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Protrusion of Cu-TSV under different strain states

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Abstract

A phase-field-crystal (PFC) model is used to investigate the protrusion of blind TSVs under different strain states. The direction of loading applied to the TSVs has an effect on the protrusion, which is closely related to the copper grains and their orientations at the TSV edges. A nonlinear relation between protrusion and strain rate has been found, which can be explained by different mechanisms of deformation. A higher strain occurring near the top end of the TSVs leads to a larger protrusion of the blind TSVs.

1. Introduction

The semiconductor industry aims for smaller, lighter and higher-performance products. Nowadays, the planar scaling of the two-dimensional (2D) semiconductor devices based on the Moore’s law has reached its limit and how to overcome this barrier is becoming an urgent topic. The next generation packaging technology is expected to keep up with the increasing requirement of package density by using three-dimensional (3D) system integration. Chip stacking in vertical interconnection, to meet the severe demands of performance and to suppress the back-end-of-line (BEoL) layers and thus the failure of 3D packaging, posing a serious reliability problem to be solved.

Meanwhile, the packaging materials are approaching the nano-scale. As an example, nanowires have been considered as interconnects in future nano-devices [6]. IMEC has also proposed a new program called advanced nano-interconnection, to meet the severe demands of performance of advanced interconnects [7]. As the dimension of the packaging materials reduces, the material microstructure is becoming a more and more salient factor, especially considering its random and statistical nature [4]. There exist a few studies aiming for relating the microstructural factor to the copper protrusion of TSVs. An electron back-scattered diffraction (EBSD) technique used by Jiang et al. revealed the grain growth process of polycrystalline copper during thermal cycling [3]. Messenmaeker et al. established a statistical model linking the protrusion height and the microstructure by studying a large ensemble of TSV protrusions [4].

To provide better understanding of the root cause of copper TSV protrusion, the strain or stress state presenting in the TSVs needs to be determined. There are a few experimental studies attempting to analyze the stress in the TSVs. Nanoindentation is used by Che et al. to measure the residual stress in the TSV [8]. Okoro et al. measured the stress of the TSVs of different diameters using a micro-Raman spectroscopy [9]. Liu et al. used synchrotron X-ray microdiffraction to measure the microscale thermomechanical strain in-situ [10]. As a supplement, simulation on TSV protrusion considering the microstructure can provide more details. In a recent work, we reproduced the process of copper protrusion of TSV using a phase-field-crystal (PFC) model, revealing the microstructural evolution at the atomic scale [11].

In this study, we investigate the protrusion behavior of the TSV under different strain states. The remainder of this paper is organized as follows. First, the PFC method is briefly reviewed. Then, different strain states applied to the TSV structures are discussed. Different kinds of strain states are studied, including the directions of loading, the strain rate and the distributions of strain along the edges of TSV.

2. Methods

In PFC model, the lattice of a crystalline material is represented as an order parameter \( \rho \). The order parameter represents the local time-averaged atomic density of a material system. In addition, developed by Wu et al., a two-point correlation function is introduced, and the corresponding two-model PFC model is used to simulate a square lattice in two dimensions [12]. In the 2D case, the two-mode order parameter is written as [12]:

\[
\rho = \rho + A \cos(q_x) + \cos(q_y)) + B \cos(q_x) \cos(q_y)
\]

where \( \rho \) is the average density. \( A \) and \( B \) are related to the amplitudes of two sets of density waves. \( q \) is a parameter related to the lattice constant, hereinafter referred to as \( a \approx 0.25nm \), with the relationship \( q = 2\pi/a \). In the 2D simulation, a square lattice corresponds to the \{100\} crystallographic plane of copper. Then, the free energy of the material system is written as [12]:

\[
F[\rho] = \int \text{d}r \left\{ \frac{\rho}{2} \{ r + (\nabla^2 + 1)\}^2(\nabla^2 + Q^2)^2\rho + \frac{\rho^5}{5} \right\}
\]

where \( r \) is the scaling temperature and \( Q^2 = 2 \) is a constant. Finally, the evolution of the microstructure is given by solving the governing equation of the PFC model [12]:

\[
\frac{\partial \rho}{\partial t} = \nabla^2 \frac{\delta F}{\delta \rho}
\]

The model configuration of our TSV structure is shown in Fig. 1. The solid gray lines mark out the edges of the TSV, showing a trapezoid TSV. Note that the TSV is a blind via in this study. To mimics mechanical loading to the TSVs, we used the technique introduced by Stefanovic et al. in [13]. Solid external layers are added to surround the TSV manually. The top layer of TSV is set as the lattice with a \( 0^\circ \) orientation and serves as a solid cover. Moreover, the grain orientations of other external layers are adjusted to accommodate the corresponding grains at both edges of the TSV. In the PFC model, the free energy is modified by adding a “penalty term” with the form:

\[
F[\rho] = F[\rho] + \int \text{d}r M(\tilde{r}) [\rho(\tilde{r}, t) - \rho(\hat{r}(\tilde{v}, t), t)]
\]

where \( M(\tilde{r}) \) is nonzero only in the external layers, except for the top cover layer. With the “penalty term” applied, the atoms inside the external layers are motivated to move with a...
strain with a...plot in Fig. 3b. It can be
seen that for grain 1, the largest protrusion is caused by the
strain with a...grain 1 and 2 are measured and plotted in Fig. 3b. It can be
considered.

But in this model, the microstructural effect was not
considered. Next, we will show how the protrusion is
influenced by the strain rate until...the strain rate.

