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# Crystallographic Structure and Mechanical Behaviour of SnAgCu Solder Interconnects under a Constant Loading Rate

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## Abstract

With the continuing increase of the integration density in electronics, dimensions of interconnections for electronic components have been miniaturized to a scale that is comparable to those of their crystallographic structure. For instance, a SnAgCu solder joint in the flip chip package can contain only one or a few grains. In this case, the mechanical behaviour of the micro-joint is expected to shift from a polycrystalline-based to single-crystal one. Considering the further miniaturization, both the crystallographic structure and mechanics of each component ( $\text{Ag}_3\text{Sn}$ ,  $\text{Cu}_6\text{Sn}_5$  and  $\beta\text{-Sn}$  matrix) within a grain and the adjacent SnCu interface will play an important role in the reliability of the micro-joint due to their size comparable with that of a grain, irregular geometry, their heterogeneous distribution and considerably different properties. In addition, at such a small scale, the non-local effect on deformation of  $\beta\text{-Sn}$  should be taken into account to interpret mechanical interactions between components. In this paper, a shearing test, in which it is possible to apply a constant loading to a SnAgCu joint is designed to investigate mechanics of substructure within a SnAgCu grain and near the SnCu interface.

## 1 Introduction

In electronics, solder alloys are usually utilised in the manufacture of joints as the main connecting medium between components and Printed Circuit Boards (PCBs). Due to the mismatch of coefficients of thermal expansion (CTE) for these components, the integrity and mechanical performance of solder joints attracts attention since their melting temperature ( $T_m$ ) are relatively low. For instance, the ambient temperature of SnAgCu solder, one of the most promising Pb-free alloys, is above  $0.5 T_m$ (K). When a package's temperature varies during its service, an external load is applied to a joint, ultimately leading to failure. To predict the life of solder joints, a considerable amount of investigation is conducted on the mechanical and damage characteristics of solder materials. However, most of these studies are based on bulk specimens. With the continuous increase in the complexity and functions of integrated circuits in electronic products, the size of solder joints for interconnections has to continue decreasing to enable the highest possible extent of compactness. When solder joint's dimensions reach a certain level, the size effect on its mechanical behaviour becomes pronounced. For instance, a solder joint in a flip chip package has been miniaturized to dimensions below  $100 \mu\text{m}$  in commercial applications. At such a small scale, a solder joint may be formed with only one or a few grains [1, 2]. Its microstructure and mechanical behaviour is expected to shift from those for a

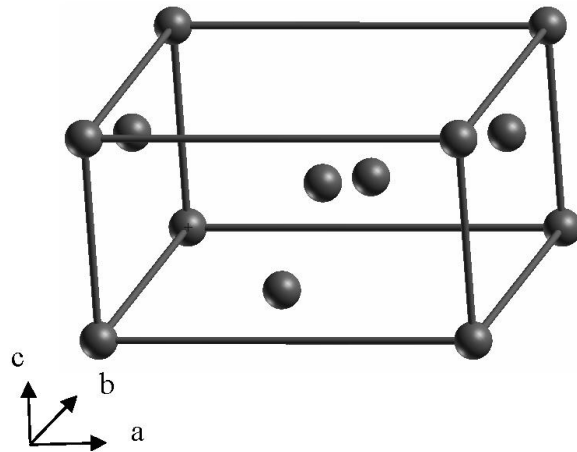
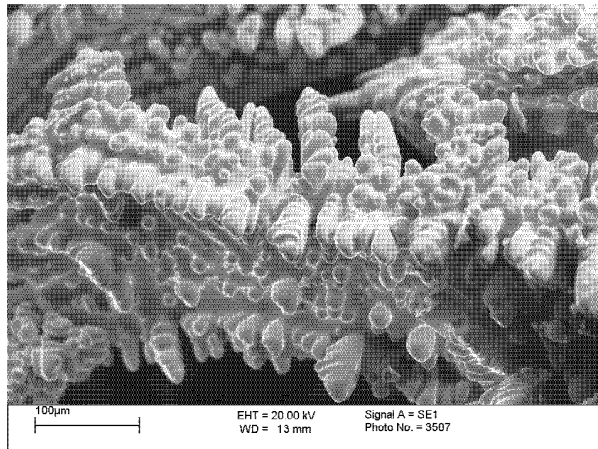


Fig. 1 Body-centered tetragonal unit cell of  $\beta\text{-Sn}$ . Dimensions: 0.58318 nm (along a and b) and 0.31819 nm (along c).

