Computational Materials Science 97 (2015) 1–5

Contents lists available at ScienceDirect

Computational Materials Science

journal homepage: www.elsevier.com/locate/commatsci

Modeling a copper/carbon nanotube composite for applications in electronic packaging

Ying Feng *, Susan L. Burkett

Department of Electrical and Computer Engineering, The University of Alabama, Tuscaloosa, Alabama 35487, USA

ARTICLE INFO

Article history:
Received 4 June 2014
Received in revised form 2 October 2014
Accepted 5 October 2014
Available online 24 October 2014

Keywords:
Copper/carbon nanotube composite
Modeling
Current density
Through silicon vias
Electronic packaging

ABSTRACT

A model is developed to determine the current density for a copper/carbon nanotube matrix configured as through silicon vias, an appropriate structure for interconnect applications. The electrical behavior of aligned carbon nanotube bundles mixed with copper at varying ratios is studied. The impact of the carbon nanotube dimensions and joule heating on electrical properties are analyzed. The results are compared for copper combined with single-walled carbon nanotube bundles and copper combined with multi-walled carbon nanotube bundles. The results suggest that through silicon vias filled with a copper/carbon nanotube matrix exhibit a more homogeneous current distribution with reduced skin effect compared to vias filled with only copper.

1. Introduction

Through silicon vias (TSVs) are vertical electrical interconnects passing through a set of stacked die [1]. This novel interconnection approach has been used to create high performance three dimensional (3D) systems by stacking integrated circuits (ICs) previously optimized for a specific function. Development of TSV technology, using copper (Cu) as the conductor, has enabled many applications that benefit from increased bandwidth, reduced signal delay, and improved power management. However, the electromigration of Cu atoms creates reliability problems due to high current density [2–4]. In addition, the performance of Cu interconnects is affected by the stress associated with a mismatch in thermal expansion coefficients. Another factor to consider is that skin effects limit the use of Cu in high frequency applications.

Carbon nanotubes (CNTs) have been proposed to replace Cu as an interconnect material due to their high current carrying capacity ($>10^9$ A/cm^2) [5,6], superior mechanical properties, and high electromigration resistance [7,8]. Theoretical studies [9–13] have compared the performance of CNT interconnects to that of Cu and demonstrated the applicability of CNTs in 3D packaging. These modeling studies considered CNT bundles with a maximum packing density. The smallest possible density of CNTs reported for interconnect applications is on the order of 10^{14} tubes/cm^2 for single-walled nanotubes (SWNTs) with a diameter of 0.8 nm [14]. The density is difficult to achieve for state-of-the-art chemical vapor deposition processes. For horizontally grown CNT bundles, the density that can be achieved is typically in the range of $\sim 10^{10}$ tubes/cm^2 or less [15].

Therefore, it is beneficial to investigate a novel materials system consisting of a mixture of Cu and CNTs. Chai et al. report formation of a Cu/CNT composite interconnect using electroplated Cu to fill the space between CNT arrays inside a SiO_2 via [7]. In the same fashion, we are conducting experimental studies on filling a Si via with a Cu/CNT composite by electroplating Cu after growth of vertically aligned MWNTs. In this approach, Cu fills the space among the outermost sheets of CNTs, providing a conducting material in the voids. The composite material should exhibit an electrical resistance somewhere between pure Cu and pure CNT bundles. Investigation of the electrical behavior of the Cu/CNT interconnect system can be used to guide experimental work when fabricating a new interconnect scheme.

In this work, we developed a model to study the current density distribution of a Cu/CNT composite interconnect. Our work was motivated by the work of [9] where their focus was the electrical behavior of TSVs that are fully filled by pure CNTs, including either SWNTs or MWNTs. Perhaps a more practical situation is one in which CNTs do not completely fill the TSV, leaving some open space [16,17]. This incomplete filling will cause the overall current carrying ability to be lower than expected. In our model, we consider CNTs filling TSVs with a variety of densities and make the

---

* Corresponding author at: 342 HM Comer, Box 870286, Dept. of Electrical and Computer Eng., The University of Alabama, Tuscaloosa, AL 35487-0286, USA. Tel.: +1 205 765 6630.

E-mail address: ying.feng@ua.edu (Y. Feng).

http://dx.doi.org/10.1016/j.commatsci.2014.10.014
0927-0256/© 2014 Elsevier B.V. All rights reserved.

assumption that Cu fills the space in between CNTs. The Cu/CNT filling model considers a practical situation due to the difficulty in completely filling a via with perfectly vertically aligned CNTs. This approach will provide guidance for experimental work on filling TSVs with Cu/CNTs. The electrical behavior of vertically aligned CNT bundles mixed with Cu at varying ratios is described in this paper. The impact of the CNT dimensions and joule heating on electrical properties has been analyzed. A comparison is performed for Cu combined with SWNT bundles and Cu combined with MWNT bundles. The modeling results suggest that TSVs filled with a Cu/CNT matrix exhibit a more homogeneous current distribution with reduced skin effect compared to vias filled with pure Cu. The CNTs with select diameters combined with Cu are suitable for electronic packaging applications in the high frequency domain. Specifically, SWNTs with diameters no less than 2 nm and MWNTs with diameters in the range of 30–100 nm possess improved electrical behavior than CNTs with diameters out of this select range.

