

ABSTRACT

Title of Dissertation: ANISOTROPIC MULTI-SCALE MODELING
FOR STEADY-STATE CREEP BEHAVIOR
OF OLIGOCRYSTALLINE SnAgCu (SAC)
SOLDER JOINTS

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Heterogeneous integration is leading to unprecedented miniaturization of solder joints. The overall size of solder interconnections in current-generation microelectronics assemblies has length-scales that are comparable to that of the intrinsic heterogeneities of the solder microstructure. In particular, there are only a few highly anisotropic grains in each joint. This makes the mechanical response of each joint quite unique. Rigorous mechanistic approaches are needed for quantitative understanding of the response of such joints, based on the variability of the microstructural morphology.

The discrete grain morphology of as-solidified oligocrystalline SAC (SnAgCu) solder joints is explicitly modeled in terms of multiple length scales (four tiers of length

scales are used in the description here). At the highest length-scale in the joint (Tier 3), there are few highly anisotropic viscoplastic grains in each functional solder joint, connected by viscoplastic grain boundaries. At the next lower tier (Tier 2), the primary heterogeneity within each grain is due to individual dendrites of pro-eutectic β -Sn. Additional microscale intermetallic compounds of Cu_6Sn_5 rods are located inside individual grains. Packed between the dendrite lobes is a eutectic Ag-Sn alloy. The next lower length-scale (Tier 1), deals with the microstructure of the Ag-Sn eutectic phase, consisting of nanoscale Ag_3Sn IMC particles dispersed in a β -Sn matrix. The characteristic length scale and spacing of the IMC particles in this eutectic mix are important features of Tier 1. Tier 0 refers to the body-centered tetragonal (BCT) anisotropic β -Sn crystal structure, including the dominant slip systems for this crystal system.

The objective of this work is to provide the mechanistic framework to quantify the mechanical viscoplastic response of such solder joints. The anisotropic mechanical behavior of each solder grain is modeled with a multiscale crystal viscoplasticity (CV) approach, based on anisotropic dislocation mechanics and typical microstructural features of SAC crystals. Model constants are calibrated with single crystal data from the literature and from experiments. This calibrated CV model is used as single-crystal digital twin, for virtual tests to determine the model constants for a continuum-scale compact anisotropic creep model for SAC single crystals, based on Hill's anisotropic potential and an associated creep flow-rule.

The additional contribution from grain boundary sliding, for polycrystalline structures, is investigated by the use of a grain-boundary phase, and the properties of

the grain boundary phase are parametrically calibrated by comparing the model results with creep test results of joint-scale few-grained solder specimens. This methodology enables user-friendly computationally efficient finite element simulations of multi-grain solder joints in microelectronic assemblies and facilitates parametric sensitivity studies of different grain configurations.

This proposed grain-scale modeling approach is explicitly sensitive to microstructural features such as the morphology of: (i) the IMC reinforcements in the eutectic phase; (ii) dendrites; and (iii) grains. Thus, this model is suited for studying the effect of microstructural tailoring and microstructural evolution. The developed multiscale modeling methodology will also empower designers to numerically explore the worst-case and best-case microstructural configurations (and corresponding stochastic variabilities in solder joint performance and in design margins) for creep deformation under monotonic loading, for creep-fatigue under thermal cycling as well as for creep properties under isothermal aging conditions.

ANISOTROPIC MULTI-SCALE MODELING FOR STEADY-STATE CREEP
BEHAVIOR OF OLIGOCRYSTALLINE SnAgCu (SAC) SOLDER JOINTS

by

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Dedication

To my grandmother, Fengzhi Liu.

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Chapter 1: Introduction

1.1 Background and Motivation

Solder interconnects provide mechanical, electrical, and thermal connections between different structures/materials to achieve proper functionality in microelectronic packages. Their behavior and failure mechanisms are critical to the reliability of integrated packaging systems. Sn-based lead-free solder alloys are widely accepted as a reliable alternative to lead-bearing solders, due to their environmental compliance, affordability, acceptable performance, and their suitability as a direct substitute for Pb-based solders in electronic assemblies.

Sn-Pb alloys have eutectic colonies of lamellar Sn and Pb, where the anisotropic deformation of Sn is accommodated by the softer Pb phase, thus reducing the degree of anisotropy of viscoplastic properties. In contrast, Sn-based solder alloys contain more than 90% β -Sn, and the intrinsic anisotropy of Sn leads to significant differences in the fundamental thermomechanical properties, distinguishing SAC alloys from eutectic Sn-Pb solders, particularly in their microstructure and associated mechanical behavior. As-fabricated SAC solder joints normally consist of only a few highly anisotropic grains. This oligocrystalline microstructure within each microscale solder joint and orientation-dependent grain properties renders each joint with unique thermomechanical behavior. This anisotropy in initial microstructure results in significant piece-to-piece variability among the performance of different joints under similar or even identical applications

The development of heterogeneous integration has led to solder interconnects located in complex structures (such as three-dimensional wafer-level packages and multi-die stacks) and subject to quite demanding loading conditions (Lau et al., 2018). Appropriate material properties are necessary for numerical simulations in order to accurately assess their performance and reliability within the system. Extensive studies have been conducted to characterize the mechanical properties of SAC alloys, however, the results vary not only between groups but also between multiple measurements of the same group (Cuddalorepatta et al., 2010; Ma and Suhling, 2009). This is usually attributed to the stochastic variations in the microstructure of each joint, which typically consists of only a few highly anisotropic grains, in either discrete or interlaced morphology (Arfaei et al., 2013; Daszki and Gourlay, 2021). Moreover, the miniaturization of packages leads to an increase in the number of I/Os and a decrease in pitch size, which also reduces the size and volume of individual solder joints. The solder joint may be of similar length scale as the grain size, in microbumps. In addition, research has been conducted to achieve precise control of electronic manufacturing by incorporating the nucleants (Ma et al., 2017) or directional solidification (Gu et al., 2019) to control the grain orientation in single-crystal solder joints. Orientation-dependent and microstructure-sensitive properties should be clearly understood for grain morphology selection, assuming that in the near future, the microstructure of Sn-based solder joints will move from a stochastic outcome to deterministic control.

In view of these facts, both testing and modeling schemes should be based on representative anisotropic grain-scale microstructures.

1.2 Problem Statement

Although SAC interconnects are usually modeled as isotropic homogeneous bodies in numerical simulations, in reality they are neither isotropic nor homogeneous. The stochastic orientation and arrangement of a few grains in each joint, together with the inherent anisotropic properties of each grain, gives each joint a stochastic microstructure, resulting in unique thermomechanical response of each joint. Grain-scale testing has been used in the literature to characterize solder properties, to gain insight into possible variabilities between specimens, and to study the effects of microstructure. Further, the test results help to understand the influence of microstructure and its correlation with mechanical response and variability, through a grain-scale modeling methodology. The literature reveals a strong need for additional testing and modeling approaches for grain-scale assessment of steady-state inelastic behavior of few-grained SAC solder joints is necessary. To accomplish this, properties of both individual grains and the accommodating grain boundaries are necessary. This study will be limited to steady-state creep behavior.

1.3 Literature Review

1.3.1 Anisotropy of β -Sn

Since SAC alloys contain more than 90% β -Sn phase and commonly exhibit oligocrystalline microstructure (Lee et al., 2010), understanding and accurately quantifying the anisotropic properties of β -Sn is critical as a starting point for analyzing and predicting the orientation-dependent behavior of SAC grains. β -Sn crystal has a body-centered tetragonal (BCT) structure, with lattice parameters $a=b=5.83 \text{ \AA}$ and $c=3.18 \text{ \AA}$ ($c/a=0.545$), as shown in Figure 1.1. This crystal structure, with lower symmetry than the cubic structure, leads to a high degree of anisotropy in its thermal expansion (Deshpande and Sirdeshmukh, 1962; Xian et al., 2017), stiffness (Rayne and Chandrasekhar, 1960) and diffusivity (Huang et al., 2015), thereby affecting thermo-mechanical behavior and electromigration.

The six elastic constants for mechanical behavior of single crystal β -Sn have been measured by multiple researchers using different methods. Although there are several discrepancies among these values, the results reported by Rayne & Chandrasekhar (1960) and Kammer et al. (1972) have been experimentally verified to a certain extent. Based on Rayne's data, the maximum ratio of elastic stiffness along different directions is about 3 at room temperature and can exceed 4 at 423 K. The ratio of CTE along [001] and [100] is about 2. Subramanian and Lee (2004) conducted elastic analysis of the stress tensor due to thermo-mechanical mismatch between two adjacent grains, as a consequence of temperature change. The computed results indicated significant 3D stress at the grain boundaries and important effects of Sn

anisotropy on the reliability analysis of Sn-based solder alloys. As one of the most important mechanical properties at high temperature, creep will significantly affect the actual deformation response and durability under cyclic loading. β -Sn melts at a low temperature of about 505 K, so even at room temperature, the homologous temperature is higher than 0.5, which makes it important to consider viscoplastic deformation of SAC single crystals.

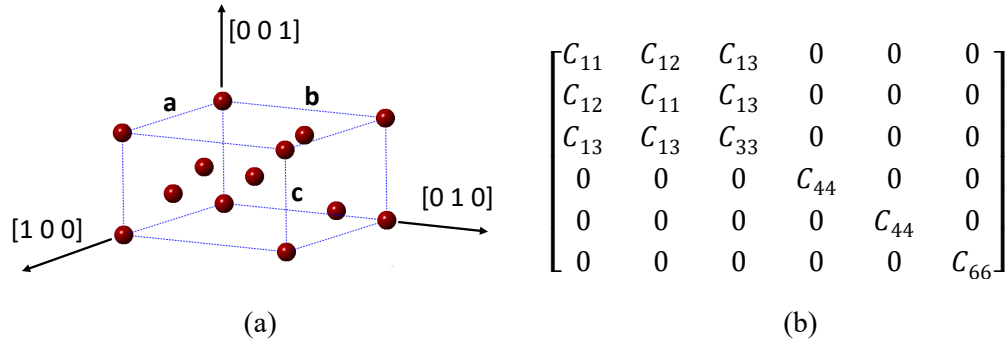


Figure 1.1 β -Sn: (a) Body body-centered tetragonal (BCT) crystal structure; (b) The matrix of stiffness constants.

1.3.2 Heterogenous microstructure of SAC solder joints

Although a great deal of work has been done to characterize the thermo-mechanical properties of Sn-based solder alloys, there are considerable discrepancies across different studies between experimental measurements and the model constants subsequently extracted from the test results. One reason for this discrepancy is attributed to differences in microstructure. Functional SAC solder joints commonly exhibit oligocrystalline (up to a few grains) morphology in either discrete or interlaced structures, with stochastic distribution of grain orientations (Bieler et al., 2008; Telang and Bieler, 2005). The behavior of these individual grain-scale solder

joints may be quite different from that of bulk polycrystalline specimens (Kariya et al., 2005; Sahaym et al., 2013).

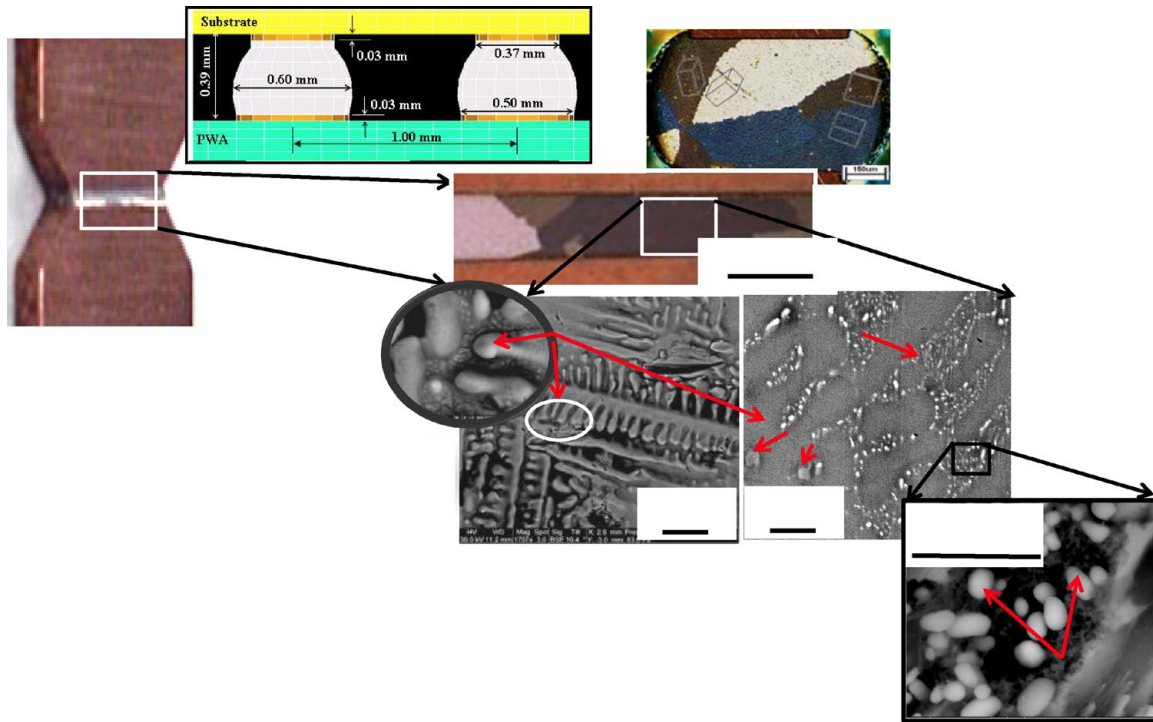


Figure 1.2 Typical microstructure of SAC solder joints (Mukherjee et al., 2014)

More than 90% of SAC alloys are β -Sn, which is one of the most anisotropic elements due to its body-centered tetragonal (BCT) crystal structure. The intrinsic anisotropy of β -Sn promotes the formation of heterogeneous microstructures during solidification, therefore leading to complex properties and unique microstructure of each joint. In addition, there are different solidification paths in the Sn-Ag-Cu ternary system, which complicates the non-eutectic solidification and makes it very sensitive to the alloy composition, cooling rate and post-soldering thermal aging (El-Daly et al., 2013; Sungkhaphaitoon and Plookphol, 2018; Zhao et al., 2004). The effects of these microstructural features, like dendritic morphology, intermetallic compounds (IMCs) coarsening, and inter-particle spacing, and so on, are measured quantitatively (Arfaei

et al., 2011; Chauhan et al., 2013; Fu et al.; Gu et al., 2021; Han et al., 2012). Moreover, the processes that lead to changes in these characteristics, such as cooling rate, isothermal aging, doping, etc., and the consequent influence on the behavior of solder joints are also investigated (Chuang et al., 2012; Darbandi et al., 2014; Lee and Huang, 2016; Maleki et al., 2014; Ochoa et al., 2004; Tsao, 2011; Yifei et al., 2008). For example, Ochoa's group (Ochoa et al., 2003) studied the effect of cooling rate on bulk Sn-3.5Ag solder. Different media were used to control the cooling rate: water, air and furnace. Increasing the cooling rate was reported to decrease both the dendrite size and the dendrite arm spacing. Thus, rapid solidification reduces the diffusion time, and then produces finer dendritic microstructures. Tensile tests have shown that the mechanical behavior is strongly influenced by the changes in microstructure caused by the cooling rate. Lee and Huang (2016) examined 4 locations in a continuous cooling experiment, with step-down cooling rates of 63°C/s, 21°C/s, 9°C/s and 2.5°C/s. With SEM inspection, the estimated size of β -Sn dendrite is approximately 30 μm^2 , 380 μm^2 , 550 μm^2 and 620 μm^2 respectively. And the corresponding volume fraction of β -Sn is about 27.8%, 42.5%, 50.2% and 55.3%, respectively. Cooling rate was also reported to affect the aspect ratio and morphology of Ag_3Sn IMC particles. In the continuous cooling test mentioned above, the morphology of the Ag_3Sn IMC particles transformed from particle shape to needle shape, then to plate shape, and finally to leaf shape, with decreasing cooling rate. The mechanical properties, such as yield strength, ultimate tensile strength, and microhardness were found to change with different solidification rates.