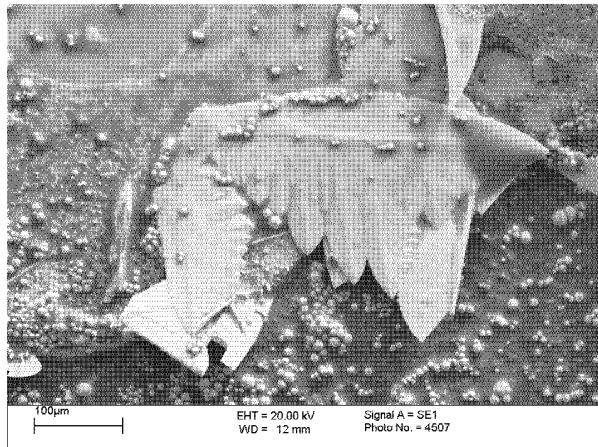
polycrystalline aggregate to ones for a single crystal. Since  $\beta\text{-Sn}$ , the matrix of SnAgCu solder has a contracted body-centred tetragonal (BCT) structure as shown in Fig. 1, a solder grain is expected to show considerable anisotropic behaviour. In this case, crystal features, such as the grain size and orientation, may become key factors to reliability of the micro-joint.

Generally, there are three major types of mechanical behaviour for a solder joint in electronics: elastic, thermal expansion and those that are inelastic. The anisotropic characteristics from all of these mechanisms have been demonstrated for SnAgCu grains; in [3], Matin investigated the response of an unconstrained solder alloy under an isotropic thermal cycling load and first attributed its fatigue damage to the anisotropic thermal expansion and elastic properties of  $\beta\text{-Sn}$  matrix. Later on, our mechanical tests on a joint under a shear load have shown that only one major slip system is activated in each grain, indicating the highly lattice-dependent local inelastic behaviour of SnAgCu grains [4]. Based on these findings, a constitutive equation was proposed for SnAgCu crystals to describe the local microstructure-dependent mechanical behaviour of such micro-scale joints [5]. These investigations establish the basic relationship between the solder's mechanical performance and crystallographic features at a grain level.

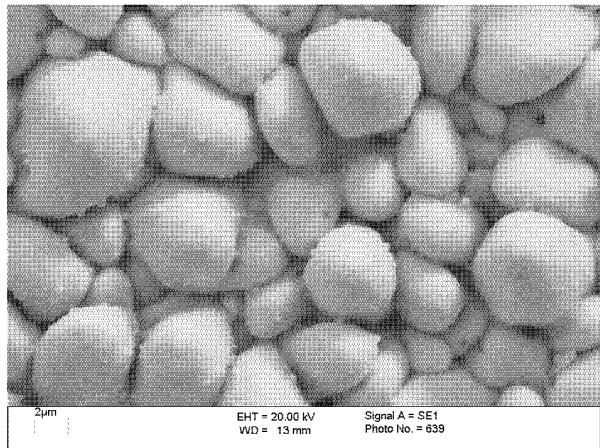
When solder joints are further miniaturized, not only the grain size and orientation, but also crystallographic structure and mechanics of each component (e.g.  $\text{Ag}_3\text{Sn}$ ,  $\text{Cu}_6\text{Sn}_5$



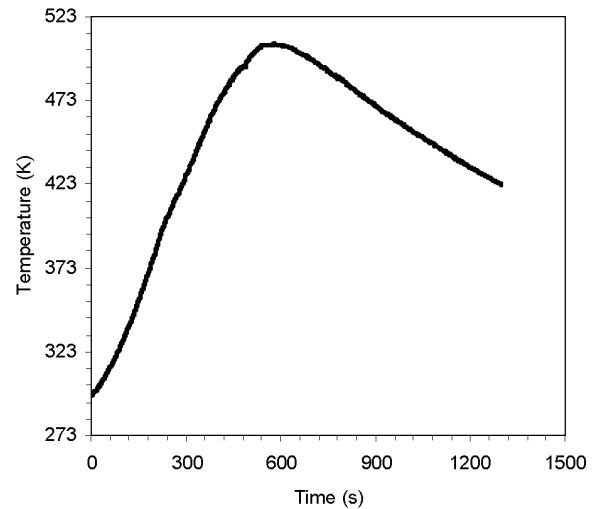
**Fig. 2 Sn dendrites formed in liquid Sn<sub>3.8</sub>Ag<sub>0.7</sub>Cu solder during solidification [8]**



**Fig. 3 Ag<sub>3</sub>Sn plates formed in molten Sn<sub>3.8</sub>Ag<sub>0.7</sub>Cu solder**



**Fig. 4 Sn<sub>6</sub>Sn<sub>5</sub> formed between Sn<sub>3.8</sub>Ag<sub>0.7</sub>Cu solder and the Cu substrate after solidification.**



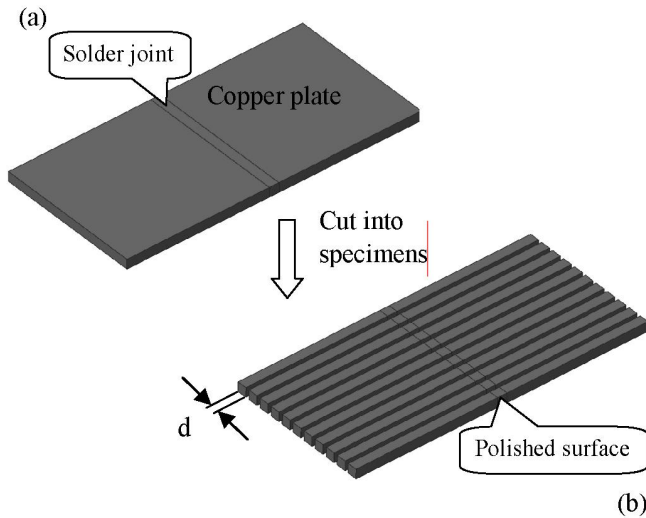
**Fig. 5 Temperature change in tests. The maximum temperature and cooling rates are 507K and 0.13K/s, respectively**

