Formation Mechanisms of Thermal Fatigue Crack Networks in Sn-Ag-Cu Die-attach Joint in High Speed Thermal Cycling

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To investigate the mechanisms by which fatigue crack networks form in die-attach joints in power semiconductors, high-speed thermal cycling test was performed using a Si/Sn-Ag-Cu/Si specimen and the formation process of fatigue crack networks in the solder layer was observed. Fatigue cracks were found to emerge around intermetallic compounds in the β-Sn dendrite boundaries or from the high-angle (high-Σ) grain boundaries of β-Sn generated by continuous dynamic recrystallization. In all of these cases, the subsequent cycles caused the individual cracks to propagate in a cross shape and to become connected to each other, resulting in the formation of fatigue crack networks. Finite element method (FEM) analysis confirmed that the solder layer was in a state of equibiaxial tensile and compressive creep in the direction parallel to the joint surface of the solder layer during high-speed thermal cycling. FEM analysis also indicated that equibiaxial tensile creep is the driving force behind fatigue fractures. FEM analysis results for the cross-shaped micro-cracks confirmed that equibiaxial tensile creep in the period of decreasing temperature caused the cross-shaped cracks to open and propagate. Further, these propagated cracks became connected to each other to form fatigue crack networks.

Key Words: Power Module, Die Attach Joint, Lead-free Solder, Thermal Fatigue Crack Networks, Finite Element Analysis

1. Introduction

In power semiconductor devices, the die-attach joints that connect the semiconductor to the insulated substrate can fracture due to fatigue caused by cyclic thermal stresses occurring during operation, and the resulting decrease in thermal dissipation leads to failure of semiconductor devices. It was previously thought that if Pb-rich solder was used in the die-attach materials, the fatigue fracture would occur due to cracks that started at the corner of a die-attach joint propagating in the direction horizontal to the joint surface1). However, it has been recently reported that when Sn-based lead-free solder alloys are used for the die-attach material, the fatigue cracks are connected to each other, forming networks (thermal fatigue crack networks), as shown in Fig. 13). The life of die-attach joints in power semiconductor devices has conventionally been designed based on the assumption that thermal resistance increases due to horizontal fatigue crack propagation in the solder layer4). However, in the formation of thermal fatigue crack networks in die-attach materials, the increase in thermal resistance is insensitive to the progression of the fracture5), which poses difficulties in reliability design of power semiconductor devices. To date, no studies have reported on the mechanisms of thermal fatigue crack networks, and clarification is urgently required.

The authors previously proposed performing high-speed thermal cycling test on die-attach joint specimens of Si/Solder/Si to investigate the formation mechanisms of thermal fatigue crack networks6). It was confirmed in that study that horizontal fatigue cracks did not occur because there was no mismatch in the thermal expansion coefficients between the materials of the upper and lower solder layers and that thermal fatigue crack networks were formed instead. Furthermore, that study indicated that...

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**Fig. 1** X-ray transmission image of thermal fatigue crack networks in die-attach layer subjected to power cycling3).
thermal fatigue cracks initiated near the cluster of intermetallic compounds in the solder layer or at the β-Sn grain boundary generated by dynamic recrystallization. However, the driving force behind fatigue crack generation and propagation was not clarified and the formation mechanisms of thermal fatigue crack networks remain unclear. To establish methods for predicting the thermal fatigue life of die-attach joints, the detailed mechanisms of thermal fatigue crack networks need to be clarified.

In the present study, high-speed thermal cycling test was performed on joint specimens of Si/Sn-Ag-Cu/Si and the mechanisms of thermal fatigue crack networks were explored by detailed observation of the fracture microstructures and the finite element method (FEM).

2. Procedure

2.1 Specimen

A Si/Solder/Si joint specimen was used in the study. The specimen was prepared using two silicon chips (10 mm × 10 mm × 0.625 mm) connected by Sn-3.0mass%Ag-0.5mass%Cu (hereafter mass% omitted) solder alloy that was 300-μm thick. Fig. 2 shows the dimensions of the specimen.

2.2 High-speed thermal cycling test

High-speed thermal cycling was applied to the specimen. Fig. 3 shows a schematic diagram of the high-speed thermal cycling test. The specimen was placed on a ceramic heater on a cooled plate at a temperature of 313 K, and then thermal cycling was applied to the specimen at high speed. The maximum surface temperature of the specimen was 448 K and the minimum was 323 K, and the surface temperature alternated between the maximum and minimum every 3 s. After the given cycles of high-speed thermal cycling were applied, microstructural observations were made via X-ray transmission, optical microscope, scanning electron microscope (SEM), and electron backscatter diffraction (EBSD).

