from the time scale, the behavior of the stripe does not depend on the particular material at hand. The actual value of I_0 and A can then be extracted from fitting with experiments. In fact, this simulator depends on a single parameter: the ratio between the stress current *per resistor*, which is the ratio of the total stress current I and the sample width, and I_0. This ratio sums up all the stressing elements: applied current, temperature, material properties.

3. Discussion and results

3.1. Resistance behavior and time to failure statistics

The usual method of assessing the quality of integrated circuits interconnects is based on destructive experiments in which a large number of stripes are stressed until breakdown, providing data for the calculation of failure statistics.

This experimental data can be compared with the output of the simulator, which can perform a complete run in a few minutes on a Linux PC, providing rapidly the corresponding failure statistics.

The resulting distribution of time to failure is lognormal, as is commonly observed in experiments [7,2], Fig. 1.

Furthermore, Fig. 1 shows the variation of the failure distribution for two different simulated current stress levels, in good agreement with experimental data.

It is worth noting that currents, failure times and geometric dimensions are all expressed in arbitrary units. Hard numbers depend on material properties and are beyond the scope of this work. Nevertheless, this "middle scale simulator" provides several insights on the nature of the electromigration phenomenon and is a powerful, robust and simple tool which can be used for interpret different experimental observations.

Figs. 2 and 3 show a comparison of simulated durability and experimental data obtained from copper [6]. A well known parameter used to describe electromigration phenomena is the Black exponent [1], which can be obtained by fitting the logarithmic plot of MTF versus J. Both simulated (Fig. 2) and experimental (Fig. 3) values are in the range of commonly observed values (1–3 [21,22]). To obtain the the experimantal values indicated in Fig. 3, the authors excluded the high current points, ascribing their accelerated failure to excessive joule heating [6].

However, by directly comparing of Figs. 2 and 3, it is possible to consider unnecessary the joule heating explanation postulated by the authors of [6], since the same accelerating failure at high currents is also reproduced by the model, which does not take joule heating into account. As for another effect which will be discussed later, this acceleration can be explained as a *middle scale effect* which arises only from the physical structure of the sample and does not require an *ad hoc* additional mechanism to be explained.

Perhaps, the most important structural parameter of a thin polycrystalline metal film is the grain size; for this reason we closely examined the relationship between failure statistics and grain size distribution. Even if most experimental studies concentrate on MTF, industrial applications depend on *predictability* as much as on

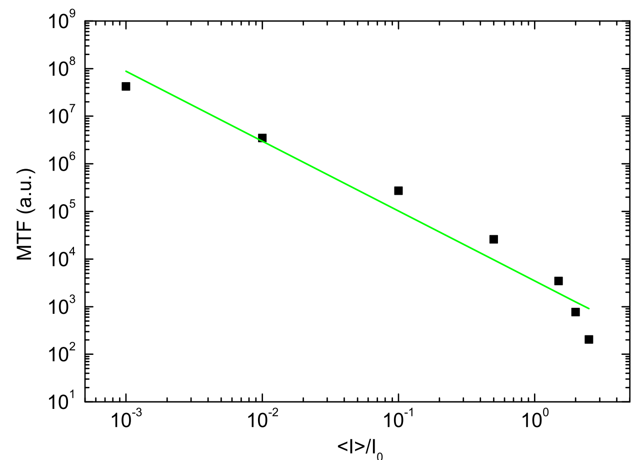

Fig. 2. Simulated MTF as a function of stress current; the fitting line shows the Black exponent (1.47).

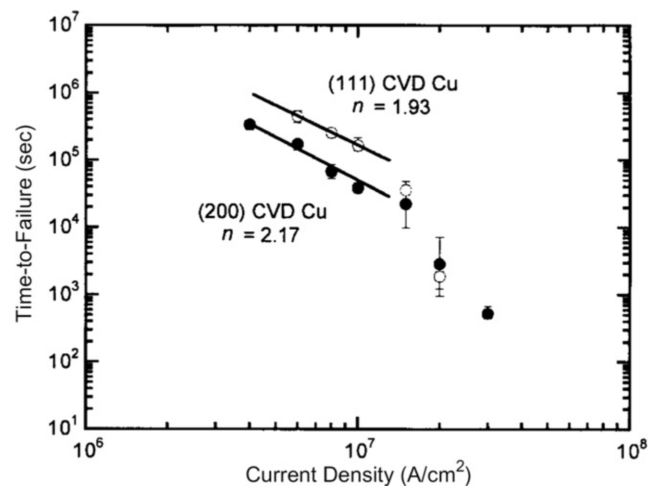

Fig. 3. Experimental time to failure as a function of stress current (from Fig. 4 of [6]).

reliability, since electromigration can lead to a small, but not negligible, percentage of early failures even in an overall reliable deposition process. This particular aspect can be evaluated by measuring deviation time to failure (DTTF). Unfortunately DTTF data is seldom available, as the deposition of a grain size controlled metal film is not easy. However [23], provides experimental MTF and DTTF data as a function of the ratio w/d of stripe width to grain diameter, obtained from 2.2 μm Al–2%Cu–0.3%Cr lines, annealed with a wide range of different conditions to modify their grain sizes. Fig. 4 shows the comparison of this results with corresponding simulations of constant width stripes, characterized by different grain diameters. Considering that for each w/d the statistical ensemble is limited, we can say that the behavior is well captured by the simulations, without any fitting except for the timescale ($A = 10^{-6}$).