intermetallic compounds (IMCs),  $\beta$ -Sn matrix and Sn dendrites for SnAgCu solder) within a grain play an important role in their reliability since some of these components, such as Sn dendrites and Ag<sub>3</sub>Sn plates are able to reach the same scale as that of the grain, as shown in Figs. 2 and 3. Considering their different properties [6], internal anisotropic character, irregular shape and distribution, the intra-granular behaviour is considerably heterogeneous. In addition, at such a small scale, the mechanical behaviour of a metal/alloy may be no longer localized due to the movement of dislocations, the natural mechanism of plastic deformation for metals and alloys [7]. This not only determines the internal behaviour of  $\beta$ -Sn, but also influences adjacent components. Therefore, to capture the principle mechanisms for such a grain, one should both investigate the formation behaviour of each components [8], and, study their individual and interacting mechanics within a grain.

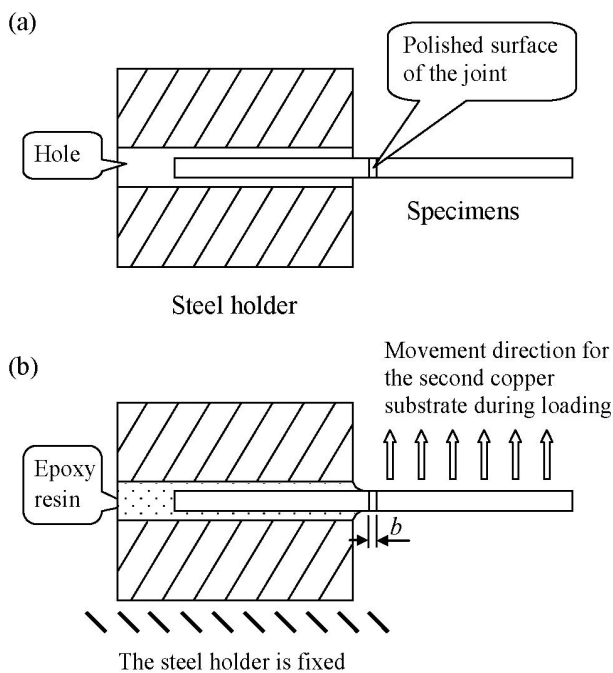
In this paper, an experiment is designed to apply a shearing deformation to a SnAgCu grain with a constant loading rate. To characterize the deformation behaviour of substructures within the SnAgCu grain, transmission electron microscopy (TEM) is employed to study crystallographic characteristics of a loaded local area. A Focus Ion Beam (FIB) system, which is capable of locally selecting and excising the areas of interest, is used for TEM sample preparation. The present paper mainly focuses on an area near the SnCu interface.

## 2 Experiments

In experiments, a commercial solder paste, Sn<sub>3.8</sub>Ag<sub>0.7</sub>Cu, is used. The diameter of solder balls ranges from 8  $\mu$ m to 12  $\mu$ m, and the flux comprises 13% of the paste by weight. It is specially designed for a fine pitch flip chip assembly, and therefore suitable for the small joint geometry used in the test. The solder joints are formed between two substrates using a Planer T-TRACK<sup>©</sup> reflow oven. Figure 5 shows the temperature change that a solder joint experiences



**Fig. 6 Procedures to prepare specimens. (a) Sample formed in oven. (b) Specimens for the mechanical test.  $d \approx 1 \text{ mm}$ .**



**Fig. 7 Constraints and loading conditions for a joint in the shearing mechanical test**

in the oven. To precisely control the size of a joint, two substrates are fixed on two linear stages, respectively. The size of a solder joint ( $b$  in Fig. 7) is determined by the relative movement of these stages, the resolution of which is  $1 \mu\text{m}$ . For a reflow cycle, stages are placed into the oven together with a specimen. To resist the high temperature in the oven, stages are made of steel. This also helps to reduce the dimension change from temperature variation due to its low CTE. The substrates are made of copper plates (99.9% purity) so to provide reliable bonding with the solder being rigid

enough for the subsequent mechanical tests. The dimensions of the substrates are  $15 \times 15 \text{ mm}^2$  with a thickness  $1 \text{ mm}$ . Figure 6(a) gives the specimen's configuration. After the reflow, the plate is cut by a low-speed diamond saw into several specimens with their longitudinal axes perpendicular to the joint line as shown in Fig. 6(b). The depth of the specimens ( $d$  in Fig. 6(b)) is approx.  $1 \text{ mm}$ . Finally, one of the specimen's cross-sections is carefully ground and polished for microstructural observation.