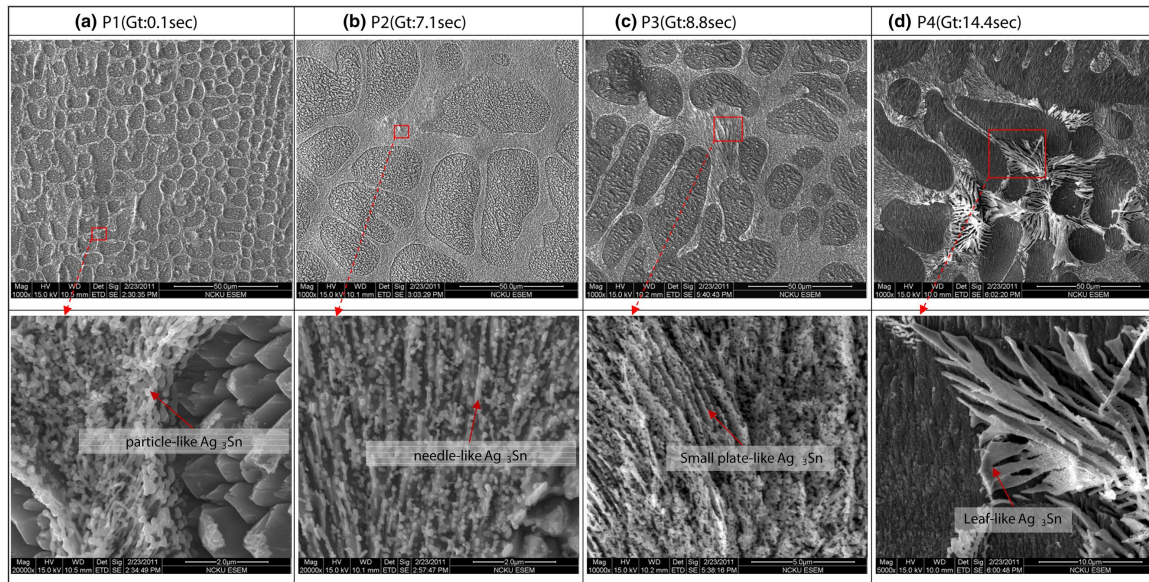


Figure 1.3 3D morphology of Ag_3Sn compounds in the eutectic phase at different cooling rates (Lee and Huang, 2016)

With the endeavors toward component miniaturization and weight reduction in advanced electronic packaging industry, there is a continuous increase in I/O density and corresponding shrinkage in solder joint dimensions. The reduction in characteristic joint size will change the solidification rate and microstructure in SAC joints. Mueller et al. (2007) compared solder joints of different diameters (as shown in Fig. 1.4) and found that the average dimensions of Sn dendrites reduces with decreasing solder ball size and that the microstructure morphology of larger joint is scalable to that of smaller one. Kinyanjui et al. (2005) measured the mean width of the Sn dendrite arm and observed that it grew monotonically with respect to the joint diameter.

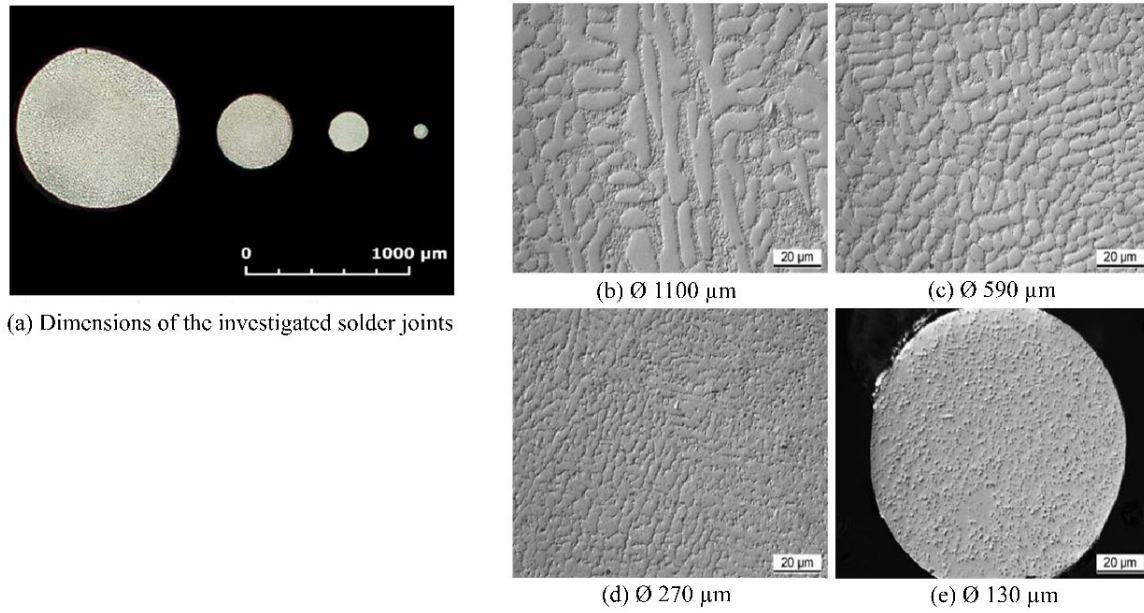


Figure 1.4 Effect of size on microstructure of solder joints (Mueller et al., 2007)

As the size of the solder joints is reduced to a few tens of microns, the volume reduction increases the fraction of the joint occupied by the interfacial IMC layers (Wang et al., 2009), as shown in Figure 1.5, and therefore changes the internal stress/strain concentration gradient (Khatibi et al., 2012; Lee et al., 2008). Choudhury and Ladani (2016) conducted systematic numerical experiments to analyze the effect of IMC thickness on the stress distribution in the microbumps. The thickness of the scallop-type Cu_6Sn_5 IMC layer was varied from 0 to 80 μm relative to the entire joint height of 100 μm . Contour plots of in-plane shear stress are provided in Figure 1.a. Joints with thicker IMC layers show stiffer response and higher yield stress under shear deformation, due to the higher yield property of Cu_6Sn_5 . In addition, the loss of solder joint volume increases the impact of contaminants, which are unintended elements from adjacent structures/materials, and changes the phase equilibrium and microstructure (Park et al., 2010; Wang et al., 2019; Yang et al., 2010).

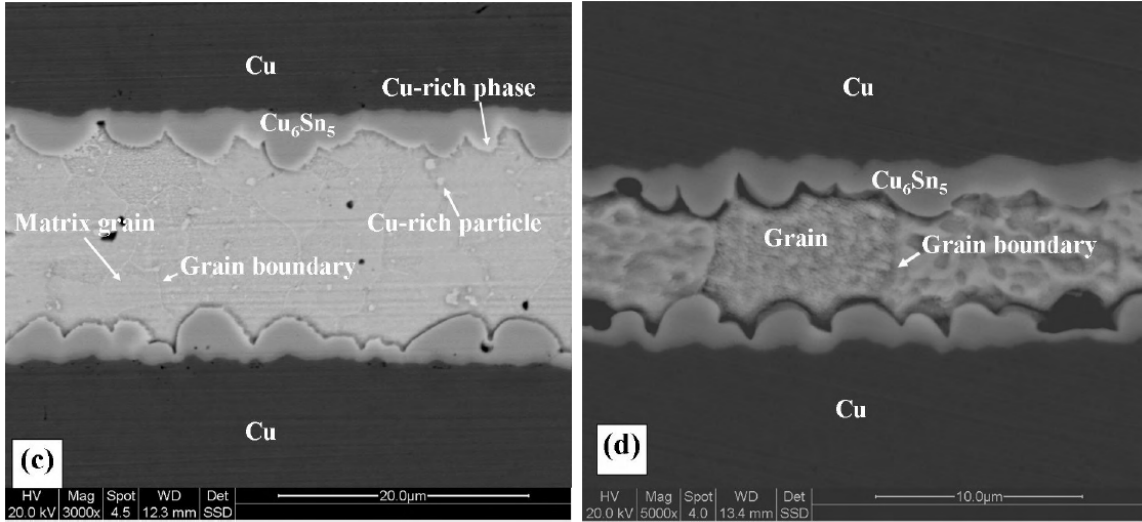


Figure 1.5 Cross sections of Cu/Sn/Cu solder joints with different stand-off height: (a) 100 µm, (b) 50 µm, (c) 20 µm and (d) 10 µm (Wang et al.)

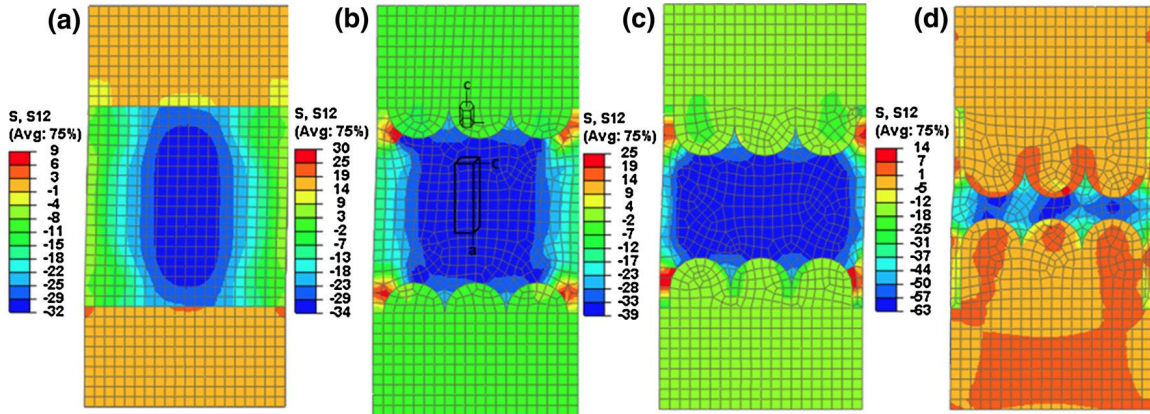


Figure 1.6 Contour plot of in-plane shear stress for solder joint with different IMC thickness: (a) 0, (b) 20 µm, (c) 40 µm, (d) 80 µm,

1.3.3 Crystal viscoplasticity modeling

The development of viscoplasticity models for single-crystal materials has been pursued from many aspects. MacLachlan et al. (2001) proposed a macroscopic single crystal model to capture the stress rupture and creep behavior of Ni-base superalloys, which are simplified as a single-phase material, in terms of the damage mechanisms

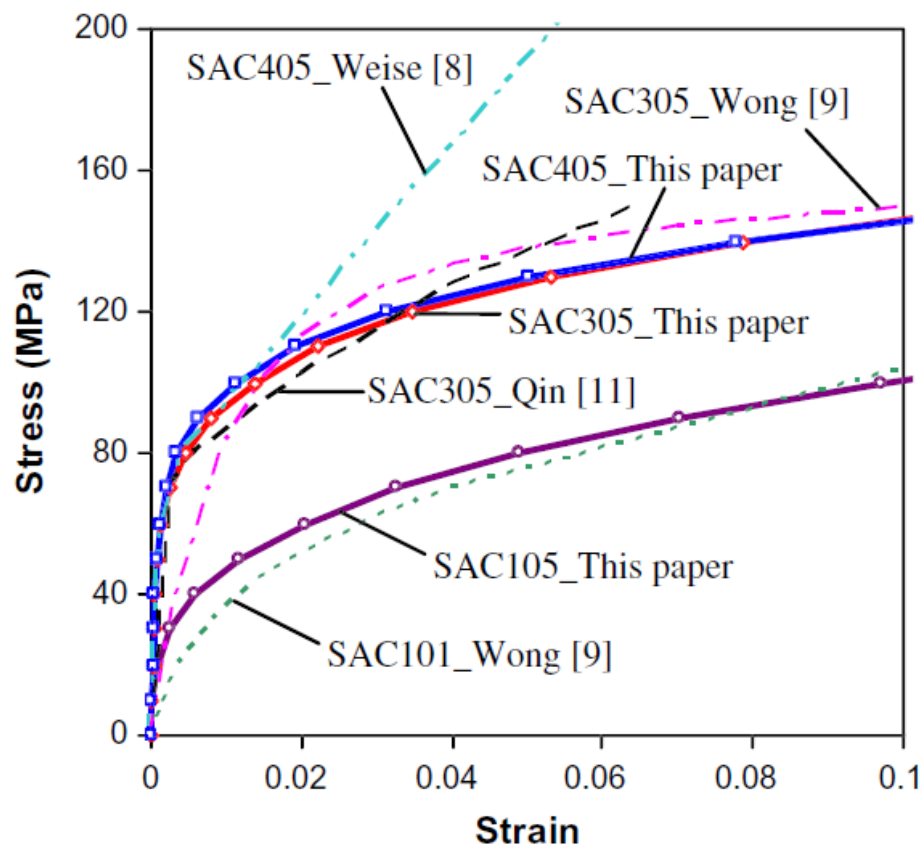
and slips on specific systems. A constitutive model was developed for the creep resistance of single crystal nickel-based superalloys within a thermodynamic frame (Prasad et al., 2006; Prasad et al., 2005), in which the anisotropic creep response is incorporated in terms of the stored energy and the rate of dissipation functions. Ma and co-authors developed a crystal viscoplasticity model for single-crystal Ni-based superalloys, accounting for the underlying deformation modes and their interactions (Ma et al., 2008). The dependence of creep on multiple features, such as the scale of the microstructure, channel thickness, and volume fraction of precipitates, was captured in this formulation. Estrada and co-workers extended this method in a displacement-based integration code to model 3-D creep-fatigue interactions (Estrada Rodas and Neu, 2018). Le Graverend and co-workers presented a viscoplastic formulation (le Graverend et al., 2014) developed in the crystal plasticity framework for another Ni-based single crystal superalloy (Cailletaud, 2009) and introduced new internal variables to take into account the microstructure evolution and the effect of mechanical and thermal history. Later, this microstructure-sensitive crystal viscoplastic model was coupled with a phenomenological hardening-based damage density function, embedded in an anisotropic formulation (le Graverend, 2019). Constitutive relation for the kinematics of single-crystal FCC metals was modeled based on the crystallographic shearing rates of the slip systems (Austin and McDowell, 2011). Zhu and co-authors focused on the influence of the composition on the creep behavior of Ni-based single crystals, and modeled the creep resistance according to the climb of dislocation and the rate of escape from the trapped configurations (Zhu et al., 2012). Mukherjee and co-workers proposed a mechanistic