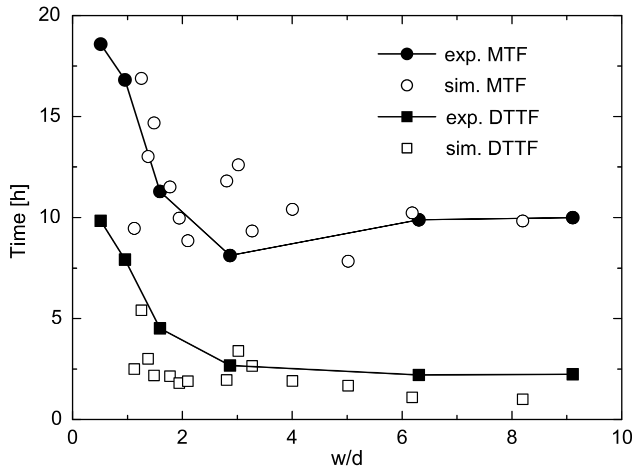

Fig. 4. Simulated and experimental (from [23]) MTF and DTTF data obtained with stripes of fixed width (2.2 μm) and different grain diameters. In simulation we have assumed $A = 10^{-6}$ and $\langle I \rangle / I_0 = 1$.

Simulated MTF data as a function of line width, (obtained changing the line width used in the simulations and keeping a constant grain size), can be compared with analogous data for copper CVD damascene lines stressed at 8 MA/cm^2 from [6]. As can be seen from Fig. 5 the simulator reproduce the measured data.

Indeed, both simulation and experimental data show an MTF reliability peak, for stripes which are, in both cases, slightly narrower than average grain size (simulation grain diameter, 13.82 a.u., $w/d_{\text{sim-peak}} = 0.72$; experimental median diameter 0.29 μm, which corresponds to an average diameter of 0.46 μm, $w/d_{\text{exp-peak}} = 0.68$). Examining the layout of simulation samples one can observe that in the width range of the peaks a structural transition takes place, in which a *grain boundary path*, i.e., a complete connection going end to end of the stripes composed only by grain boundary segments disappears, as illustrated in the inset of Fig. 5(above). As the stripe width is reduced, the probability that a single grain spans the whole cross section of the stripes approaches one, and no grain boundary path is possible. It is worth noting that the simulations reproduce this observed behavior without the need to postulate an *ad hoc* effect of the confining trench on the grain structure of the material, as the authors of [6] instead propose. This'structural resonance' is, in our opinion, another typical example of middle scale phenomenon, which can be explained simply as a consequence of the grain structure of the sample.

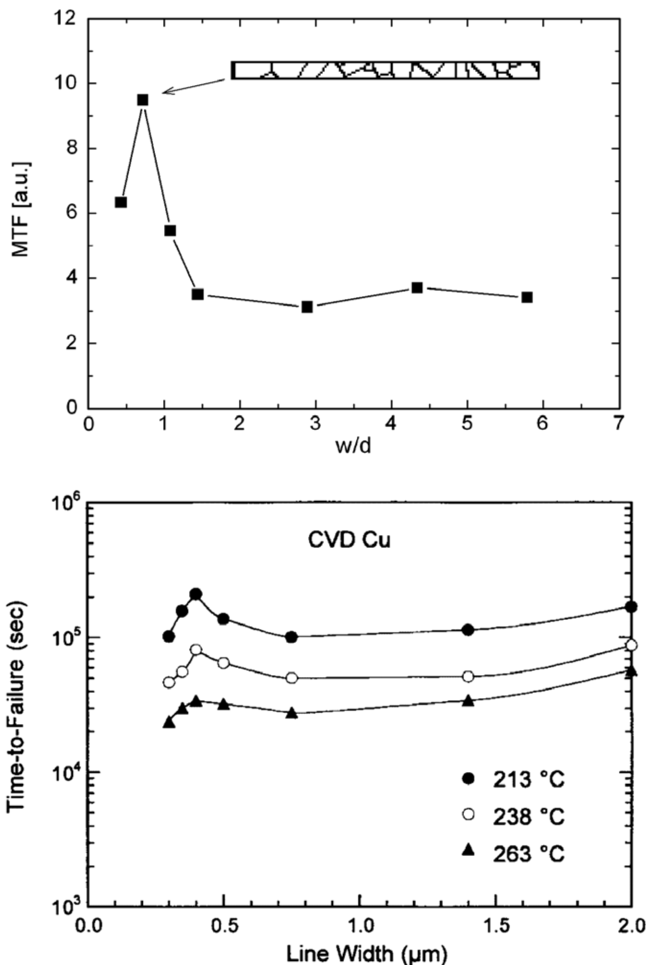

Fig. 5. Simulated MTF (above) and experimental (below; Fig. 15a of Ref. [6]) obtained from samples with variable width and constant average grain size (0.46 μm).