To enable a constant-rate and low-speed load on the joint, mechanical tests are carried out on an Instron 5848 Micro-tester. A problem with a standard testing method is that the geometry of the joint is considerably small. When a sample is assembled in the tester, a pre-load is applied to the soft solder joint due to a large mismatch in the grips' geometry. This inevitably influences the final result. To solve this, a cuboidal steel holder is prepared. In the holder, a hole, the area of which is slightly larger than the specimen's cross-section, is made as shown in Fig. 7(a). Before testing, the holder is fixed on one of the tester's grips with all movement constrained. The Cu substrate on one end of the specimen is inserted into the hole as shown in Fig. 7. The other substrate (opposite end) is fixed on the tester's second grip, the movement of which is controlled by the Micro-tester. Then the hole in the steel holder is filled in with Epoxy resin, making sure that the resin does not touch the joint. After 24 hours of curing, the epoxy resin is fully hardened, and the specimen is assembled in the Micro-tester in a stress-free state.

During the mechanical test, the second Cu substrate moves together with the secondary grip in the vertical direction as shown in Fig. 7(b), leading to a shearing mode of load. Since the yield point of pure copper is much higher than that of Sn3.5Ag0.7Cu solder, when the solder joint yields, the copper substrates are still in the elastic condition. At the same time, the Young's modulus of the SnAgCu solder is much less than that of copper. Under loading, nearly all the movement of the second substrate is transferred to the joint, especially in case of large deformation. Therefore, the applied engineering shear strain rate  $\dot{\gamma}$  on the joint is approximately:

$$\dot{\gamma} = \frac{\dot{U}_{\text{substrate}}}{b}, \quad (1)$$

where  $\dot{U}_{\text{substrate}}$  is the rate of the second substrate and  $b$  is the distance between substrates (it is the distance between the middle points of interfaces for the real specimens). It should be mentioned that the epoxy resin can reduce the shear strain rate due to its relative low stiffness. To reduce this effect, the epoxy resin applied is one of the hardest available; the hole in the holder is also made as small as possible to increase the rigidity.

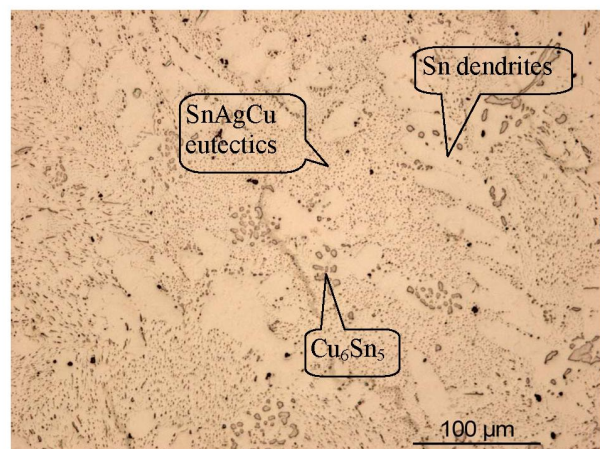
Before the mechanical test, both scanning electron microscopy (SEM) and an optical microscopy accompanied by polarized light (PL) are employed to examine grain features and microstructure in the solder joints. To characterize the deformation and damage behaviour of substructures within SnAgCu grains, transmission electron microscopy (TEM) is employed to study crystallographic characteristics of local areas after loading. The TEM sample



is prepared by means of a Focus Ion Beam (FIB) system, which is capable of locally selecting an area of interest. The mechanical test is carried out at the room temperature.

## Results and discussion

### 1 Crystallographic structure of SnAgCu grains



**Fig. 8 Bright-field optical image of a large Sn<sub>3.8</sub>Ag<sub>0.7</sub>Cu solder joint.  $b = 1000 \mu\text{m}$ .**

Fig. 8 is an optical image of a large solder joint, where  $b$  is  $1000 \mu\text{m}$ . It presents the typical microstructure of SnAgCu solder: the alloy is mainly composed of SnAgCu eutectics, which contains the Sn matrix and  $\text{Cu}_6\text{Sn}_5$  and  $\text{Ag}_3\text{Sn}$  IMC particles; at some areas, Sn dendrites are formed, which are usually surrounded by SnAgCu eutectics. Sometimes, large  $\text{Ag}_3\text{Sn}$  plates, which are not presented in Fig. 8, are formed in the solder. Recent studies by electron-backscattered diffraction (EBSD) and polarized light microscopy (PLM) shows that a Sn dendrite and the adjacent Sn matrix for eutectics have the same crystal orientation, indicating that they are substructures of one SnAgCu grain [1, 2]. To interpret crystallographic structures of such a grain, the key point is to understand the irregular formation of Sn dendrites. Under ideal conditions, e.g. when the cooling rate is extremely low, only eutectics can be formed in Sn<sub>3.8</sub>Ag<sub>0.7</sub>Cu alloy; no dendrite should be present. However, with most manufacturing processes, e.g. reflow conditions used in the present paper as shown in Fig. 5, a solder joint usually experiences a degree of under-cooling, and deviates from the equilibrium solidification. Our experiments show that Sn dendrites are first formed in the liquid SnAgCu solder under this condition. The dimension of a Sn dendrite can reach several hundred micro-meters as shown in Fig. 2. This is a reason for a large size of the grain, which makes a micro-joint contain only one or a few grains. The large-scale dendrites consume a considerable amount of Sn in the liquid solder. When the solidification continues, SnAgCu eutectics begin to form. Since heterogeneous nucleation needs less energy, the growth of SnAgCu eutectics is based on the existing Sn dendrites. Therefore, a dendrite and the matrix of the adjacent SnAgCu eutectics have the same crystal orientation, which finally form one SnAgCu grain. Since the Sn dendrite is the nucleation core of a grain, its original crystal orientation