2.3 Finite element method (FEM) analysis

For the FEM analysis, thermal-structural coupled analysis was used to consider the temperature distribution in the specimen. Fig. 5 shows the FEM model. The FEM model was created so that it had quarter symmetry. A 20-node hexahedral solid element was used for the model. Material properties used in the FEM analysis are shown in Tables 1 and 2. Heat transfer coefficient in the cooled plate was determined by inverse analysis so that the surface temperature of the specimen at the time of the highest temperature in the analysis result coincided with the temperature distribution in the test. The temperature contours at the Si surface
at the time of the highest temperature are shown in Fig. 6. In terms of the material properties used for structural analysis, solder was treated as an elastic creep body and the other constituent materials were treated as elastic bodies. The elastic properties of the ceramic heater and grease were the same as those of Si, so that no stress was generated between the specimen and the heater. The creep constitutive equation for Sn-3.0Ag-0.5Cu obtained from a separate test followed Norton’s law, as shown in Eq. (1)\(^7\).

\[
\dot{\varepsilon}_s = 1.26 \times 10^{-3} \sigma^{8.77} \exp \left( \frac{-60 \text{kJ/mol}}{RT} \right)
\]

where \(\dot{\varepsilon}_s\) is the steady state creep strain rate (s\(^{-1}\)), \(\sigma\) is the stress (MPa), \(R\) is the universal gas constant, and \(T\) is the temperature. The solver used was general-purpose code ANSYS ver. 18.1.

3. Results and discussion

3.1 Results of thermal cycling test

Fig. 7 shows X-ray transmission images of the microstructure of the solder layer at various thermal cycles. Separate specimens were used for the X-ray transmission observation of the individual cycles shown. No fatigue damage was observed until 1000 cycles under the conditions in this study. In the X-ray transmission images after 3000 and 4000 cycles, several white parts appeared that seemed to be the initiation points of damage at positions different from the solidification defects (voids). From 10000 cycles onwards, the fatigue damage became mutually connected with these connected points forming a fatigue crack network. However, fatigue cracks were not observed parallel to the joint surface from the joint edge.

3.2 Microstructural observation of damage

The findings obtained by observing the microstructures of damage that occurred at 3000 cycles by optical microscope were that there were two fracture modes depending on the occurrence or non-occurrence of recrystallization of the solder layer. The following sections describe the results of the microstructural observation.

3.2.1 Microstructure damage without recrystallization

Fig. 8 shows optical microscope images of the fatigue damage progression in the solder layer slightly below the joint interface. Polishing for observation was performed from the silicon side. Bright field images are shown in the top panel and polarized images are shown in the bottom panel. In this specimen, the damage started in the area without recrystallization. Microstructures specific to Sn-Ag-Cu alloys that have both a eutectic layer consisting of granular intermetallic compounds crystallized in \(\beta\)-Sn dendrite boundary and \(\beta\)-Sn were observed, and micro-cracks were confirmed in areas where damage was observed on X-ray transmission images. These cracks seemed to have initiated from the intermetallic compounds near the boundary between the eutectic layer and \(\beta\)-Sn dendrite. The micro-cracks then developed into star-shaped damage, and the cracks at the tips of star-shaped damage then propagated and developed into cross-shaped fatigue cracks. These cross-shaped
cracks became connected to each other, eventually forming fatigue crack networks that were visualized on the X-ray transmission images. As the damage progressed, recrystallized grains were observed around the damage due to the stress concentration in the crack tip field, whereas damage without recrystallization occurred considering that recrystallized particles were not observed around the initial micro-cracks.

3.2.2 Damage microstructure of fractures with recrystallization
Fig. 9 shows optical microscopic images of the damaged part of a specimen that differs from the specimen in Fig. 8. In the initial damage stage, the microstructure of the solder layer was composed of fine grains with a diameter of 20 μm, which were not seen in the initial microstructure. The solder layer was recrystallized by the high-speed thermal cycles. As shown in Fig. 9, the fatigue cracks initiated in the grain boundary of fine grains formed by recrystallization and propagated along the grain boundary. Even in the case with recrystallization, the cracks grew macroscopically in mutually orthogonal directions. The cracks that occurred in this way became connected to each other, forming a fatigue crack network, as in the case without recrystallization. Whether or not the damage involves recrystallization depends on the crystallographic orientation of the solidified microstructure. It should be noted that the formation of a fatigue crack network seems to mostly involve recrystallization and the progress of recrystallization during the course of thermal cycles is closely related to the formation of a fatigue crack network.