multi-scale modeling framework that describes the anisotropic transient and steady-state creep behavior of single-crystal SnAgCu alloy, based on its heterogeneous microstructure and dislocation mechanics (Mukherjee et al., 2016). Brehm and Glatzel (1999) proposed a constitutive model to describe the anisotropic creep behavior of Ni-based single crystal, by extending the Haasen-Alexander model to multiple coupled slip systems, in which individual dislocations interact with each other. As a simplification, this model development was restricted to single phase. This method was implemented in numerical simulation to analyze the orientation-dependent creep behavior of two-phase single crystals (Preußner et al., 2009).

1.3.4 Characterization and modeling of the mechanical behavior of SAC solder joints

The stochastic initial microstructure of oligocrystalline SAC solder joints results in significant piece-to-piece variability among the performance of different joints under similar or even identical applications. Nguyen compared his elasto-plastic curves of ternary solder alloys with other literature's, finding obvious differences in the hardening region for samples tested by different groups but of the same compositions (Nguyen and Park, 2011), as well as significant variations in stress level for samples with different Ag contents but at the same strain range, as shown in Fig. 1.2 (a). Vianco et al. reported a significant variability in the compression creep behavior for the as-cast 95.5Sn-3.9Ag-0.6Cu solder joints. Differences in the shape of creep curve, strain magnitude and strain-rate were attributed to the discrepancies in the joint microstructure (Vianco et al., 2004a, b). A comparison of experimental results between Schubert et al. (Schubert et al.) and Pang et al. (2004) showed

considerable differences in the values of parameters. A closer examination pointed out that the variations in two sets of data reflect changes in microstructure during testing. Cuddalorepatta et al. measured creep responses for five SAC305 specimens, which followed the same fabrication process. Although tested at similar stress level (20 MPa) and the same temperature (25 °C), the results exhibited a large variation.



(a)

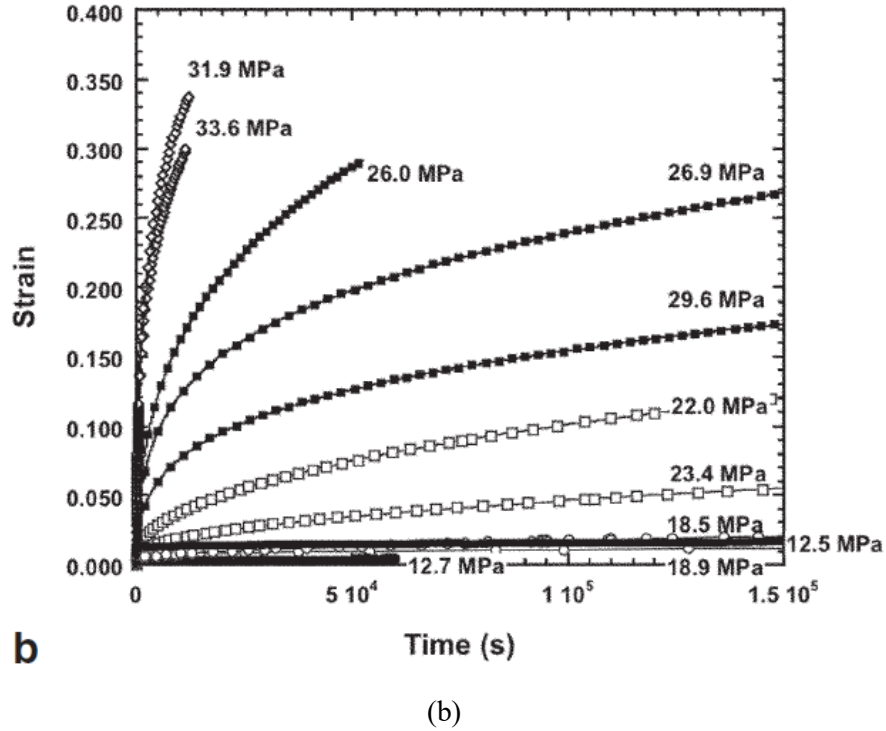


Figure 1.7 (a) Comparison of elasto-plastic curves for the solder alloys (Nguyen and Park, 2011). (b) Creep strain versus time for as-cast samples tested 25 °C (Vianco et al., 2004b).

To better understand the mechanical behavior of SAC joints during applications, modeling approaches need to be based on its heterogeneous microstructure and be able to capture the anisotropy presented in BCT Sn (primary phase in SAC alloys). Although the anisotropic mechanical responses of SAC solder joints have attracted extensive interest and Crystal Plasticity Finite Element Method (CPFEM) has been used to describe plastic behavior of SAC alloys from single crystal to joint-scale specimens, the modeling of anisotropy in elasticity and creep response of SAC joints remains an ongoing challenge.

Considering the inevitable influence of this heterogeneous microstructure, multiscale modeling has been proposed to better characterize the behavior of different materials, usually classified into concurrent and hierarchical approaches according to

the bridging methodology (Chandra et al., 2018; de Pablo and Curtin, 2007; Groh et al., 2009; Tan et al., 2021). Maleki and his colleagues (Maleki et al., 2013, 2016) created statistically representative volume elements (RVEs) for SAC405 in three-dimensional finite element (FE) modeling, which preserves the characteristics of the actual microstructure obtained through tomographic images. Numerical homogenization was performed sequentially on the microscopic scale (within the eutectic mixture) and mesoscopic scale (including dendrites, surrounding eutectic phases and IMC) to extract the overall elastic-plastic behavior of the solder joint during isothermal aging. For simplicity, the anisotropy of Sn was not considered by Maleki. Mukherjee and co-authors (Mukherjee et al., 2016) proposed a mechanical model based on microstructural features and dislocation motions along the three most facile slip systems, to predict the anisotropic transient as well as steady-state creep response of SAC305 single crystals. Xu et al. (2021) focused on the effect of morphology and size of IMCs on the early-stage creep of directionally solidified SAC305 samples. In the FE analysis, RVEs representing eutectic mixtures of three different microstructures were modeled as particle-reinforced matrix composites, while the β -Sn was modeled by a dislocation-based crystal plasticity method. After homogenization, changes in creep resistance were determined based on the microstructural evolution caused by aging.

1.3.5 Gaps in the Literature

Although previous studies have provided insights into the correlation between the intrinsic microstructure and mechanical behavior of SAC alloys, both in terms of bulk specimens and microscale functional joints, there are still several unresolved issues.

- Anisotropic elasticity of SAC crystal is not available, neither from experimental measurements nor from analytical modeling.
- Effect of morphology variations inside the SAC crystal on its elastic modulus has not been quantified
- No mechanics based anisotropic modeling to capture the secondary creep behavior of β -Sn crystal observed in conventional creep tests
- No grain-scale modeling for steady-state creep analysis on SAC joints containing multiple grains
- Accommodation of grain boundary viscoplastic behavior in oligocrystalline SAC joints has not been quantified
- No prediction of variability in the viscoplastic response of SAC joints with different grain orientations, morphologies, and arrangements
- Variations encountered in the reliability and failure analysis of SAC joints cannot be predicted on the basis of microstructure and dislocation mechanisms

1.4 Scope of this Dissertation

The remainder of this dissertation is organized as follows. Chapter 2 introduces the thermo-mechanical microscale (TMM) system and grain-scale specimens used for mechanical testing, and for characterizing the typical microstructure of oligocrystalline SAC305 solder joints. Chapter 3 describes in detail the anisotropic multiscale modeling framework for the elastic behavior of oligocrystalline SAC solder joints. Chapter 4 presents a multi-tier Crystal Viscoplasticity (CV) modeling approach and a corresponding continuum constitutive modeling approach, which aims to describe the anisotropic steady-state creep behavior of single-crystal β -Sn.

Chapters 5 and 6 present the multiscale modeling strategy for the secondary creep response of oligocrystalline SAC solder joints, focusing on the anisotropic behavior of individual crystals and the contribution of grain boundaries, respectively. This dissertation concludes in Chapter 7 with Summary & Discussion, Limitation and Future Work.

Chapter 2: Experimental System and Test Specimen

The mechanical test system used in current work is introduced in this chapter, including a brief description on the design and fabrications of specimens. The custom-built experimental system used to characterize mechanical properties of solder materials at functional length scale is introduced Section 2.1. As a well-established system, this setup has been used to test several interconnection materials, such as lead-tin solders, lead-free solders and sinter paste/adhesive. The detailed description of this test setup, related calibration procedure and additional improvements are provided in previous dissertations (Haswell, 2001; Zhang, 2004). A brief introduction is provided here for completeness. The specimens used for TMM tests is provided in Section 2.2.

2.1 Test System

The customized test system, named as “Thermo-Mechanical-Microscale (TMM) setup, was first designed by Haswell (Haswell, 2001) aiming to conduct monotonic constitutive tests and cyclic durability tests, at temperature ranging from room temperature up to 200°C. The test setup and its shear grips are shown in Fig. 2.1 (a). Mechanical tests are controlled by a lead-zirconate-titanate (PZT) high-resolution linear actuator for close-loop operation, with a total traveling range of 90μm. The actuator is directly connected to a flexible link, which transfers displacement to the movable grip through the holding shaft. The shaft is sleeved by a low-friction linear bushing, to protect the actuator from bending and off-axis loads during installation and tests.

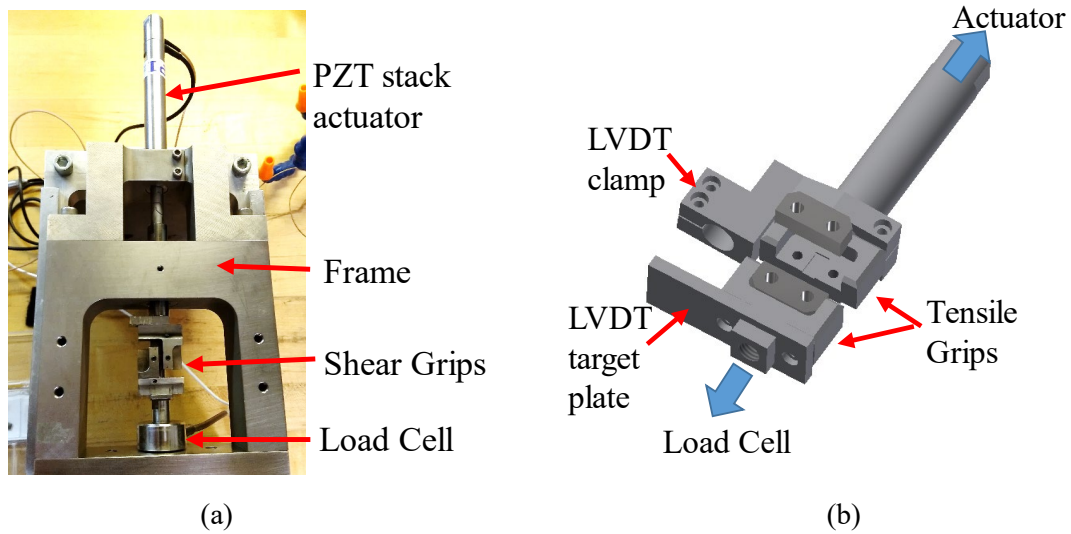


Figure 2.1 TMM test setup with different grips: (a) test system with shear grips (b) 3D drawings for tensile grips

2.2 Test Specimen

The initial design of the TMM system aimed to characterize mechanical behavior of solder joints using shear specimens, whose dimensions are similar to those of functional interconnects (100~1000 μm). The length scale (shear loading across the 200 μm width) is critical for specimens to capture the typical microstructure of solder joints in applications, especially for those oligocrystalline, highly anisotropic Sn-based interconnects.

The shear specimens used in this work were modified based on the Iosipescu shear test method and are able to produce a very uniform stress field in the specimen gage zone, due to the 90° notch angles on both sides of joint. As shown in Fig. 2.2 (a), the typical solder joint is about 0.2 mm wide, 3 mm long and approximately 1mm long. Two pieces of copper platens are used to mimic the OSP pad finish and transform loadings from grips.

The TMM system can also be equipped with tensile grips to conduct uniaxial tension tests. The joint-scale tensile specimen is depicted in Fig. 2.2 (b). Copper platens with curvature in the end connected to solder joints were designed to produce a wider gripping area and gradually taper into a narrow gage zone in the joint. The dog-bone shape specimens aimed to yield a uniform stress distribution at the mid of joints. Due to the constraints of copper platens, stress concentration was found in the edges of specimen, which was inevitable considering the joint-scale nature of the specimen. Since copper has a higher modulus than commonly used solder materials, most deformation is expected to occur in the joint. Hence the effect of stress concentration should be insignificant.