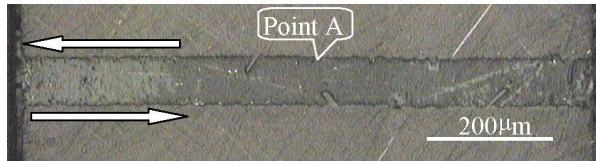
determines that of the entire grain. This is one of the key factors that determines substructures and mechanical performance of a SnAgCu grain. Besides Sn dendrites,  $\text{Ag}_3\text{Sn}$  plates are another irregular component in the SnAgCu joints, as illustrated in Fig. 3. In fact, these plates are formed ahead of Sn dendrites. Therefore, they are relatively independent of SnAgCu grains: they can either form within a grain or go through several grains. Sn dendrites, SnAgCu eutectics together with  $\text{Ag}_3\text{Sn}$  plates form the basic elements of the SnAgCu grain. Their geometry and distribution determine the grain's structure. Both Sn dendrites and  $\text{Ag}_3\text{Sn}$  plates are single crystals. At the same time, they are both formed in the liquid solder. However, their morphology is considerably different. It is probably that this difference mainly results from their internal crystalline structures. Obviously, the external factors also play important roles. For instance, rapid cooling can not only reduce the arm spacing of a dendrite due to more undercooling, but also suppress the formation of  $\text{Ag}_3\text{Sn}$  plates from less growth time.

### 2 Mechanical behaviour within a SnAgCu grain near the interface with the Cu substrate

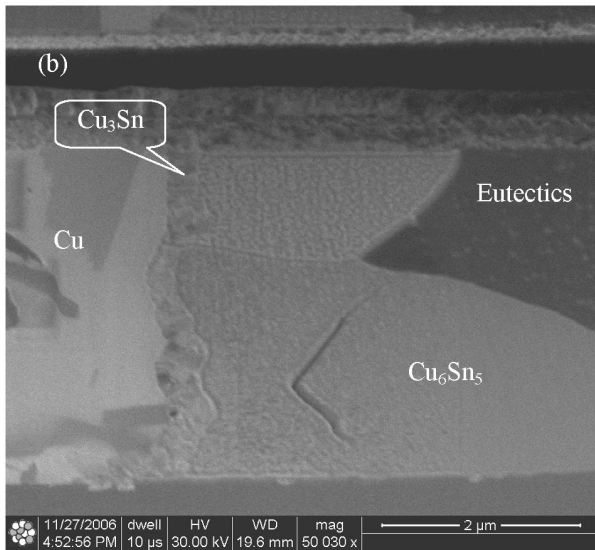
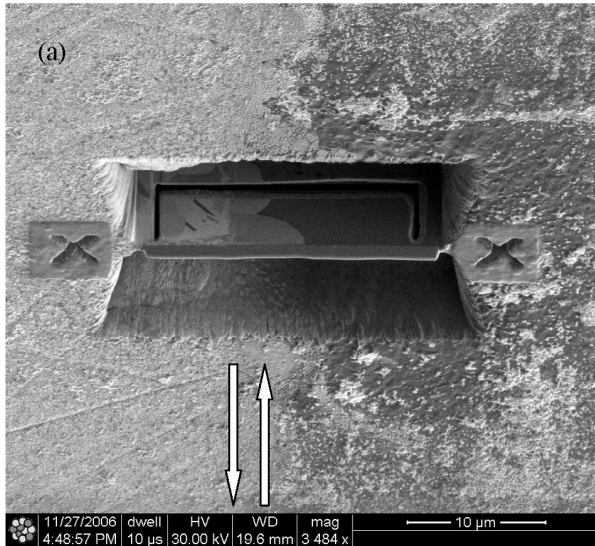
To study the crystal behaviour of metals/alloys at the meso-scale, a typical way is to simulate the response of a micro-joint between two impenetrable walls under a shearing load. At such a small scale, the inelastic behaviour of a crystal are proposed to be non-localized: dislocations move across the crystal along certain slide systems, piling up at hard particles in the matrix or the impenetrable walls, leading to an hardening effect [7, 9]. The experiment is specially designed to reproduce these models with the aim to identify the basic mechanics for SnAgCu crystals. Fig. 9 gives the PLM image of the entire specimen before mechanical tests. The gap between the two Cu substrates,  $b$ , is  $100 \mu\text{m}$ . The width of the joint is  $1000 \mu\text{m}$ , which is 10 times that of  $b$  to reduce the geometry effect from the joint's edges. This corresponds to the periodical boundary conditions in the non-local crystal-plasticity model. As discussed, due to the formation of Sn dendrites, SnAgCu alloys have the ability to generate large-scale grains. Therefore, only two grains are presented in the cross-section of the prepared joint: a small one on the left side and a relatively large one on the right with different colors. Details of the use of the PLM to identify SnAgCu grains can refer to [1]. During the mechanical test, with the loading rate  $0.1 \mu\text{m/s}$ , the minimum capacity of the microtester, is applied to one of the Cu substrates. According to Eq. 1, the shearing strain rate is  $1 \times 10^{-3}/\text{s}$ . The specimen at first is loaded for 200 seconds (equal to 20% shearing deformation), then held in the tester for 24 hours to release the residual stresses. Normally, a uniform distribution of slip bands will then appear on the surface of each grain [5].