Fig. 10 shows the change in crystallographic orientations at up to 3000 thermal cycles when damage begins to appear in the X-ray transmission image. The images on the left show grain boundary misorientation of β-Sn (grain boundary characterization) and those on the right show the orientation mapping of β-Sn grains. Individual specimens were used for the EBSD analysis of each cycle, and the figure is not the result of continuous observation with the same specimen. Fine subgrains emerged at 1000 thermal cycles, and the low-angle (low-Σ) grain boundaries (subgrain boundaries) continuously became high-Σ grain boundaries as the number of cycles increased beyond 1000 cycles. Fig. 11 shows the relationship between the number of cycles and the average misorientation angle. The misorientation angle increased sharply when the cycles exceeded 1000. Then the change in the misorientation angle seemed to be saturated from 3000 cycles onwards and recrystallization was completed. Because β-Sn is a dynamic recovery type of metal with high stacking fault energy, fatigue deformation causes continuous dynamic recrystallization in Sn-Ag-Cu alloys that have β-Sn as the matrix phase. Continuous dynamic recrystallization is common in materials with high stacking fault energies. It occurs when low-Σ grain boundaries are assembled from dislocations that form within the grain. When the metals are subjected to continued stress, the subgrains rotate, which increases the...
misorientation angle and creates a high angle-grain boundary\(^{13,14}\). The phenomenon of increasing average misorientation angle with more cycles, as shown in Fig. 11, corresponds to continuous dynamic recrystallization. ß-Sn had a body-centered tetragonal structure with a \(c/a\) axis ratio of 0.55. Therefore, there were no grain boundaries with low-\(\Sigma\) values in ß-Sn and the grain boundaries formed by the recrystallization had high-\(\Sigma\) values, which became fracture sites. In fractures with recrystallization, the high-\(\Sigma\) grain boundaries that became fracture sites were generated by thermal cycles, and the cracks that initiate at the grain boundaries developed into fatigue damage.

### 3.2.3 Driving force of fatigue crack networks formation

Microstructural observations indicate that fatigue crack networks are formed by crack propagation that starts from the periphery of intermetallic compounds or from grain boundaries with high-\(\Sigma\) generated by continuous dynamic recrystallization, and these cracks become connected to each other. However, because crack initiation and recrystallization require a driving force, the driving force behind the formation of fatigue crack networks was investigated using FEM analysis.

Figs. 12 and 13 show the contours of axial stresses and creep strain in the \(x\) and \(y\) directions parallel to the joint surface and in the \(z\) direction toward the thickness of the solder layer at the maximum and minimum temperatures. The solder layer was under biaxial compressive stress in the direction parallel to the joint surface while the temperature was increasing, and was under biaxial tensile stress while temperature was decreasing. Fig. 14 shows the hysteresis loops of stress-creep strain in the central part of the solder layer in the \(x\), \(y\), and \(z\) axial directions and the \(xz\) shear direction. The creep deformation of solder dominated in the \(x\) and \(y\) directions, and their hysteresis loops coincided with each other. Stress in the \(z\) direction was almost zero and no shear deformation occurred in the center area of the solder layer. The hysteresis loops showed that the solder layer underwent equibiaxial tension-compression deformation during thermal cycles. Because the specimen used in the study had a structure in which the solder was sandwiched between silicon plates, there were no differences in thermal expansion coefficients between the top and bottom layers and no shearing deformation occurred. However, thermal expansion of the solder layer during the period of increasing temperature was constrained by the low thermal expansion of the top and bottom silicon plates, so the solder layer was in a state of equibiaxial compressive stress in the direction horizontal to the joint surface. This compressive stress caused the solder layer to undergo compressive creep deformation in the direction parallel to the joint surface. However, the solder layer shrunk during the period of decreasing temperature, so the solder creeps in the direction opposite to the direction in which the compressive creep occurred during the period of increasing temperature and the solder layer underwent equibiaxial tensile creep deformation in the direction parallel to the surface of the solder layer. The cross-shaped cracks observed by optical microscope and fatigue crack networks formed by the linkage of the subsequent cracks were caused by the equibiaxial tensile and compressive stress parallel to the joint surface. The fact that the equibiaxial stress causes fatigue crack networks to form has
also been reported by studies on thermal fatigue in steam-pipes in electric power plants\(^{15-17}\). However, when the stress state deviates from the equibiaxial state, fatigue cracks occur in the direction vertical/perpendicular to the principal strain axis\(^{15-17}\).

In addition, because plastic deformation of the solder was incompressible (constant volume), the plastic strain in the z direction of the solder layer increased due to the compressive creep deformation in the x and y directions during the period of increasing temperature, as shown in Fig. 14. Therefore, the thickness of the solder layer increased during this period. However, the thickness of the solder layer shrunk due to the tensile creep deformation in the x and y directions when the temperature started to decrease. Because the deformations due to increasing and decreasing temperature were not identical, the compressive creep strain in the x and y directions remained at the minimum temperature and the positive strain remained in the z direction in the solder layer. Accumulation of positive strain in the z direction by repeated thermal cycling resulted in an increase in the thickness of the solder layer. In fact, upon test completion, increased thickness of the solder layer was confirmed. The residual compressive strain widened the crack width, as observed on X-ray images.