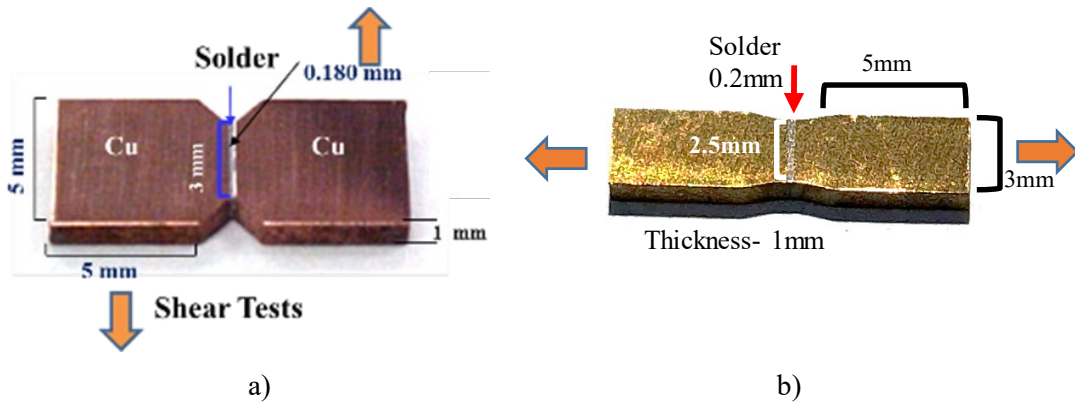


Figure 2.2 TMM Specimens: (a) for shear testing (b) for tensile testing

The copper platens are manufactured by electrical discharge machining (EDM) process for a precision geometry with low residual stresses and good surface finishes. Tight tolerances assist to produce identical platens, which is critical for fabricating repeatable solder joints with desired dimensions. For each new batch of platens, at least 10% of them were randomly picked for standard quality check on dimension, asymmetry, parallelism, and perpendicularity. After pairing under an optical

microscope, 4 pieces of platens (2 pairs) of similar heights were mounted in the corners of grinding fixture and ground with 1200-grit silicon carbide paper, for a smooth, flat and oxide-free soldering surface. Platens were paired again after initial grinding to ensure the soldering surfaces of the same length and parallel to each other. Possible mismatches, such as overlapping edges or round corners, should be checked and avoided carefully.

Matched pairs were cleaned thoroughly before soldering, to remove any residual debris and oxides for an optimal soldering surface. Each platen was first cleaned with isopropyl alcohol (IPA) using a soft bristle brush, then dipped into one rosin flux and placed on a preheated hot plate at 130°C for a few seconds. After active flux removing oxidations from the copper surfaces, platens were removed from the hot plate and cleaned with IPA again. This cleaning process was repeated thrice or more if needed.

Platens ready for soldering were assembled in an alignment fixture. A shim was placed in the middle of two copper pieces to create the gap region for a desired joint width, which is about 180 μm in current study. The soldering procedure adopted in this study was strictly follow the same method used by Haswell, Zhang, and Cuddalorepata, in order to facilitate comparisons of the mechanical behavior of the various solder compositions tested with the current methodology. Soldered specimens were examined for fillet size, void densities, and planarity. Admissible specimens were wrapped in high-temperature Kapton tape and conditioned at 0.8 homologous temperature (80% of absolute melting temperature) for 100 hours to obtain a stabilized microstructure in the joint and relax any residual stresses remaining from

the prior reflow or grinding processes. Aged specimens were gently ground and polished to remove any oxide layers formed during the isothermal conditioning, using standard metallography preparation procedures.

Before testing, prepared specimens were inspected and characterized individually for microstructural features and geometric parameters. All information was record for future analysis. In particular, the void densities, intermetallic layer at the interface and fillets are examined. This examination aimed to eliminate defective specimens, such as those with high void contents, weak interfacial boning and unusual microstructural features (pre-existing cracks) or joint geometries (skewed, asymmetric joints). Further details about specimen preparation could be found in previous dissertations.

The calibration of both multi-scale modeling approaches on elasticity and creep necessitates single crystal joint-scale specimen. For samples dominated by a single grain, the simple stress conditions applied on the specimen frame could be transformed to crystal coordinates, without considering the effects of loads sharing among different crystals and the relative deformation between neighboring grain boundaries.

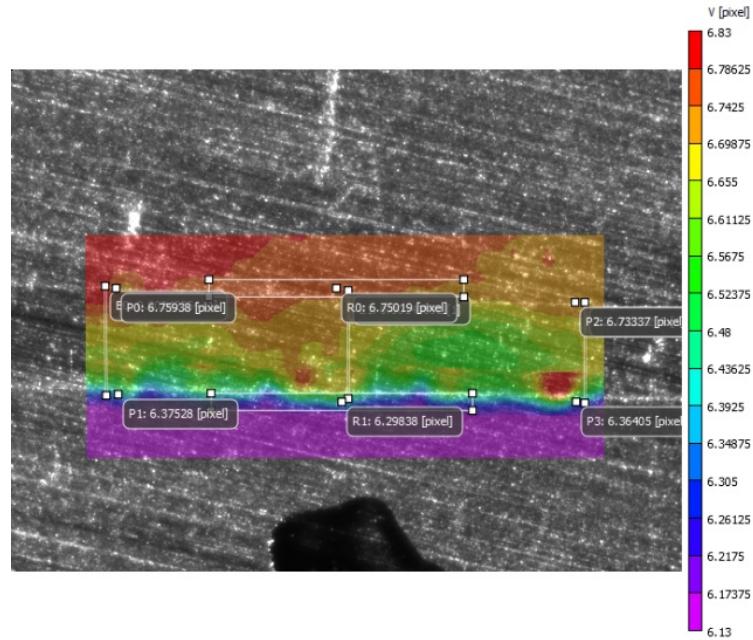
For the procedures of specimen preparation used in this study, slowing down the cooling rate will increase the probability of single-crystal specimen. One example of single-crystal joint fabricated with extremely slow cooling rates is shown in Fig. 2.3. A trial-and-error method with varying cooling slopes was applied to investigate the number of crystals within TMM solder joints.



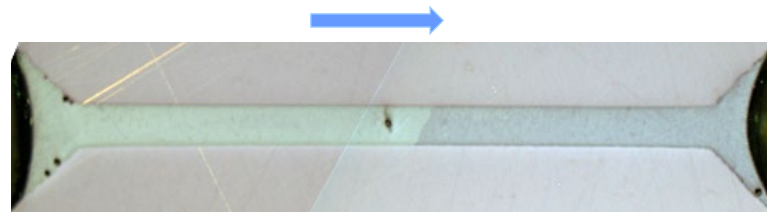
Figure 2.3 Cross-polarized image of a single-crystal tensile specimen

2.3 Additional Displacement/Deformation Measurements

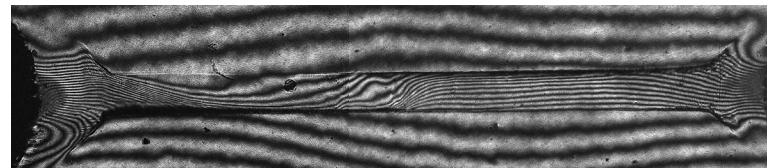
In the TMM system, a Solartron linear variable differential transformer (LVDT) and its target plate are mounted on the two pieces of grips separately, to control and measure the deformation. Although the compliance of the load train (from the copper platens and grips) is compensated during the post-processing, the measurement of LVDT sensor on a single-crystal specimen contains deformations of both crystal and intermetallic compounds layers. In order to capture the in-situ deformation of the crystal precisely, two other techniques are considered: Digital Image Correlation (DIC) and High-sensitive Moiré interferometry. Example measurements of two methods on the solder joints are presented in Fig. 2.4.



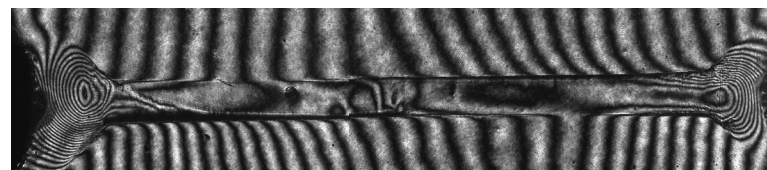
(a)



TMM shear specimen tested with constant loading



Moiré measurement in the horizontal direction



Moiré measurement in the vertical direction

(b)

Figure 2.4 Deformation Measurements of (a) DIC and (b) Moiré interferometry

Chapter 3: Elastic Behavior of Oligocrystalline SnAgCu (SAC) Solder Joints Based on an Anisotropic Multi-scale Predictive Modeling Approach

Abstract

Lead-free electronic interconnections made of Tin-rich solder alloys usually contain only a few highly anisotropic grains, rendering their overall thermo-mechanical behavior highly dependent on each crystal's morphology and orientation. Miniaturization and heterogeneous integration will further reduce the length-scale of interconnections and exacerbate this piece-to-piece variation among different solder joints. The objective of this paper is to predict the elastic response and intergranular stresses in oligocrystalline SAC (SnAgCu) solder joints, starting with orientation sensitive anisotropic predictive models of the elastic behavior of single crystals. The properties of the single crystal is, in turn, predicted by a multi-scale method, where each grain is modeled as a collection of Sn dendrites embedded in an eutectic Sn-Ag matrix. The eutectic phase, in turn, is modeled as an effective homogenized composite material consisting of nano-scale Ag_3Sn particles embedded in a highly anisotropic tin matrix. All homogenization for prediction of single-crystal elastic properties is based on composite micromechanics, using Eshelby's method and Mori-Tanaka homogenization. Elastic response of few-grained solder joints is then numerically predicted from the anisotropic behavior of the single crystal, by explicitly modeling the grain morphology in finite element analysis (FEA). Stress distributions along grain boundaries are simulated and analyzed in terms of the misorientation angle between neighboring grains. The mismatch in von Mises stress along the

boundaries varies up to 55% for grain structures considered here. This multi-scale predictive modeling approach is explicitly sensitive to microstructural features such as the morphology of: (i) the intermetallic compound (IMC) reinforcements in the eutectic phase; (ii) dendrites; and (iii) grains. Thus, this modeling approach is ideally suited for: (i) parametric studies of the effect of microstructural tailoring on solder joint thermo-mechanical behavior and (ii) examining the effects of microstructural evolution caused by static and cyclic thermo-mechanical aging. This work forms the starting point for future development of microstructurally based anisotropic models of crystal-scale inelastic behavior.

Key words: Lead-free solder, anisotropic elasticity, heterogeneous microstructure, multiscale homogenization, coarse-grained finite element model

3.1 Introduction

Ternary SnAgCu (SAC) alloys have been widely used in the electronics industry to replace Pb-Sn solder materials. Unlike the Pb-based alloys, as-solidified SAC joints contain only a few highly anisotropic grains, as shown in Figure 3.1 (a). The thermo-mechanical behavior of different joints therefore exhibits significant piece-to-piece variability, due to the variations in grain structure and intragranular microstructure [1]-[7]. These variations are usually stochastically dependent on the fabrication method and composition. This paper presents a systematic multi-tier modeling approach for mechanistic estimation of the anisotropic elastic behavior of SAC single crystal as well as the elastic load-displacement characteristics of polycrystalline joints. This modeling approach is important because it allows

parametric investigation of the effect of the micro-morphology of the SAC alloy on the elastic behavior. More importantly, this approach provides the starting point for microstructurally based models for predicting crystal-scale inelastic behavior (plasticity and creep).

The microstructure of SAC solders has been well documented in the literature [8]-[10]. Within each SAC crystal, the pro-eutectic β -Sn is in the form of dendrites, surrounded by a eutectic Sn-Ag phase, which is composed of nanoscale Ag_3Sn precipitates embedded in a pure β -Sn matrix. Microscale and nanoscale precipitates of intermetallic compounds (IMCs) Cu_6Sn_5 and Ag_3Sn are found in the bulk and microns-thick layers of IMC are found near the interface between the solder and the copper bond-pads. The interfacial IMC species depends on the pad and surface plating materials.

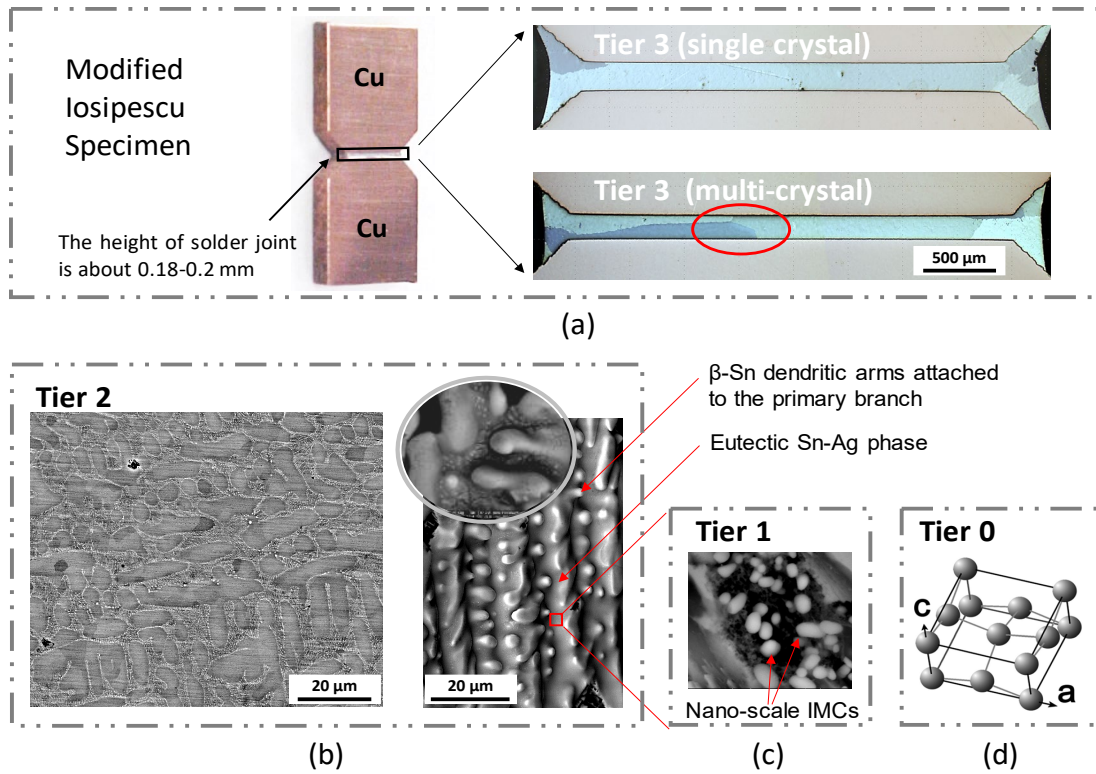


Figure 3.1 Heterogeneous multiscale hierarchical microstructure within SAC305 solder joints: (a) Tier 3: Grain morphology of typical ball grid array (BGA) and specimen used in custom-built thermo-mechanical micro-scale (TMM) test system; (b) Tier 2: β -Sn dendritic morphology within each grain; (c) Tier 1: Typical morphology of eutectic Sn-Ag region within each grain; (d) Tier 0: BCT crystal structure of β -Sn

The microstructure of tin-based lead-free solders is known to be affected by several factors, such as composition, solidification conditions (melting conditions, time above melting point, cooling rates), and surface finish materials [11]-[19]. Even with identical fabrication processes, SAC solder joints on the same components could exhibit stochastically different distributions of grain size and orientation. Electron backscatter diffraction (EBSD) orientation imaging microscopy (OIM) scans are widely used for analyzing microstructural features, such as crystal orientation and distribution. Although cyclic twinned crystal structures are often observed in as-

fabricated BGA joints in the form of beach ball structure, the grain orientations of different joints are stochastically distributed [1][20]-[24]. In some instances, the different grains have been observed to have an intercalated structure [8]-[10]. This microstructure of SAC solder joints renders considerable variability in their performance and reliability [25]-[27].