To investigate the evolution of substructures within a grain, a cross-section, which is perpendicular to both the polished surface of the joint and the Cu/solder interface, is prepared by means of FIB as shown in Fig. 10(a). To reduce the effect of both the joint's and grain's boundaries, the section is prepared in the middle of the joint (Point A in Fig. 9). This also approximates the middle position of the larger grain. Fig. 10 (b) focuses at the Cu/joint interface on the





**Fig. 9** PL image of a small Sn3.8Ag0.7Cu solder joint before mechanical tests.  $b = 100 \mu\text{m}$ . Arrows indicate the shearing loading direction.

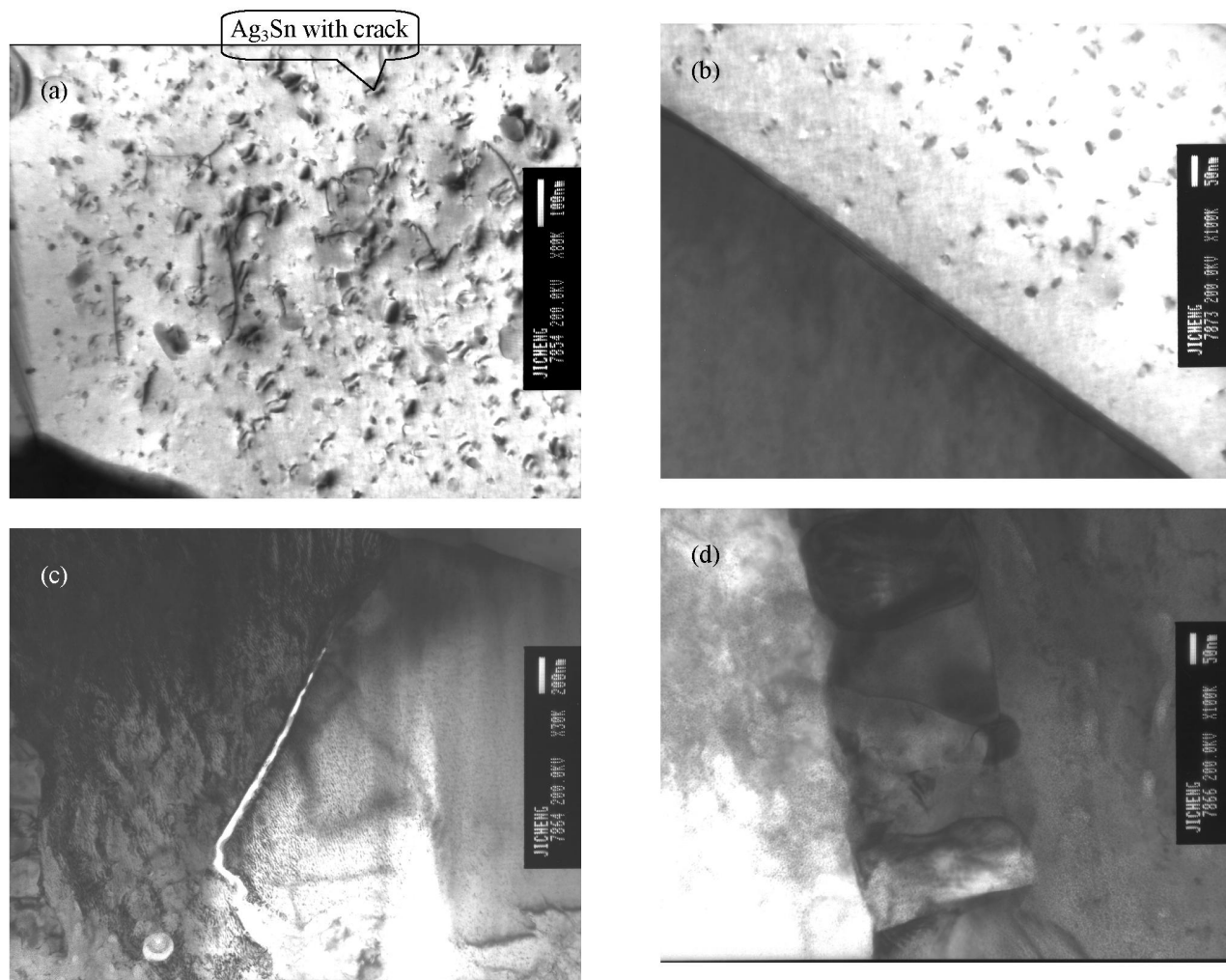


**Fig. 10** Cross-section within a loaded SnAgCu grain at point A in Fig. 9. (a) Investigation area; (b) local ion image. Arrows indicate the shearing loading direction.