2. Modeling details

2.1. CNT sheets in TSVs

A CNT can be viewed as a sheet of graphene that has been rolled up forming a tube. Depending on the number of sheets, the tubes are categorized as either SWNTs or MWNTs. SWNTs are composed of just one sheet with a diameter less than a few nanometers. MWNTs contain at least two sheets. Fig. 1(a) shows a schematic representation of a MWNT with four sheets. The outermost sheet can reach approximately 100 nm in diameter. There is a space that exists between two sheets due to van der Waal's forces; this space, $\varDelta$, is 0.34 nm wide. The outermost sheet's diameter, $D_{\max}$, is nearly 1.2 to 2.8 times larger than the innermost sheet's diameter, $D_{\min}$ [18]. We assume an average value of 2 in this work, thus the maximum number of sheets, n_{sheet}, in a MWNT is:

$$n_{\text{sheet}} = 1 + Fix\left(\frac{D_{\max} - D_{\min}}{2\varDelta}\right) \tag{1}$$

where *Fix* (.) returns the integer portion of the number resulting from that operation.

Fig. 1(b and c) illustrates schematic diagrams of cross sectional views of CNT bundles and a TSV filled with the Cu/CNT composite, respectively. The circles demonstrate SWNTs or the outermost sheets of MWNTs. The distance between two tubes, d, is shown in Fig. 1(d). When CNTs are of the highest packing density, the minimum value of d is 0.34 nm in consideration of van der Waal's forces. To estimate the total number of CNTs in a TSV, we assume the area occupied by each CNT is equivalent to a square shape with a width of (D_{CNT} + 0.34 nm). The tube quantity, n, is calculated by:

$$n = \frac{\pi D_{\text{TSV}}^2}{4(D_{\text{CNT}} + d)^2} \tag{2}$$

D_{TSV} and D_{CNT} refer to the diameters of a TSV and each CNT cylinder, respectively. The area corresponding to the CNT bundles in a via is given by $n \times (D_{\text{CNT}} + 0.34\ \text{nm})^2$. In the highest density case,

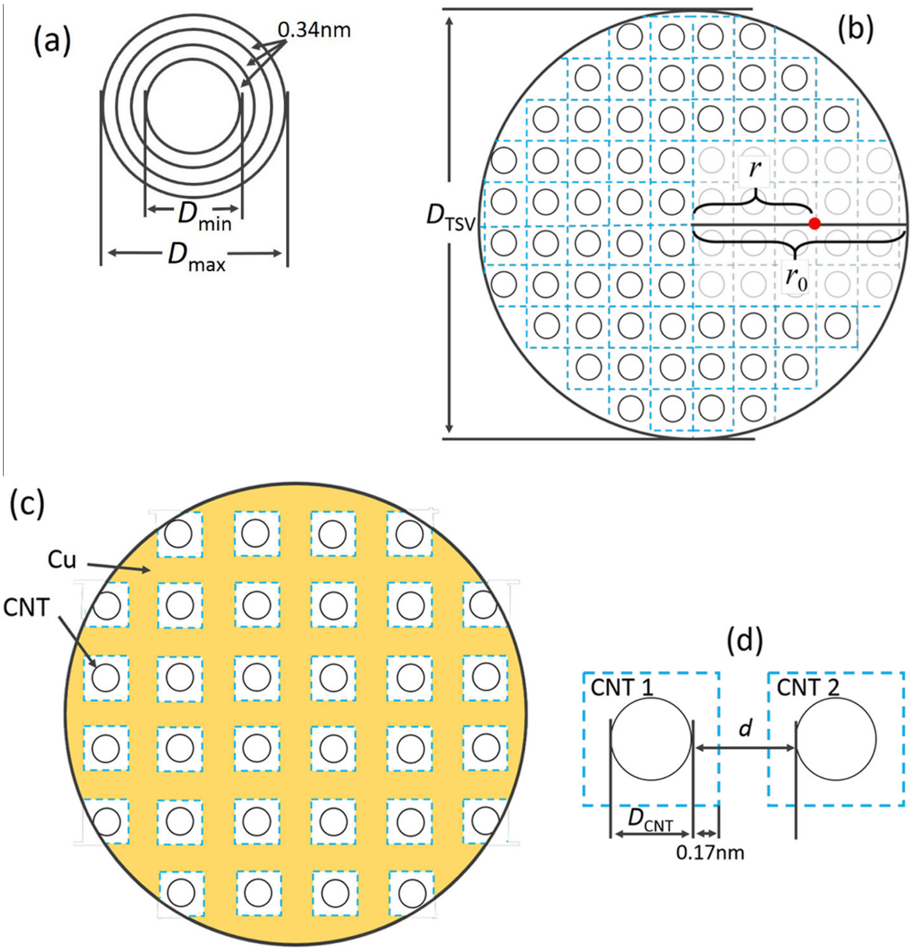

Fig. 1. Schematic diagrams of: (a) graphene sheets in a MWNT; (b) cross sectional view of a TSV full of dense CNT bundles; (c) cross sectional view of a TSV filled with Cu/CNT composite; and (d) two separate CNTs in a TSV.