3.2. Electromigration noise vs MTF

Electromigration is usually accompanied by a typical noise, in the frequency range from a few milliHertz to 1 Hz [24]. It is generally recognized [12,25–27] that this noise should exhibit a $1/f^{\gamma}$ frequency dependence with a *noise exponent* γ typically close to 2 and always well above 1 [12]. This noise is thought to be connected with the process of vacancy creation and hence its total power should be related to the intensity of the electromigration process.

Since the electromigration noise is superimposed on a linear increase of resistance with time, noise spectra are obtained from the resistance output of simulations by Fast Fourier Transform (FFT), after the average linear increase is subtracted from the resistance time series. The FFT is applied to moving time windows, in order to track the evolution of noise spectrum as the electromigration damage proceeds [20].

Fig. 6 shows the noise power spectra obtained from a typical Monte Carlo run. It can be seen that, placing the transformation window in two positions, one in the beginning of the run and the other slightly before break down, total noise powers which differ of more than an order of magnitude are obtained.

This spectra can easily be explained as the effect of small independent step increases in the resistance which are induced by single damage events [20]. While this independence is reasonable for the initial phase of the electromigration damage and leads to random walk of resistors and therefore to $1/f^2$ spectrum, in the advanced stages of stripe damage a degree of correlation arises, which leads to the well known γ fluctuations [12,20].

After we verified that our model can provide distributions of time to failure statistics and noise properties in agreement with

experiments, we used it to investigate the correlation between failure time and initial total noise power, that has been suggested several years ago [28–30], on a large ensemble of structures.

We have performed simulations on an ensemble of 15 groups of 10 stripes each, recording failure time and initial total noise power. In these simulation several important geometric parameters were varied, from current level, to grain dimensions. Indeed, this last parameter has a strong effect on stripe reliability since, as already stated, electromigration is triggered at the grain boundary level. Furthermore, the different reliability properties of interconnections with different grain sizes are well known and have been recently reassessed in copper lines [6].

Fig. 7 shows the scatter plot of initial noise power versus time to failure of the mentioned 150 simulation runs, along with the linear fit line. The figure deserves two main comments. First of all, there is a correlation between failure time and noise level (correlation factor −0.56, p-factor negligible), signifying that initial electromigration noise activity is an index of the successive evolution of the system. Secondly, although noise power levels exhibit a quite high dispersion from the fit line, such dispersion tends to decrease as we move towards lower noise powers and longer time to failure. Fig. 8, instead, shows that the MTF tends to increase when the standard deviation (SD) of the noise power of a group of simulations decreases. These results confirm that a low and consistent (low SD) noise level can be used as a EM quality indicator for metal lines.

This means that the predictive value of electromigration noise is higher for the most enduring lines, where other methods (like MTF-based methods), are particularly impractical, or, in an industrial environment, too costly to be used.

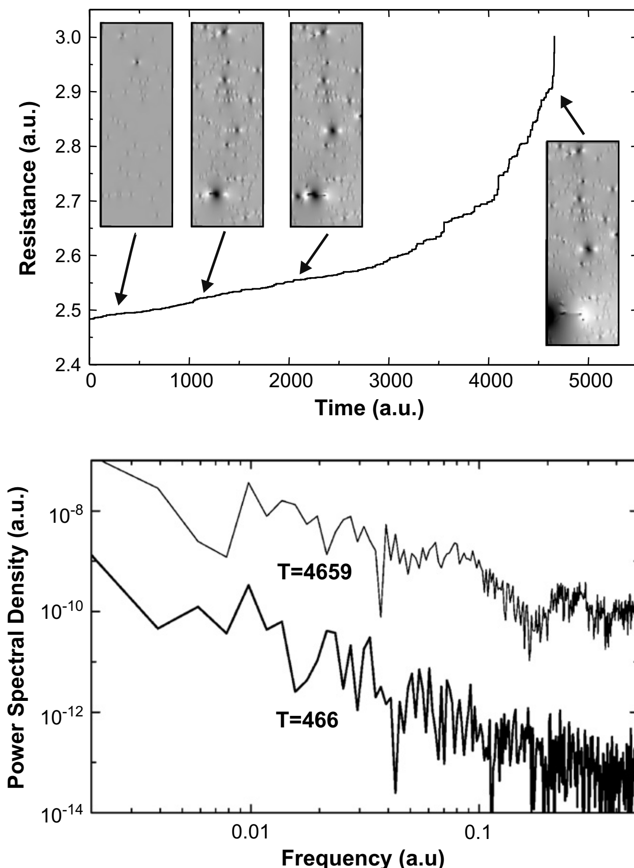

Fig. 6. A typical simulation run showing resistance increase, inserts show damaged areas in the sample (above); noise power calculated with a FFT window in a initial and later stage on the simulation showing 2 orders of magnitude increase in noise power (below).