cross-section. A typical sandwich IMC structure for Sn-based alloys soldered on the Cu substrate is presented: on the Cu substrate, there is a thin layer of  $\text{Cu}_3\text{Sn}$  particles; between the  $\text{Cu}_3\text{Sn}$  layer and the solder joint, a thick layer of  $\text{Cu}_6\text{Sn}_5$  IMCs is formed. The  $\text{Cu}_6\text{Sn}_5$  layer on the cross-section is composed of two coarse particles. On the larger one, which is closer to

the joint's polished surface, there is a crack across the entire  $\text{Cu}_6\text{Sn}_5$  particles. On the solder side, there are some white IMC particles in the joint, indicating that this area is composed of SnAgCu eutectics.

To further characterize the evolution and damage behaviour due to deformation, the cross-section is lifted up by a precision-controlled probe and milled by the ion beam for TEM observation. It is well known that the SnAgCu solder alloy is considerably soft. A small force during polishing may lead to re-crystallization of the  $\beta$ -Sn matrix on the polished surface. This can change the substructure of a grain, and subsequently influence its mechanical behaviour. To eliminate this factor, a careful check is carried out over the entire SnAgCu area of the cross-section. All the checked positions provide the same diffraction pattern, indicating that this is a single crystal; no recrystallization occurs; and therefore, the achieved results are reliable. This also indicates that the applied loading conditions cannot cause re-crystallization, which is considered as one possible mechanism for the failure of a SnAgCu joint during thermal cycling [10]. Fig. 11 (a) presents an image of this area with a large amount of dislocations present. Actually, the distribution of dislocations is not uniform. In some areas, practically no dislocation can be found. This may be due to heterogeneous deformation within a grain, on the one hand; on the other hand, dislocations may be released since the cross-section is not constrained with regard to all degrees of freedom during the thinning process. It is found that the section is bent during this process, which does not occur in an unloaded sample. Inside the  $\beta$ -Sn matrix, there is a large number of small  $\text{Ag}_3\text{Sn}$  IMCs. It is well known that these particles (or fibres depending on the manufacturing processes) are able to reinforce the alloy since they can block the movement of dislocations. Many studies have been conducted on the strengthening mechanisms of particles in metals/alloys, and it is still an area of active research [11]. A common explanation is that dislocations have a lower energy at the particle/matrix interface compared to that in the matrix. In this case, particles can attract dislocations during their movement. In order to detach from particles, an additional load is required during deformation. In this theory, it is generally considered that dislocations climb over particles before detachment, and it was found in experiments that dislocations can be pinned by  $\text{Ag}_3\text{Sn}$  particles [12]. However, in our tests, cracks are found in these particles, as noted in Fig. 11(a). It is probably that these cracks result from the movement of dislocations: they pile up at the front of particles, resulting in a high residual shearing stress. When the stress reaches a certain level, particles are fractured and sheared, and dislocations go across particles through the cracks to release the residual stresses. Note that the result is only achieved from one loading test. To consistently investigate the strength mechanism, more loading conditions, e.g. the varying loading rate, deformation level and temperature, should be considered. After deformation, dislocations should move across the entire grain. According to the model based on non-local crystalline plasticity, dislocations can pile up at the impenetrable walls. In the specimen, these walls correspond to the  $\text{Cu}_6\text{Sn}_5$  IMC layer.



**Fig. 11 TEM image of local loaded areas. (a) within SnAgCu grain; (b) SnAgCu/Cu<sub>6</sub>Sn<sub>5</sub> interface; (c) interfacial Cu<sub>6</sub>Sn<sub>5</sub> IMCs; (d) interfacial Cu<sub>3</sub>Sn IMCs**