3.2.4 Formation mechanisms of fatigue crack networks in the solder layer

Fig. 15 shows a schematic diagram of the formation mechanisms of fatigue crack networks. In the fractures without recrystallization, micro-cracks initiated at the interface between the intermetallic compounds and β-Sn phase generated by equibiaxial tensile creep developed into a cross shape. In the fractures with recrystallization, however, the following fracture mechanisms were predictable. Continuous dynamic recrystallization progressed by equibiaxial creep deformation occurring with thermal cycling as the driving force, which led to the generation of high-Σ grain boundaries. Furthermore, the equibiaxial tensile creep caused cracks to occur from the high-Σ grain boundaries, which propagated along the grain boundaries in a cross shape from a macroscopic perspective. In any case, because the entire area of the solder layer was in a state of equibiaxial stress, these cracks occurred across the entire area of the solder layer and new cracks were initiated while cross-shaped cracks were propagating. Ultimately, individual cracks became connected to each other and a fatigue crack network was formed.

3.3 Reproduction of fatigue crack network formation by FEM analysis

It was presumed that fatigue crack networks form by cracks propagating and connecting by equibiaxial tensile creep during the period of increasing temperature. To verify this, a qualitative reproduction of the formation of fatigue crack networks was examined by FEM analysis.

First, under the assumption that equibiaxial tensile and compressive stress cause cross-shaped micro-cracks to occur, an FEM model was created by adding multiple cross-shaped micro-cracks, each 200-μm wide, in the solder layer of the Si/solder/Si joint specimen. Fig. 16 shows the solder layer of the FEM model with the addition of the multiple micro-cracks. The high-speed thermal cycles were applied to the FEM model. Based on the creep strain energy density distribution determined from the FEM analysis results, fatigue damage of the solder layer was developed according to the following process. The cross-shaped cracks were made to propagate for a certain length and then new cracks were added to the solder layer based on the creep strain energy density distribution, and the FEM analysis was performed again. The cracks were made to propagate for a certain length again. The final crack length was set to the total crack length in the specimen subjected to 10000 cycles of high-speed thermal cycling.

Fig. 17 shows the contours of creep strain energy density at each stage of fatigue damage progression at the minimum
temperature. At the initial damage stage shown in Fig. 17 (a), it was confirmed that the added cross-shaped micro-cracks were opened into a star shape due to the equibiaxial tensile creep generated during the period of decreasing temperature. The star-shaped crack opening reproduced the crack shape observed in the damaged microstructures shown in Fig. 6. In addition, the creep strain energy densities concentrated at all tips of the cross-shaped cracks by opening under a state of equibiaxial tensile creep became identical, and thus cracks were predicted to propagate in the shape of a cross, as shown on the X-ray images. Because the entire area of the solder layer was under a state of equibiaxial stress, as the temperature cycling proceeded, cracks propagated in the shape of a cross and concurrently new cracks emerged in the solder layer. However, stress and creep strain were relaxed in the vicinity of the cracks, due to which the creep strain energy density was low and new cracks did not appear in the vicinity of the cracks. Subsequently, a number of new cracks were added to an area slightly distant from the existing cracks and FEM analysis was performed again. The existing cracks propagated and new micro-cracks were initiated, as shown in Fig. 17 (b). Finally, each crack further propagated, as shown in Fig. 17 (c). In Fig. 17 (c), the propagated cross-shaped cracks became connected to each other and network-shaped cracks were formed. Thus, it was confirmed by the FEM analysis that fatigue crack networks were formed by cross-shaped cracks repeatedly initiating and propagating, as caused by equibiaxial creep. To predict quantitative fatigue life, however, the frequency of crack initiation, remains to be investigated in future research.

4. Conclusion

High-speed thermal cycle testing was performed using a Si/Solder/Si joint specimen and the process by which fatigue crack networks formed in the solder layer was investigated. The findings were as follows:

1) Initial cracks initiated in the vicinity of intermetallic compounds in the β-Sn dendrite boundary, or from high-Σ grain boundaries formed by continuous dynamic recrystallization. However, dynamic continuous recrystallization in the entire solder layer was caused to occur by subsequent fatigue cycles and cracks propagated mostly along the high-Σ grain boundaries.

2) Macroscopically, each crack propagated in a cross shape and connected to each other to form fatigue crack networks.

3) FEM analysis confirmed that the solder layer was in a state of equibiaxial tensile and compressive creep with the direction parallel to the joint surface. The equibiaxial tensile and compressive creep acted as the driving force for fatigue damage and continuous dynamic recrystallization.

4) FEM analysis of cross-shaped micro-cracks also confirmed that fatigue cracks were propagated by equibiaxial tensile creep during the period of decreasing temperature, causing cross-shaped cracks to open and propagate and the further interlinking of these cracks with each other.

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