The oligocrystalline microstructure of SAC joints undergoes recrystallization during thermomechanical cycling [28-31]. Researchers have shown by detailed OIM examinations of BGA solder joints damaged by thermomechanical cycling, that recrystallization near the bond pads results in fine-scale grain structure, localization of high-angle grain boundaries and distributed micro-cracking [see for example, 24]. Furthermore, within each grain there is considerable coarsening of the pro-eutectic dendritic structure and the eutectic IMC precipitates [32,33]. This evolving microstructure implies that the thermo-mechanical properties of SAC interconnects will constantly change under life-cycle loading conditions. This stochastic variability and evolution of the microstructure makes it challenging to forecast the instantaneous stress state, the evolving stress history and the resulting long-term reliability of SAC solder joints in applications.

The inevitable miniaturization in heterogeneous integration brings the dimensions of interconnects down to the size of single SAC crystals. During the past ten years, considerable attention has been paid to the anisotropic behavior of SAC grains, since analysis of joints based on homogeneous isotropic properties is inadequate for addressing the variations of mechanical behavior across different joints at this length scale. SAC alloys contain more than 90% Sn, and body-centered tetragonal (BCT) Sn

is well known for its anisotropy. Thus, the elastic behavior of SAC crystals is highly dependent on their orientation. Although the anisotropic elasticity of Sn crystals has been studied by several researchers [34-39], that of single crystal SAC has received less quantitative attention. Instead, a majority of the literature has resorted to using isotropic elastic constants measured from polycrystalline SAC specimens [40-44]. A few researchers have used anisotropic elastic constants of pure Sn as substitutes for the elastic response of SAC crystals [45-49].

Some researchers have also studied the evolution of the elastic properties due to isothermal and thermo-mechanical aging. [33, 40-44, 50-52] Cai et al. [53] measured isotropic elastic modulus of polycrystalline solder samples aged for various durations (0-6 months) at 100 °C. Reductions observed in the elastic modulus were empirically modeled as a function of aging time. A parallel study on the microstructure evolution revealed that the degradation of mechanical properties under isothermal aging correlates with microstructural coarsening within each grain. Maleki et al. [54, 55] used a combination of synchrotron x-ray and focused ion beam/scanning electron microscopy tomography techniques to visualize the evolution of 3D microstructure inside SAC solder grains at different length scales. After solidification the intermetallic compounds (IMCs) within the eutectic phase are found to grow in a preferred direction. During isothermal aging at 150 °C, the needle-like Ag_3Sn and rod-like Cu_6Sn_5 IMCs in the eutectic phase exhibit a continuous growth in size and decrease in aspect-ratio, and gradually coarsen into fewer and larger ellipsoidal particles after 144 h. The evolution in the microstructure can be identified by the morphology and distribution of the IMC particles in the eutectic region. After 296 h

of aging, the eutectic region coarsens and diffuses to the extent that the dendritic structure of the pro-eutectic Sn cannot be distinguished any more. The evolving aspect ratios of IMCs and Sn dendrites, the volume fraction of each constituent and the morphology of the dendritic features all contribute to the changes in the elastic properties of SAC joints due to aging.

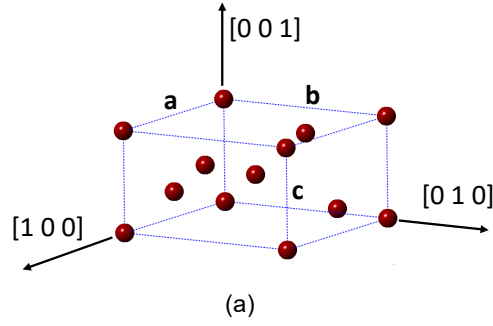
Although considerable attention has been paid to correlate the evolving isotropic properties of SAC grains with their microstructural evolution [1, 5, 56], a mechanistic connection between the micro-structure and resulting anisotropic mechanical behavior hasn't been quantified. Microscale SAC305 solder joints exhibit significant anisotropic elasticity in the as-fabricated state, due to the oligocrystalline microstructure and the anisotropy of single crystal Sn. The differences in the elastic properties between SAC crystal and Sn crystal and the influence of microstructure variations on this elastic behavior of joints need to be determined. This paper evaluates the anisotropic elastic modulus of SAC305 crystal based on its multi-scale heterogeneous microstructure and evaluates the influence of evolving microstructures on the elastic behavior of SAC crystal. Stress and strain distribution along the grain boundaries were characterized quantitatively through finite element analysis (FEA) of selected joint architectures, as a function of crystallographic grain orientations. This understanding of the anisotropic SAC single-crystal behavior is an important precursor to the analysis of grain-boundary sliding and decohesion, which are typical failure mechanisms of SAC solder joints in thermomechanical fatigue. This work also forms the starting point for future development of microstructurally-based anisotropic models of crystal-scale inelastic behavior.

3.2 Modeling Approach

The heterogeneous microstructure of as-fabricated SAC solder joints is analyzed here using a hierarchical bottom-up modeling strategy [56, 57]. The Mori-Tanaka average-matrix-stress homogenization approach [58, 59], widely used in matrix-inclusion composites, is applied here to determine the effect of the IMC/dendritic microstructure on the anisotropic elasticity of SAC joints. The microstructure of SAC crystal and modeling methods are briefly discussed in this section. A simplified solder joint with three crystals of different orientations is modeled in FEA to investigate the stress distribution and deformation within the joint. The grain orientations are parametrically varied to assess their effect on the elastic stress distributions in the individual grains as well as on the stress mismatches at the grain boundaries.

3.2.1 Anisotropic elasticity of single-crystal Sn

β -Sn is well known to have a body-centered-tetragonal (BCT) crystal structure, with lattice constants $a=b=5.83\text{\AA}$ and $c=3.18\text{\AA}$, as shown in Figure 3.2. The 6 elastic constants of single crystal β -Sn have been measured by multiple researchers and the results are summarized in Table 3.1. Although there are several discrepancies among these values, the results reported by Rayne [38] and Kammer [39] have been experimentally verified to a certain extent. Hence Rayne's data at 300 K are used in this paper for all subsequent calculations.



$$\begin{bmatrix} C_{11} & C_{12} & C_{13} & 0 & 0 & 0 \\ C_{12} & C_{11} & C_{13} & 0 & 0 & 0 \\ C_{13} & C_{13} & C_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{66} \end{bmatrix}$$

(b)

Figure 3.2 β -Sn: (a) Body body-centered tetragonal (BCT) crystal structure; (b) The matrix of stiffness constants

Table 3-1 Measurements of elastic constants of single β -Sn crystal (Unit: 1010 Pa)

Year	C_{11}	C_{33}	C_{44}	C_{66}	C_{12}	C_{13}	Temp.	Method	Author
1925	8.39	9.67	1.75	0.74	4.87	2.81	RT	Static Mechanical Test	Bridgeman [34]
1955	8.6	13.3	4.9	5.3	3.5	3.0	RT	Diffuse X-ray reflection	Prasad and Wooster [35]
1956	7.35	8.76	2.2	2.26	2.39	2.49	RT	Ultrasonic Attenuation	Mason and Bömmel [36]
1959	7.53	9.55	2.19	2.34	6.16	4.41	288 K	Resonance	House and Vernon [37]
1960	7.23	8.84	2.203	2.4	5.94	3.58	300 K	Ultrasonic pulse technique	Rayne and Chandrasekhar [38]
1972	7.2	8.8	2.19	2.4	5.85	3.74	301 K	Ultrasonic pulse technique	Kammer et al. [39]

The 4th order elastic compliance tensor S_{ijkl} can be determined from the six engineering elastic constants (expressed in Table 1 in Voigt's reduced notation). The elastic modulus $E(\mathbf{n})$ can be expressed as a function of S_{ijkl} and $\mathbf{n}$ [60], for β -Sn crystal's response to uniaxial stress in the direction of unit vector $\mathbf{n}$:

$$\frac{1}{E(\mathbf{n})} = S_{ijkl} n_i n_j n_k n_l \quad \text{Eq. (1)}$$

The Young's modulus of β -Sn as a function of direction in 3D space is depicted in Figure 3.3 (a), while its top view along the $-z$ direction is shown in Figure 3.3 (b). In the $(\bar{1} 1 0)$ plane, the variation of Young's modulus as it sweeps from $[0 0 1]$ to $[1 1 0]$ is very small, therefore the in-plane elasticity is close to transversely isotropic.

Directions $[1\ 0\ 0]$ and $[0\ 1\ 0]$ are equivalent to each other, due to the symmetric nature of β -Sn unit cell. In the $(0\ 1\ 0)$ plane, the Young's modulus decreases from 68.9 GPa to 22.9 GPa [5, 61], when it switches from the stiffest direction $[0\ 0\ 1]$ (c-axis of the unit cell) to the most compliant directions $[1\ 0\ 0]$ and $[0\ 1\ 0]$. The maximum ratio of elastic stiffness along different directions is about 3 at room temperature and can exceed 4 at 423K [62]. Temperature-dependent anisotropic properties, along with the oligocrystalline structure, will affect SAC joints' mechanical state and long-term reliability.

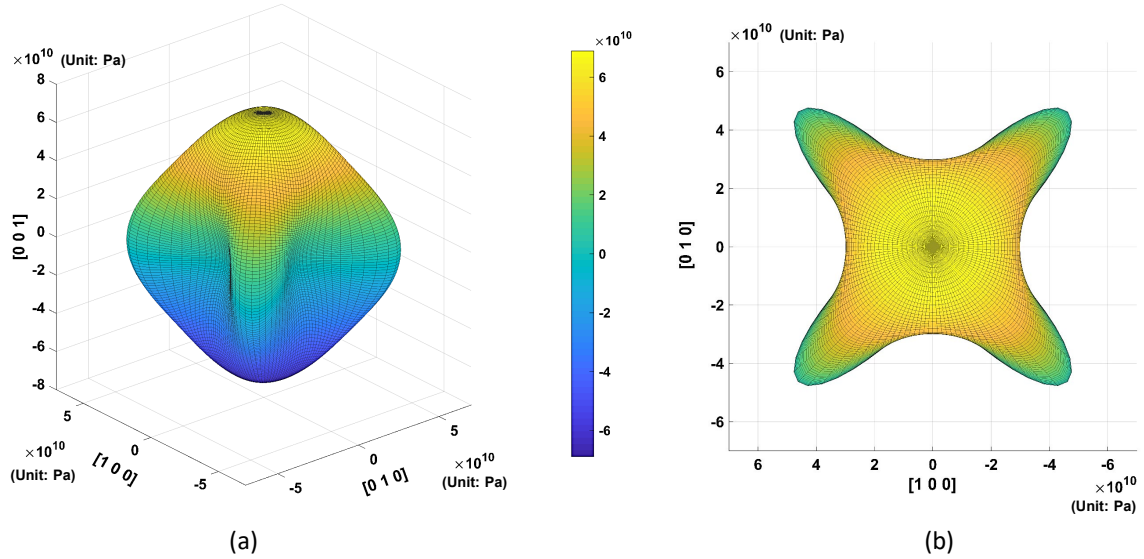


Figure 3.3 Three-dimensional anisotropic elastic properties of β -Sn crystal: (a) Isometric View; (b) Top view on the $(0\ 0\ 1)$ plane

3.2.2 Heterogeneous microstructure of SAC joints and hierarchical modeling of single-crystal SAC mechanical behavior

As-fabricated SAC joints are known to commonly contain only a few grains. Each grain consists of many β -Sn dendrites and inter-dendritic eutectic Sn-Ag phase

containing nanoscale Ag_3Sn IMC elongated ellipsoids. In addition, there are larger (microscale) Ag_3Sn and Cu_6Sn_5 IMC particles, sporadically distributed in the solder bulk or near the interfacial layers, that are not considered in the current study. The microstructure of SAC joints was divided into multiple tiers on the basis of length scales, to represent its heterogeneity. This hierarchical modeling strategy ranges from Tier 0 to Tier 3 in a bottom-up order, as shown in Figure 3.1. Tier 0 refers to the anisotropic β -Sn BCT lattice structure. Tier 1 is defined as the eutectic Sn-Ag microconstituent filling up the inter-dendritic space. As discussed earlier, this eutectic phase consists of nanoscale Ag_3Sn ellipsoidal particles that are treated as statistically uniform distributions of dispersoids, embedded in the β -Sn matrix. Tier 2 is composed of a complete single grain containing pro-eutectic Sn dendrites and a network of eutectic Sn-Ag phase surrounding them. Tier 3 represents a single joint containing a few grains.