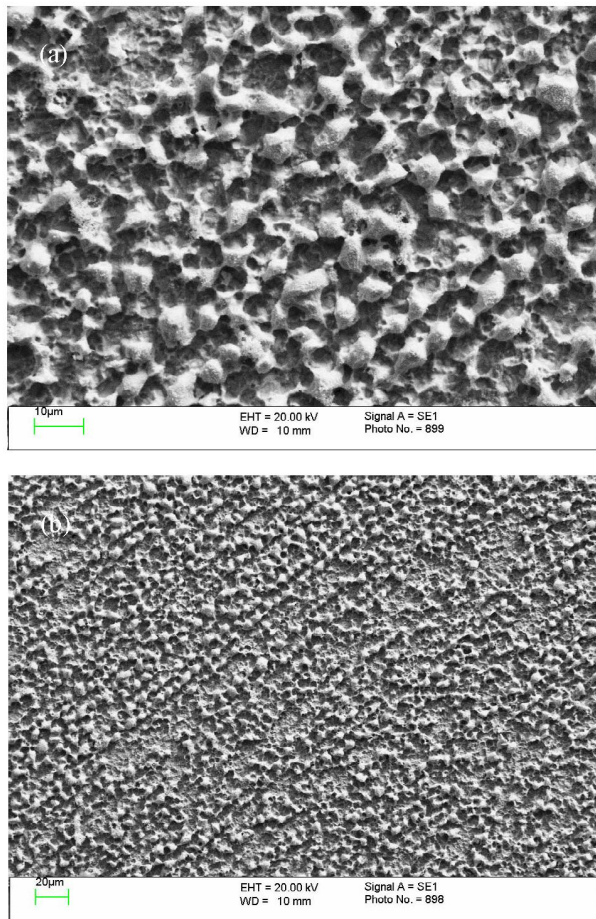
Fig. 11(b) presents an image of this area. As can be seen, no dislocation or damage is found at the Cu<sub>6</sub>Sn<sub>5</sub>/joint interface. In fact, these defects are not found in the entire interface for the two Cu<sub>6</sub>Sn<sub>5</sub> particles. This suggests that dislocations are released, for instance, from the bending during ion milling process, movement of vacancies or damage of the adjacent Cu<sub>6</sub>Sn<sub>5</sub>, as shown in Fig. 11 (c), or they never move into this area, e.g. due to a high energy required for dislocations there. The reliable bonding shows that the interfacial energy is relatively low; and this stronger bonding is able to transfer the entire mechanical deformation (stresses) to the adjacent IMC interface.

Generally, Cu<sub>3</sub>Sn layer was considered to be the weakest site at the IMC interface, especially considering the Kirkendall voids formed there. However, throughout the entire cross-section in our experiment, no damage is found in this layer. Fig. 11 (d) gives an image of this area. The only damage is a large crack formed in a Cu<sub>6</sub>Sn<sub>5</sub> particle as shown in Figs. 10(b) and 11(c). A diffraction analysis performed on both sides of the crack shows similar patterns, indicating that the crack is in one original grain and the crack is intragranular. This damage behaviour is mainly due to its

morphology and properties. As seen in Fig. 4, Cu<sub>6</sub>Sn<sub>5</sub> has a scallop shape in a joint, and propagates into the solder material. During the shearing deformation, a single Cu<sub>6</sub>Sn<sub>5</sub> particle serves as a cantilever beam to resist a bending force, since it is much harder than the SnAgCu solder. This bending force is evident by the lever effect at its bottom: when certain criteria are met, damage occurs there, and the crack rapidly goes across the entire particle due to its brittleness. This also explains why there is no damage in the smaller Cu<sub>5</sub>Sn<sub>6</sub> particle in the cross-section, which has a lower lever effect.

Based on the present mechanical test, the weakest point in the joint is at the Cu<sub>5</sub>Sn<sub>6</sub> layer. However, this finding is from only one site of the sample, and this cross-section is close to one surface of the joint. In this case, the results may be influenced by the free boundary. To obtain more information, the loaded joint is etched with an acid solution, which is able to achieve interfacial Cu<sub>6</sub>Sn<sub>5</sub> IMCs as shown in Fig. 4. Fig. 12 (a) is at a local area within the joint. It shows that nearly half the number of Cu<sub>6</sub>Sn<sub>5</sub> particles fall off, indicating that they were fully broken during deformation, which is in a similar case for the larger Cu<sub>6</sub>Sn<sub>5</sub>, while the remaining particles correspond to the small one particle in the cross-section in Fig. 10 (b). In fact, this type of failure can be generalized





**Fig. 12 Surface morphology of SnCu IMC interface after SnAgCu joint undergoes 20% shearing deformation. (a) a local area; (b) a large area.**

to the entire SnCu interface, as shown in Fig. 12(b), a large interfacial image for the loaded joint.

### Conclusions

In this paper, the formation behaviour of substructures within a SnAgCu grain is summarized. A mechanical test has been designed to apply a shearing deformation to a Sn3.5Ag0.7Cu grain with a constant loading rate. The results show that:

1. Due to the formation of Sn dendrites, SnAgCu grain can reach the same size of a solder joint so that the micro-solder joint contains one or a few grains. The orientation of the AgSnCu grain is controlled by that of original Sn dendrites. Ag<sub>3</sub>Sn are independent of the SnAgCu grain.

2. Under the loading conditions applied in the present test (room temperature, shear strain rate, deformation: 20%), dislocations are presented in the matrix of SnAgCu eutectics in the joint's body. They are not found at the Cu<sub>6</sub>Sn<sub>5</sub> interface. Ag<sub>3</sub>Sn particles in SnAgCu eutectics are fractured, which is probably due to the movement of dislocations in the matrix. In the CuSn IMC interface, a crack goes through the relative large Cu<sub>6</sub>Sn<sub>5</sub> particle in the prepared cross-section. No damage is found in the Cu<sub>3</sub>Sn layer.

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