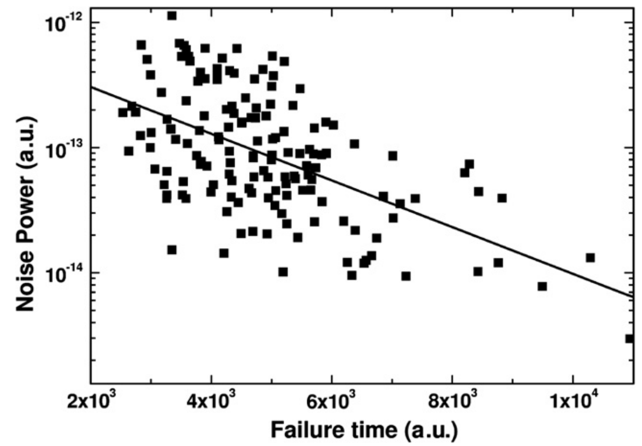

Fig. 7. Scatter plot of noise power versus failure time for an ensemble of 150 simulation runs on 15 polycrystalline lines of different geometries and grain configurations.

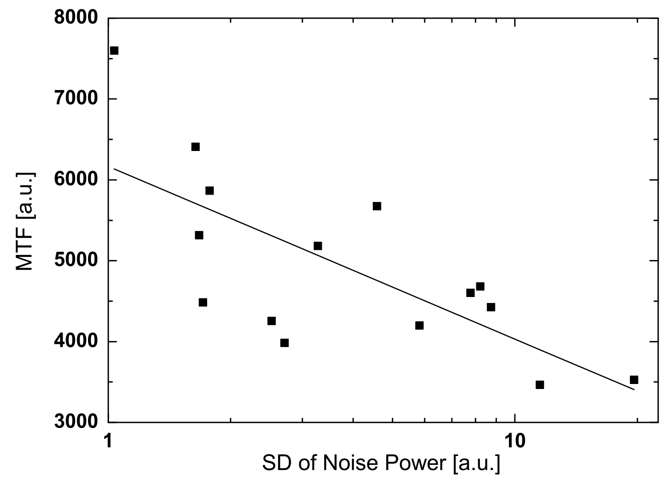

Fig. 8. MTF versus standard deviation of noise power for groups of 10 simulation runs on 15 polycrystalline lines of different geometries and grain configurations; The fitting line has a correlation factor of −0.72.

4. Conclusion

Our approach, although based on a simplified "middle-scale" model, has been able to accurately reproduce most of the statistical properties of the electromigration damage process in non-bamboo lines ($W \geqslant D$), where the polycrystalline structure of the sample plays a fundamental role in the evolution of the EM damage; this simulation approach can provide valuable results with the use of very limited computing power and time.

Perhaps the most striking result is the demonstration that the correlation between initial electromigration noise and reliability performance holds down to a per-sample basis. Although some preliminary and dated experimental results already suggest this conclusion [28–30], a compelling evidence is still lacking, and further experimental studies aimed to correlate, for interconnections of different geometries, grain sizes, and current stress, lifespan to noise power would be needed.

In our opinion, such result is fundamental both from a theoretical and a practical point of view, since it would really allow to pre-

dict the reliability properties of a batch, of a wafer, or of a part of it, on the basis of single or few noise measurements of test structures.

It is also important to stress the fact that we have shown that several experimental results that in the literature have been explained with additional "ad hoc" mechanisms, such as the accelerated failure at higher currents due to joule heating or the increased MTF in narrow stripes due to an effect of the confining trench [6], can be reproduced by simulations as an intrinsic effect of the middle scale structure of the system, without the need of including in the model specific mechanisms. Adopting Occam's razor, such additional mechanisms are unnecessary and should not be invoked. The middle-scale (polycrystalline) structure of the system seems to often dominate the behavior of stressed metal lines, at least for samples not much narrower than the mean grain size. The emerging properties are therefore more adequately captured by simple middle-scale models at a relatively high level of abstraction, notwithstanding their simplicity, while more detailed microscopic models are typically too complex to perform the simulations at the scale (in system size and evolution time) required to reproduce the experimental behavior.

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