Eshelby's equivalent inclusion method and Mori-Tanaka's average-matrix-stress homogenization approach for binary composites (Eq. 2) [63] were applied respectively in Tier 1 and Tier 2, to evaluate the overall homogenized elastic response. In Tier 1, Ag_3Sn particles are approximated as isotropic ellipsoids that are uniformly dispersed in the β -Sn matrix. In Tier 2, the lobes of dendritic pro-eutectic β -Sn are simplified as ellipsoidal inhomogeneities, surrounded by the eutectic Sn-Ag phase. The principal semi-axes of the ellipsoids in both Tiers are assumed to align with the coordinates of β -Sn crystal, in order to simplify the mechanics analysis. Meanwhile, these alignments, as extreme cases, can be used to estimate the range of homogenized elasticity due to orientation variation of inclusions. After the

homogenization, the effective elastic properties of each tier depend on the shape and volume fraction of the embedded inclusions. According to the Mori-Tanaka approximation, the average elastic properties at Tier 1 and Tier 2 are calculated by:

$$\mathbf{L} = \mathbf{L}_0 + c_1(\mathbf{L}_1 - \mathbf{L}_0)[c_0\mathbf{S}\mathbf{L}_0^{-1}(\mathbf{L}_1 - \mathbf{L}_0) + \mathbf{I}]^{-1} \quad (\text{Eq. 2})$$

Where, $\mathbf{L}$ is the effective stiffness tensor after homogenization; $\mathbf{L}_0$ is the stiffness tensor of the matrix medium; $\mathbf{L}_1$ is the stiffness tensor of the inhomogeneity; c_0 and c_1 are the volume fractions of the matrix and inclusions, respectively ($c_0 + c_1 = 1$); $\mathbf{S}$ is Eshelby's strain concentration tensor (fourth-order tensor), which is used to relate the constrained strain inside the inclusion to the equivalent eigenstrain. It is a function of the matrix stiffness tensor $\mathbf{L}_0$ and the shape of embedded inclusions. For elastic field due to ellipsoidal inclusions in anisotropic materials, Eshelby's tensor can be estimated as [63]:

$$\mathcal{S}_{ijkl} = \frac{1}{8\pi} L_{0mnkl} \int_{-1}^{+1} d\zeta_3 \int_0^{2\pi} \{G_{imjn}(\bar{\xi}) + G_{jmin}(\bar{\xi})\} d\omega \quad (\text{Eq. 3})$$

where,

$$\begin{aligned} G_{ijkl}(\bar{\xi}) &= \bar{\xi}_k \bar{\xi}_l N_{ij}(\bar{\xi}) / D(\bar{\xi}), \quad \bar{\xi}_i = \zeta_i / a_i, \\ \zeta_1 &= (1 - \zeta_3^2)^{1/2} \cos\omega, \quad \zeta_2 = (1 - \zeta_3^2)^{1/2} \sin\omega, \quad \zeta_3 = \zeta_3, \\ D(\bar{\xi}) &= \varepsilon_{mnl} K_{m1} K_{n2} K_{l3}, \quad N_{ij}(\bar{\xi}) = \frac{1}{2} \varepsilon_{ikl} \varepsilon_{jmn} K_{km} K_{ln}, \quad K_{ik} = L_{0ijkl} \bar{\xi}_j \bar{\xi}_l, \end{aligned}$$

Although Eshelby's tensor relates two symmetric strain tensors, it does not satisfy the major symmetry (i.e. $\mathcal{S}_{ijkl} \neq \mathcal{S}_{klij}$). a_i denotes the three principal half axes of the ellipsoidal inclusions, which are assumed to be aligned with the principal axes of β -Sn unit cell in sequence ($a_1 \parallel [1\ 0\ 0]$, $a_2 \parallel [0\ 1\ 0]$). In the current study, both Ag_3Sn dispersoids and Sn dendrites are simplified as prolate spheroids. The value of $\mathbf{S}$ can

be numerically estimated, using the Gaussian quadrature formula for the double integration (Eq. 4) [63].

$$\mathcal{S}_{ijkl} = \frac{1}{8\pi} \sum_{p=1}^M \sum_{q=1}^N L_{0mnkl} \left\{ G_{imjn}(\omega_q, \zeta_{3p}) + G_{jmin}(\omega_q, \zeta_{3p}) \right\} W_{pq} \quad (\text{Eq. 4})$$

3.2.3 Finite element models

As shown in the two cross-polarized images of TMM joints in Figure 3.1 (a), the as-fabricated SAC joints contain at most a few grains. The joint with one dominant grain throughout can be approximately regarded as a single crystal interconnection. Considering the volume fraction, smaller grains located in the corners have a limited contribution to joint's overall elastic stiffness, so the overall elastic behavior of the entire joint is determined by the large crystal. The other consists of multiple grains, where crystals of different orientations are represented by colors (primarily 3 different grains in this case, illustrated with 3 different shades of blue). Cross-polarized microscopy conducted on both sides of the TMM solder region, have revealed that the grain configuration remains mostly unchanged through the thickness of the joint [44, 57].

Motivated by this oligocrystalline (predominantly tri-crystal) microstructure of the tested TMM specimens (circled in red in Figure 3.1 (a)) and intergranular cracks found in tested joints, a simplified FEA model of tri-crystal solder interconnection was constructed, to investigate the stress distribution near the grain boundaries, as shown in Figure 3.4. The solder joint of 0.2 mm width (along the y direction) was connected to two copper platens. Only half of the joint (along the z direction) was modeled due to the symmetry about the XY plane. Suitable constraints were applied

on the plane of symmetry, as shown in Figure 3.4 (b). A uniform displacement (0.2 μm) was applied on the top surface of one copper platen along the Y-axis (uniaxial tensile load), while the bottom surface of the other copper platen was fully constrained to have zero displacement. The three grains are numbered 1-3, for convenience of discussion. Global coordinates of the entire joint and local coordinates indicating each crystal's orientation are depicted in Figure 3.4 (c). The crystalline systems of three grains are mutually perpendicular to each other, as the initial state. The isotropic material properties of the copper platens used in FEA are listed in Table 2. As crystals 2 and 3 in the solder are connected in series along the loading direction, this model is used to parametrically examine the effect of misorientation between Crystals 2 and 3, on the intergranular stresses. During the simulation, the orientation of Crystals 1 and 3 are fixed, while Crystal 2 is gradually rotated about the global z axis. The stress concentration due to grain misorientation is critical to the reliability of solder joints, since high-angle boundaries are closely related to recrystallization and crack propagation in the bulk interior of interconnects.

Since diffusion and dislocation movement along the grain boundaries take time to develop, and only the elastic response is considered in the current study, all inelastic deformations at the grain boundary (e.g. grain boundary sliding) were ignored. Instead, neighboring grains are assumed to have perfectly bonded interfaces. The stress/strain mismatch between crystals at the grain boundaries come from the resolved stress (boundary orientation corresponding to loading directions) and orientation-dependent elasticity.

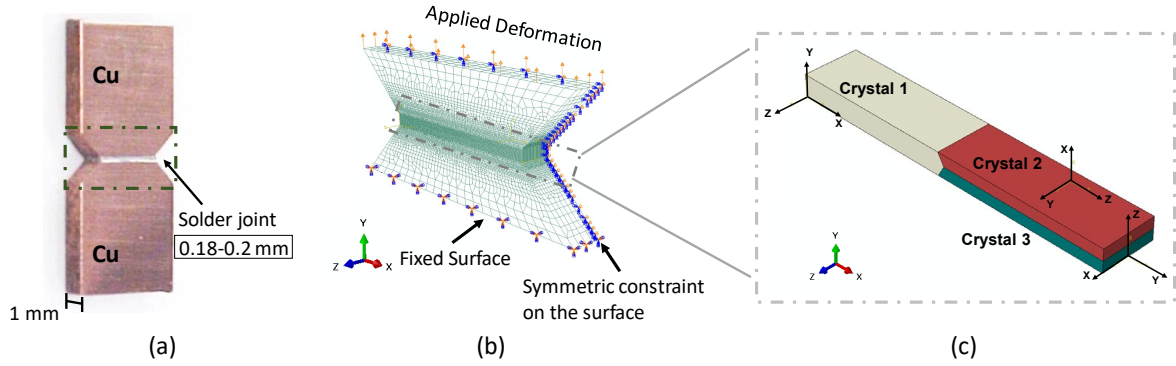


Figure 3.4 FEA model of tri-crystal specimen: (a) specimen used in custom-built thermo-mechanical micro-scale (TMM) test system; (b) model geometry and boundary conditions; (c) The tricrystal geometry with local coordinates indicating the initial orientations.

Table 3-2 Material properties of copper used in FEA

Young's Modulus	Poisson's Ratio
11 (10^{10} Pa)	0.33

3.3 Results and Discussion

In this section, parametric results are presented for the Tiers 1-3 modeling approach of Section 3.2. In Section 3.3.1, the modeling approach of Tiers 1-2 are used to estimate homogenized elastic constants for single SAC crystal. Parametric studies are conducted to study the effects of the morphology of: (i) IMC particles in the eutectic phase; and (ii) dendrites in the pro-eutectic phase. In Section 3.3.2, the finite element modeling approach of Tier 3 is used to examine the effect of grain orientation on the deformation and stress distribution in the simplified tri-crystal test joint described earlier in Section 3.2.

3.3.1 Homogenized anisotropic elastic properties of single-crystal SAC

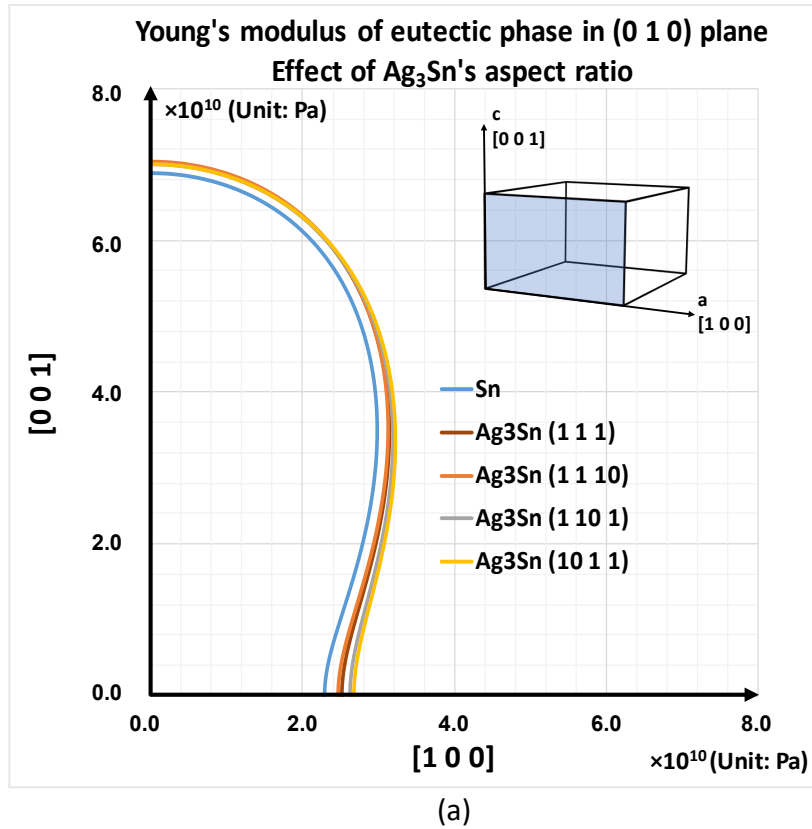
A parametric study was conducted for the properties of a SAC305 solder single-crystal, with 5% volume fraction for Ag_3Sn dispersoids in the eutectic phase, and 60% $\beta\text{-Sn}$ pro-eutectic dendrites [32]. Image processing methods are needed to determine the volume fraction of dispersoids in both Tiers, due to the existence of microscale IMCs in the bulk or near the interface of solder joints. The dendrites are first assumed to be sphere with aspect ratio (1,1,1) to isolate the influence of Ag_3Sn particles' aspect ratio.

Eutectic phase

The homogenized elastic behavior of the eutectic phase on the $(\bar{1} 1 0)$ and $(0 1 0)$ planes are plotted in Fig. 5. The four curves of different particle ratios almost overlap with each other on the $(\bar{1} 1 0)$ plane (Fig 5(a)), and are uniformly spaced from the one of $\beta\text{-Sn}$. This demonstrates that the effect of the aspect ratio of Ag_3Sn dispersoids is weak, compared to the effect of its volume fraction, when considering the elastic properties on this plane. The elastic moduli of eutectic phase containing 5% nanoscale Ag_3Sn particles increases by 2-3% in this cross section, while the increment is about 3.5-4.5% when the fraction of particles is 8%. The dashed curve is a quadratic curve with a radius of Sn's modulus in the $[0 0 1]$ direction.

The elastic stiffness of the eutectic phase (Tier 1) along the $[1 0 0]$ direction on the $(0 1 0)$ plane (Fig. 5 (b)) increases by 10% compared to that of $\beta\text{-Sn}$, when 5% spherical Ag_3Sn inclusions are modeled. The variation in the elastic behavior along the $[0 0 1]$ direction is limited (about 2%) as particles elongating along the principal directions with an aspect ratio up to 10, compared to that along the $[1 0 0]$ direction.

Particles elongated perpendicular to the (0 0 1) plane slightly decreases the elastic properties along the [1 0 0] direction, compared to that for spherical particles. The elastic stiffness along [1 0 0] increases by 15% and 17%, as inclusions elongate along the two principal directions in the (0 0 1) plane, with aspect ratios of (1,10,1) and (10,1,1) respectively. The maximum increase occurs along the direction of the long axis of the dispersoids, as expected. Particles extended in [0 1 0] direction, will also result in nearly equivalent reinforcement in the modulus along [1 0 0] and vice versa. The modulus along [1 0 0] increases up to 27% for particles with a ratio of (10,1,1), as the volume fraction of Ag_3Sn inclusions increases to 8%.