3. Results and Discussion

3.1 The direction of loading
To simulate a TSV under different strain states, the
direction of loading \( \theta \) is changed systematically from 90°
to 240°, which represents all the scenarios of the strain states
that the TSV could be subjected to. For example, the strain
with \( \theta = 180° \) means a pure compressive strain to the TSV,
while the strain with \( \theta = 150° \) represents the combination of
a compressive strain and a shear strain. Fig. 2 shows the
protrusion of three TSVs with different loadings, i.e., \( \theta = 180°, 150° \)
and 120°. The protrusions of TSVs at the time \( t = 30000 \) of the loading stage are sketched by the black dashed
curves. It can be seen that the maximal protrusion is the largest
for the second TSV. Moreover, the relationship between the
TSV protrusion and the direction of loading is plotted in Fig.
3a. The curves show that the protrusion increases then
decreases with the increasing \( \theta \) in general, with the maximal
mean protrusion occurring at \( \theta = 135° \).

A stress-driven interfacial sliding model proposed by
Kumar et al. was used to predict the protrusion height [14].
But in this model, the microstructural effect was not
considered. Next, we will show how the protrusion is
influenced by the strain rate and the direction of loading.
For the case discussed above, the orientations of the grains in
the top end of the TSVs, labelled with grain 1 and 2, are 28°
and 70° respectively, as shown in Fig. 1. The protrusion
of grain 1 and 2 are measured and plotted in Fig. 3b. It can be
seen that for grain 1, the largest protrusion is caused by the
strain with a \( \theta = 150° \), while for grain 2 \( \theta = 120° \).

Meanwhile, the protrusion of grain 2 is larger than grain 1 for
the \( \theta \) within the range [90°, 180°]. This demonstrates the
fact that the protrusion is related to the grain orientation. A
smaller difference between the grain orientation and the
direction of loading, i.e., \( \theta \), will lead to a higher protrusion.
This effect can be significantly important when the TSV
scaling is reduced into the nanometer regime where only a few
grains exist in the TSV.

Fig. 1 The model configuration of a TSV structure. The
solid gray lines mark out the edges of a trapezoid TSV. The
parallel arrows form an angle \( \theta \) with the horizontal line,
which indicate the strain applied to the TSV. The defect
atoms in the TSV are highlighted by the brighter dots. Note
that the length scales in \( x \) and \( y \) direction are dimensionless.

3.2 The effect of strain rate
The strain rate applied to the TSV also influences the
protrusion behavior. In this study, the parameter \( |\vec{v}| \) is
corresponding to the strain rate. Note that \( |\vec{v}| \) is
dimensionless because the time and length in the PFC model
are dimensionless. With the same initial microstructure, the
TSVs are applied with different strain rate from \( 4 \times 10^{-4} \)
to \( 20 \times 10^{-4} \). The mean protrusion under different conditions is plotted in Fig. 4a. It shows that the protrusion is dependent on the
strain rate. The largest protrusion occurs under the strain
rate \( 8 \times 10^{-4} \). The protrusion firstly increases with increasing
the strain rate until \( 8 \times 10^{-4} \), then decreases and finally
hardly increases within the range from \( 10 \times 10^{-4} \) to \( 20 \times 10^{-4} \).

Fig. 2 Three TSVs are applied with different direction of
loading: (a) \( \theta = 180° \), (b) \( \theta = 150° \), and (c) \( \theta = 120° \).
The black dashed curves mark out the protrusion at time \( t = 30000 \) of the loading stage.

Fig. 3 The difference of...the strain rate until
\( \varepsilon = 5\% \) under the strain rates \( 4 \times 10^{-4}, 12 \times 10^{-4}, \) and \( 16 \times 10^{-4} \), while keep increasing under the strain rate...
suggested that the local strain near the top end of TSV may be responsible for the protrusion from the observation that a TSV with a higher protrusion is subjected to a higher strain near the top end of the TSV [16].

Fig. 4 (a) The plot of protrusion vs. the strain rate from $4 \times 10^{-4}$ to $20 \times 10^{-4}$. The mean and maximal protrusion height are plotted by solid and dashed curve, respectively. (b) The mean protrusion height to the strain with four different strain rates applied are plotted.

**Table 1. The strain distribution in different regions.** The coordinate of TSV is illustrated in Fig. 1 and Fig. 5.

<table>
<thead>
<tr>
<th>Strain rate applied in different regions</th>
<th>Model No.</th>
<th>Strain rate range</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>M1</td>
<td>$1 \times 10^{-4}$</td>
</tr>
<tr>
<td></td>
<td>M2</td>
<td>$10 \times 10^{-4}$</td>
</tr>
<tr>
<td></td>
<td>M3</td>
<td>$10 \times 10^{-4}$</td>
</tr>
<tr>
<td></td>
<td>M4</td>
<td>$5 \times 10^{-4}$</td>
</tr>
</tbody>
</table>

4. Conclusions

In this paper, a two-mode PFC model is utilized to simulate the protrusion of blind Cu-TSVs. The effects of different strain states on protrusion are studied. It can be concluded that:

1) The direction of loading applied to the TSVs has an effect on protrusion, which is closely related to the grains and their orientation at the edges.

2) The protrusion is found to have a nonlinear relationship with strain rate and the largest protrusion is produced under $|\bar{p}| = 8 \times 10^{-4}$.

3) The distribution of strain along the TSV edges also influences the protrusion. The strain applied at the bottom edge of the TSVs has little effect on protrusion. A higher strain applied near the top end of the TSV leads to a larger protrusion out of the blind TSVs.
Fig. 5 TSVs with different distribution of strain along the edges. The corresponding models are (a) M1, (b) M2, (c) M3, and (d) M4 summarized in Table 1. The black dashed curves sketch the protrusion profile at $t = 30000$.

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