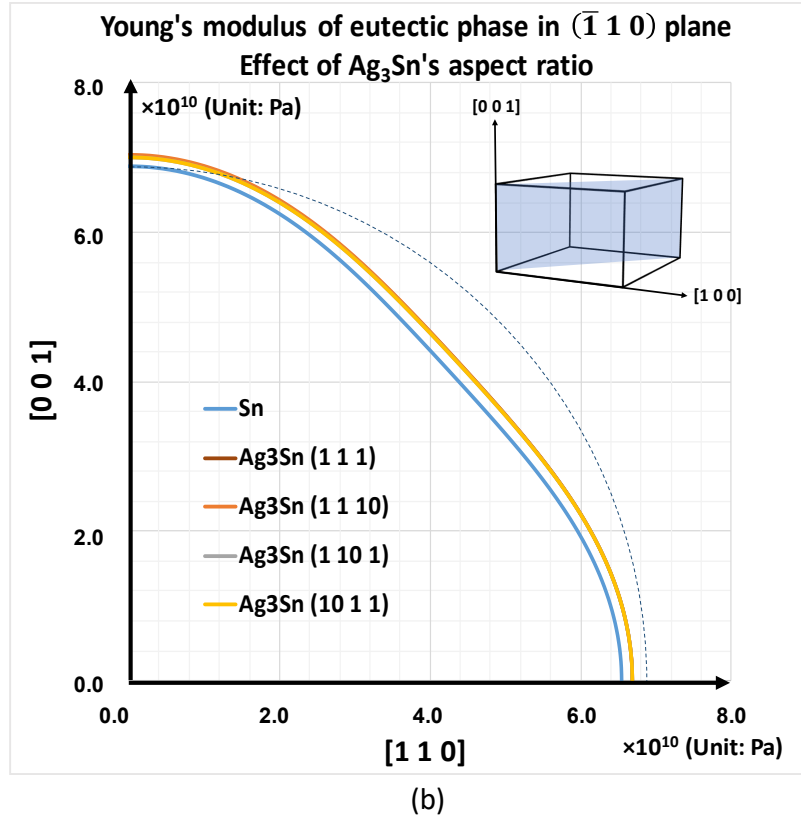
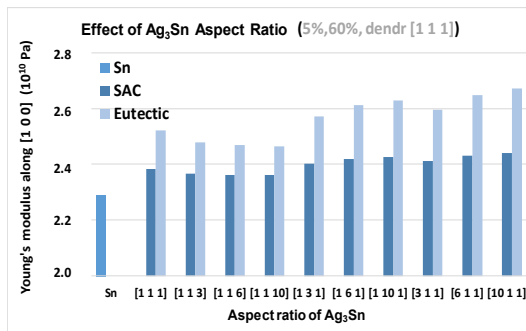


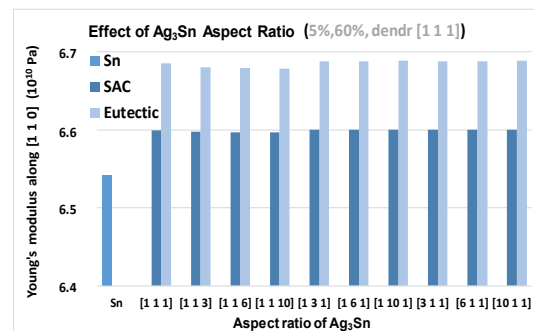
Figure 3.5 Directional elastic properties of the eutectic constituent: (a) Cross-section on the $(\bar{1} 1 0)$ plane; (b) Cross-section on the $(0 1 0)$ plane

SAC crystal

After homogenization for 40% eutectic phase and 60% dendritic pro-eutectic β -Sn phase, the elastic modulus of SAC crystal is estimated along $[1\ 0\ 0]$, $[1\ 1\ 0]$ and $[0\ 0\ 1]$ and presented in Fig. 6. In (a) to (c), the light blue histograms represent the directional moduli of the eutectic constituent, while the dark blue ones indicate that of the SAC crystal. The eutectic phase is approximately 1.8-16.6 % stiffer than the β -Sn phase because of the reinforcement from the Ag_3Sn IMC dispersoids. As a result, the homogenization process in Tier 2 shows that the absolute values of the directional moduli are found to be approximately 1-9.4 % smaller for SAC crystal than that for the eutectic phase (as seen in Fig. 6 (a) to (c)). The overall distribution of a crystal's moduli follows the same pattern as that of the eutectic matrix. The modulus along $[1\ 0\ 0]$ of SAC crystal containing spherical Ag_3Sn inclusions is 4% greater than that of β -Sn crystal. Dispersoids' elongation along $[0\ 0\ 1]$ will somewhat weaken its reinforcement in elasticity in the direction of $[1\ 0\ 0]$. As expected, the increment of modulus along $[1\ 0\ 0]$ maximizes when the ellipsoidal Ag_3Sn inclusions has its elongated axis along the same direction, and it is about 6.5% for Ag_3Sn inclusions with a ratio of (10,1,1).



(a)



(b)

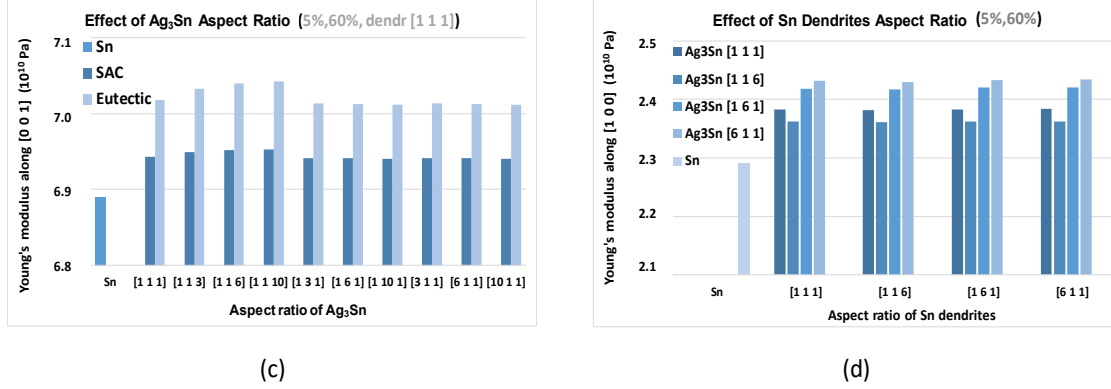


Figure 3.6 Directional elastic properties of SAC crystal with 5% volume fraction for Ag₃Sn IMC dispersoids in the eutectic phase, and 60% β -Sn pro-eutectic dendrites: (a) Along [1 0 0] direction with different aspect ratios of Ag₃Sn particles; (b) Along [1 1 0] direction with different aspect ratios of Ag₃Sn particles; (c) Along [0 0 1] direction with different aspect ratios of Ag₃Sn particles; (d) Along [1 0 0] direction with different aspect ratios of Sn dendritic lobes

The [1 0 0] elastic moduli of SAC crystals with different β -Sn dendritic shapes was compared in Fig. 6 (d). For the volume fractions examined in current work, the shape of the spheroidal Sn dendrites (aspect ratio of the principal axes) does not have a strong influence on the anisotropic elastic moduli of SAC crystal. Thus, the results from Tier 2 homogenization are applicable across a wide range of shape distributions of the dendrite lobes.

3.3.2 FEA simulations of tri-crystal joint

Parametric results are presented using the tri-crystal FEA model described in Section 2.3. As Crystal 2 is rotated about the global z axis, the intergranular stresses and strain between Crystal 2 and 3 are estimated as a function of misorientation. Based on the homogenization methods discussed above in Tiers 1-2, the elastic constants of SAC crystal in FEA were calculated and tabulated in Table 3, for 40%

eutectic phase (Tier 2) and 5% Ag₃Sn inclusions of ratio (1,3,1) within the eutectic phase (Tier 1).

Table 3-3 Table 3 Elastic constants of SAC crystal (Unit: 10¹⁰ Pa)

C ₁₁	C ₂₂	C ₃₃	C ₄₄	C ₅₅	C ₆₆	C ₂₃	C ₁₃	C ₁₂
7.32	7.35	8.93	2.23	2.23	2.42	3.64	3.63	5.96

The distribution of normal stresses (σ_{22}) along the global Y-axis for elements on the free X-Y surface is shown in Fig. 7. Large stress concentrations are found near both ends of the joints. In the reference configuration, the difference of elastic modulus along the loading direction between Crystals 2 and 3 is at the maximum. As the principal axes of Crystal 2 are rotated around the global Z-axis, this difference decreases gradually, and finally approaches its minimum when the stiffest crystalline directions of Crystals 2 and 3 are parallel to each other (rotation angle=90 degree), leaving a “Y” marker of stress discontinuity in the junction of three crystals. The average stress of elements near the grain boundary is about 35% higher than that of other elements nearby. The σ_{22} distribution on the surface elements of Crystal 1 remains almost independent of the changes in the orientation of Crystal 2.

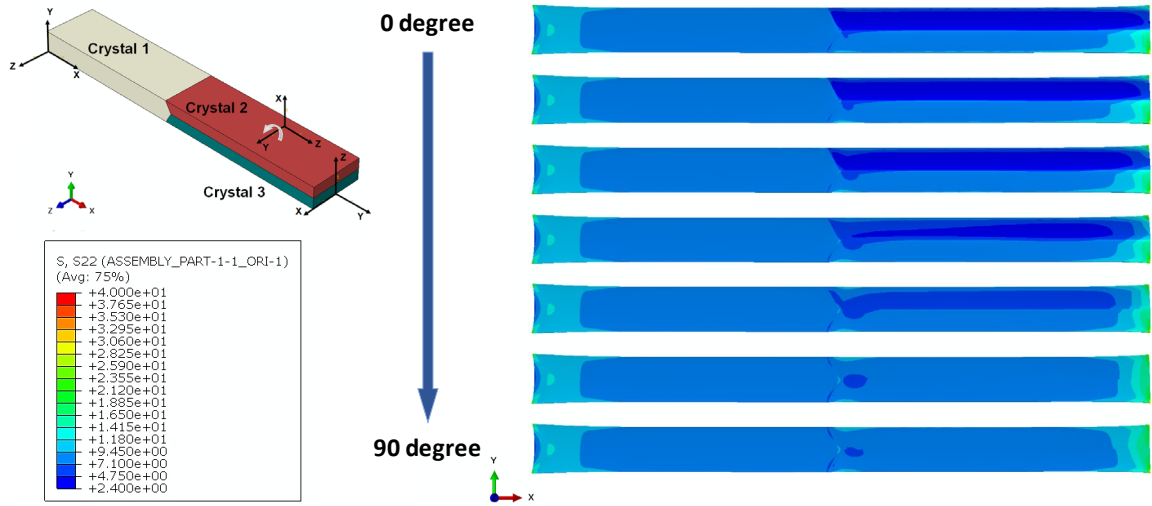


Figure 3.7 σ_{22} (MPa) contour as Crystal 2 principal axes are rotated around the global Z-axis

The sectional side view in Fig. 8 reveals that stress concentrations occur at the edges of the interface with the copper platens. σ_{22} decreases sharply near the free X-Y surface. Furthermore, the difference of σ_{22} between Crystal 2 and 3 is seen to occur only in regions close to the free X-Y surface and the edge shared by three crystals, where the stress gradients are highest. In the interior, where the stresses are relatively uniform, no such difference is observed.

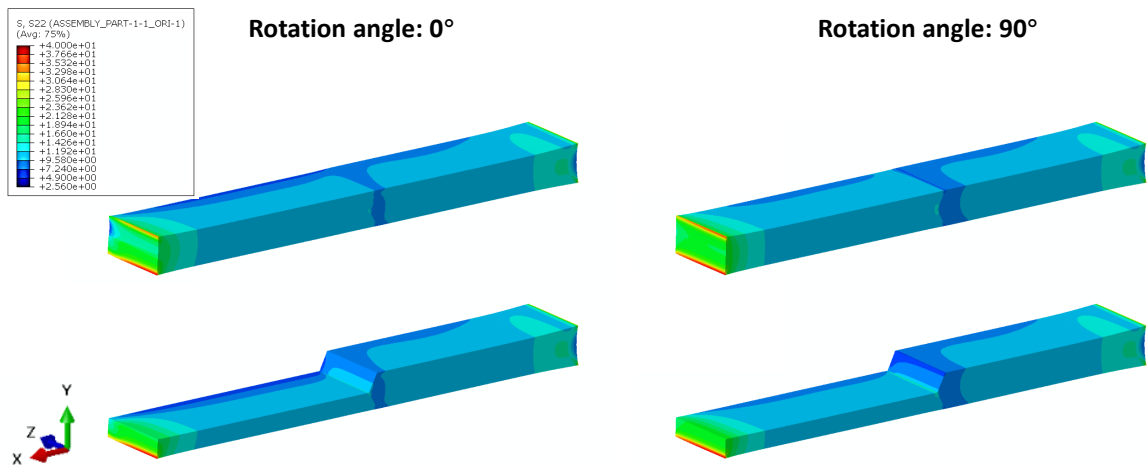


Figure 3.8 Sectional side view of σ_{22} contour

Unlike σ_{22} , the von Mises shown in Fig. 9 has discontinuities across the interface between Crystal 2 and 3, because of contribution from other stress components. These discontinuities completely disappear when Crystal 2 is rotated by 90° about the global z axis, because the elastic modulus along the loading direction of two crystals are identical.

Similar mismatches at the interface are also found in the contours of normal strain ε_{22} . Contours of σ_{22} , ε_{22} and von Mises stress in two layers of elements across the interface between Crystal 2 and 3, are depicted in Fig. 10. Mirror images are used to display the distributions on the interface between Crystal 2 and 3, in order to make the representation geometrically compatible.

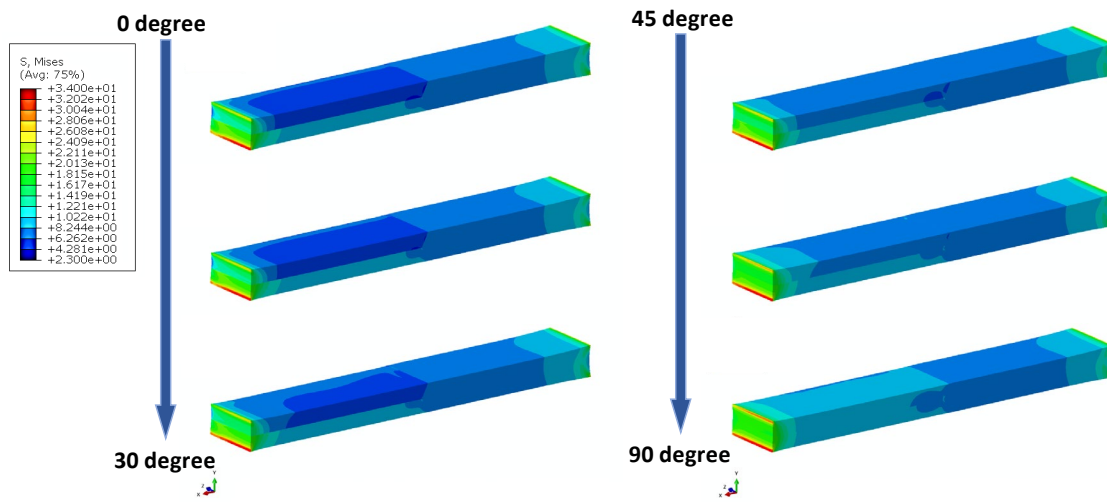


Figure 3.9 Side view of von Mises stress contour as Crystal 2 is rotated about the global z-axis

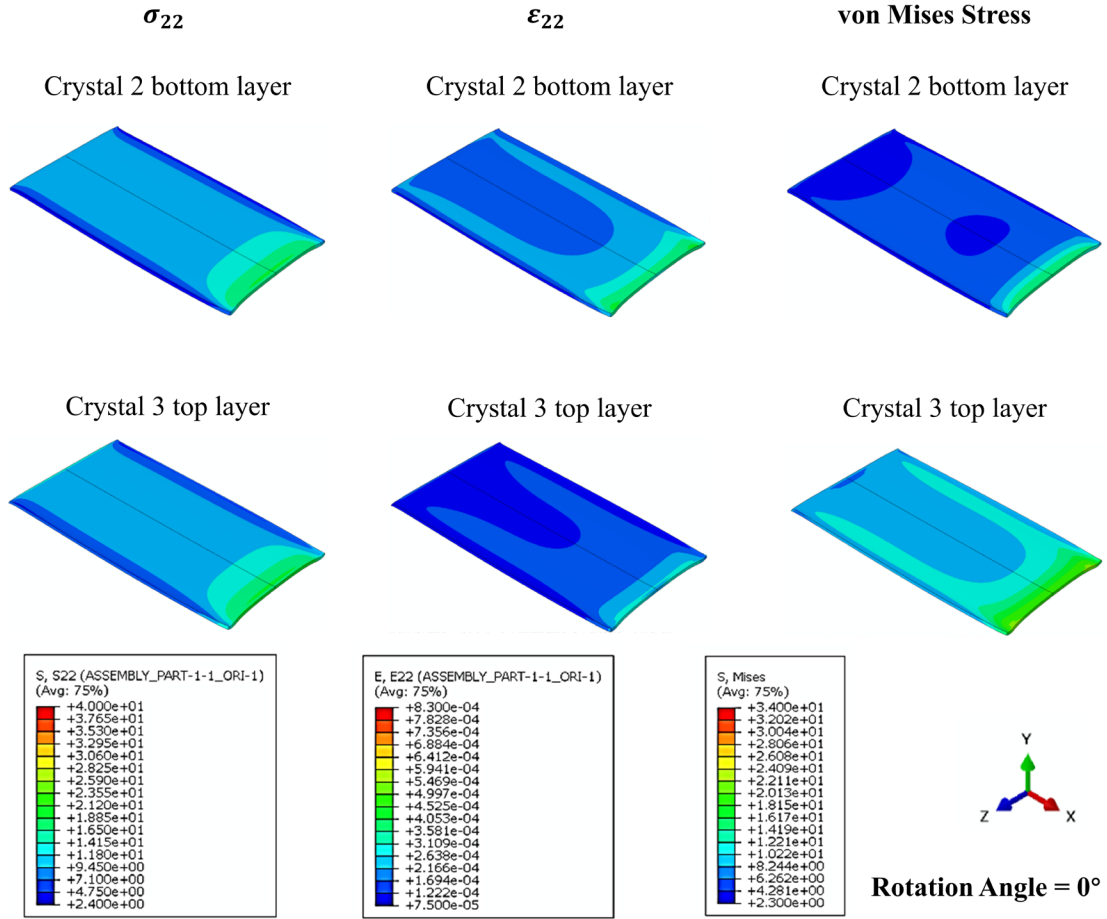


Figure 3.10 Contours of σ_{22} , ϵ_{22} and von Mises stress, in two layers of elements at the interface between Crystals 2 and 3, rotation angle = 0° (about the global z axis)

The percentage of variation between two layers of elements, which connecting to each other at grain boundary and belonging to Crystals 2 and 3 respectively, are used here to quantitatively evaluate the von Mises stress discontinuities caused by grain misorientation, as defined in Eq. (5). The variation percentage was calculated on the entire interface between Crystals 2 and 3. Its contour and projections along three principal axes are delineated in Fig. 11 (a), when the rotation angle of Crystal 2 equals to zero. Different from the contour of von Mises stress, large percentage of variations occurs in the interior of the interface. The maximum percentage is located

in the corner which is enclosed by the free X-Y surface and the edge shared by three crystal. The maximum gradient of von Mises stress at the interface was plotted as a function of Crystal 2's rotation angles about the global z axis in Fig. 11 (b). As the misorientation between Crystals 2 and 3 decreases, the absolute value of variation percentage drops from 55% to 5%. Although the stiffest crystalline directions of Crystal 2 and 3 are identical when Crystal 2 is rotated by 90°, difference of modulus along other directions results in 5% gradient in the intergranular discontinuity in the von Mises stress

$$\lambda = \frac{\sigma_{VM}^{Bottom\ layer\ of\ Crystal\ 2} - \sigma_{VM}^{Top\ layer\ of\ Crystal\ 3}}{\sigma_{VM}^{Top\ layer\ of\ Crystal\ 3}} \times 100\% \quad (\text{Eq. 5})$$

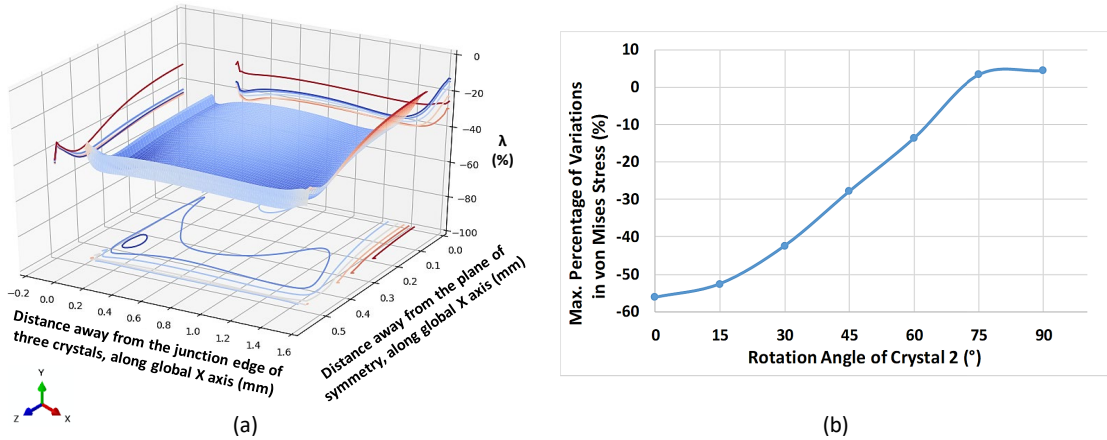


Figure 3.11 von Mises Stress variation at the interface between crystals 2 and 3: (a) Contour of variation on the entire interface with rotation angle = 90°, (b) The Max. percentage of variation as Crystal 2 is rotated from 0° to 90° about the global z-axis.

3.4 Summary and Conclusion

This paper presents a systematic multi-tier modeling approach for mechanistic estimation of the anisotropic elastic behavior of SAC single crystal as well as that of polycrystalline joints. This modeling approach is important because it allows

parametric investigation of the effect of the micro-morphology of the SAC alloy on the elastic behavior. More importantly, this approach provides the starting point for microstructurally based models for predicting crystal-scale inelastic behavior (plasticity and creep).

The anisotropic elastic behavior of a SAC single crystal was quantitatively estimated in the first part of this paper, based on multi-scale modeling of the heterogeneous microstructure. The effects of the degree of reinforcement on the anisotropic elastic constants was evaluated as a function of microstructural features, such as the morphology of the IMC reinforcements in the eutectic phase and Sn dendrites within crystals. This parametric modeling capability enables is to explore how SAC crystal properties may evolve with isothermal aging, including the limiting case (for long-time aging or slow cooling rates) where the Sn dendritic features may completely disappear. Joints of such microstructure can be treated in our modeling approach as containing only Tier 1 features and no Tier 2 morphology.

In Part 2 of the modeling approach, finite element models of polycrystalline solder joints, using the anisotropic modulus derived above, were used to analyze the elastic fields in the joint, with particular focus on the stress mismatch at the grain boundaries, as a function of the misorientation between anisotropic crystals. For two crystals connected in series along the loading direction, no apparent differences were found in the normal stress. However, the discontinuities in von Mises and normal strain ϵ_{22} at the same region are large enough to form apparent stratification at the interface. The gradient of von Mises stress at the interface varies from 5% up to 55% as a function of misorientations. This can be used to estimate the intergranular

stresses for crack propagation, especially for high-angle grain boundaries in SAC joints.

Future work will focus on test and validation of this modeling approach after this work is extended to anisotropic inelastic behavior of SAC alloys and solder joints. The methods to be used for validating response and grain boundary stresses are Digital Image Correlation (DIC) and micro-moiré. Experimental results will include the effects of inelastic deformation; hence this verification is deferred to future papers that will include predictions based on crystal-inelasticity as well as appropriate experimental verification.

Chapter 4: Anisotropic Steady-state Creep Behavior of Single-crystal β -Sn: A Continuum Constitutive Model Based on Crystal Viscoplasticity

Abstract

Body-center tetragonal (BCT) β -Sn crystals exhibit highly anisotropic properties such as stiffness and thermal expansion, which significantly affect their thermal-mechanical behavior. The homologous temperature of β -Sn is relatively high under common applications due to its low melting point, which renders Sn and Sn-based alloys viscoplastic even at room temperature. The orientation-dependent creep behavior of β -Sn specimens have been previously measured by different research groups. A dislocation mechanics based crystal viscoplasticity model is applied in this study to describe this anisotropic steady-state creep behavior of β -Sn single crystals. The model constants are calibrated with single-crystal creep test results available in the literature. The resulting creep behavior of β -Sn single-crystal is also represented with a homogenized continuum-scale finite element approach based on the use of a combined Hill-Norton approach where the creep anisotropy is represented with Hill's anisotropic potential and the creep flow rule is represented with Norton's power-law model. Estimation of the six Hill's constants for β -Sn requires multiple creep tests under specific stress states, for single crystals along crystal principal directions. In this study, these physical creep tests are replaced with 'virtual tests' conducted with the developed dislocation-based crystal-viscoplasticity model. To assess the ability of the Hill-Norton finite element approach to represent dislocation creep, the finite element simulation results are compared with results of: (i) physical tests on single

crystal specimens reported in the literature; and (ii) crystal-viscoplasticity modeling along many crystal orientations (beyond the fundamental calibration cases conducted along crystal principal directions). In future studies, this approach will be used for anisotropic finite element modeling of creep in polycrystalline specimens.

Key words: β -Sn, Anisotropic steady-state creep, crystal viscoplasticity, Hill's potential, Norton's law

4.1 Introduction

Sn-Ag-Cu alloys are widely used in electronic packaging, as replacements for SnPb solders, to provide thermal, electrical and mechanical interconnections. Since SAC alloys contain more than 90% β -Sn phase and commonly exhibit oligocrystalline microstructure (Lee et al., 2010), understanding and accurately quantifying the anisotropic properties of β -Sn is critical as a starting point for analyzing and predicting the orientation-dependent behavior of SAC grains. β -Sn crystal has a body-centered tetragonal (BCT) structure, with lattice parameters $a=b=5.83 \text{ \AA}$ and $c=3.18 \text{ \AA}$ ($c/a=0.545$). This less symmetrical crystal structure leads to a high degree of anisotropy in its thermal expansion (Subramanian and Lee, 2004; Wu et al., 2018), stiffness (Rayne and Chandrasekhar, 1960) and diffusivity (Huang et al., 2015), thereby affecting thermo-mechanical behavior and electromigration. As one of the most important mechanical properties at high temperature, creep will significantly affect the actual deformation response and durability under cyclic loading. β -Sn melts at a low temperature of about 505 K, so even at room temperature, the homologous temperature is higher than 0.5, which makes it important to consider viscoplastic deformation.

The development of viscoplasticity models for single-crystal materials has been pursued from many aspects. MacLachlan et al. (2001) proposed a macroscopic single crystal model to capture the stress rupture and creep behavior of Ni-base superalloys, which are simplified as a single-phase material, in terms of the damage mechanisms and slips on specific systems. A constitutive model was developed for the creep resistance of single crystal nickel-based superalloys within a thermodynamic frame (Prasad et al., 2006; Prasad et al., 2005), in which the anisotropic creep response is incorporated in terms of the stored energy and the rate of dissipation functions. Ma and co-authors developed a crystal viscoplasticity model for single-crystal Ni-based superalloys, accounting for the underlying deformation modes and their interactions (Ma et al., 2008). The dependence of creep on multiple features, such as the scale of the microstructure, channel thickness, and volume fraction of precipitates, was captured in this formulation. Estrada and co-workers extended this method in a displacement-based integration code to model 3-D creep-fatigue interactions (Estrada Rodas and Neu, 2018). Le Graverend and co-workers presented a viscoplastic formulation (le Graverend et al., 2014) developed in the crystal plasticity framework for another Ni-based single crystal superalloy (Cailletaud, 2009) and introduced new internal variables to take into account the microstructure evolution and the effect of mechanical and thermal history. Later, this microstructure-sensitive crystal viscoplastic model was coupled with a phenomenological hardening-based damage density function, embedded in an anisotropic formulation (le Graverend, 2019). Constitutive relation for the kinematics of single-crystal FCC metals was modeled based on the crystallographic shearing rates of the slip systems (Austin and

McDowell, 2011). Zhu and co-authors focused on the influence of the composition on the creep behavior of Ni-based single crystals, and modeled the creep resistance according to the climb of dislocation and the rate of escape from the trapped configurations (Zhu et al., 2012). Mukherjee and co-workers proposed a mechanistic multi-scale modeling framework that describes the anisotropic transient and steady-state creep behavior of single-crystal SnAgCu alloy, based on its heterogeneous microstructure and dislocation mechanics (Mukherjee et al., 2016). Brehm and Glatzel (1999) proposed a constitutive model to describe the anisotropic creep behavior of Ni-based single crystal, by extending the Haasen-Alexander model to multiple coupled slip systems, in which individual dislocations interact with each other. As a simplification, this model development was restricted to single phase. This method was implemented in numerical simulation to analyze the orientation-dependent creep behavior of two-phase single crystals (Preußner et al., 2009).

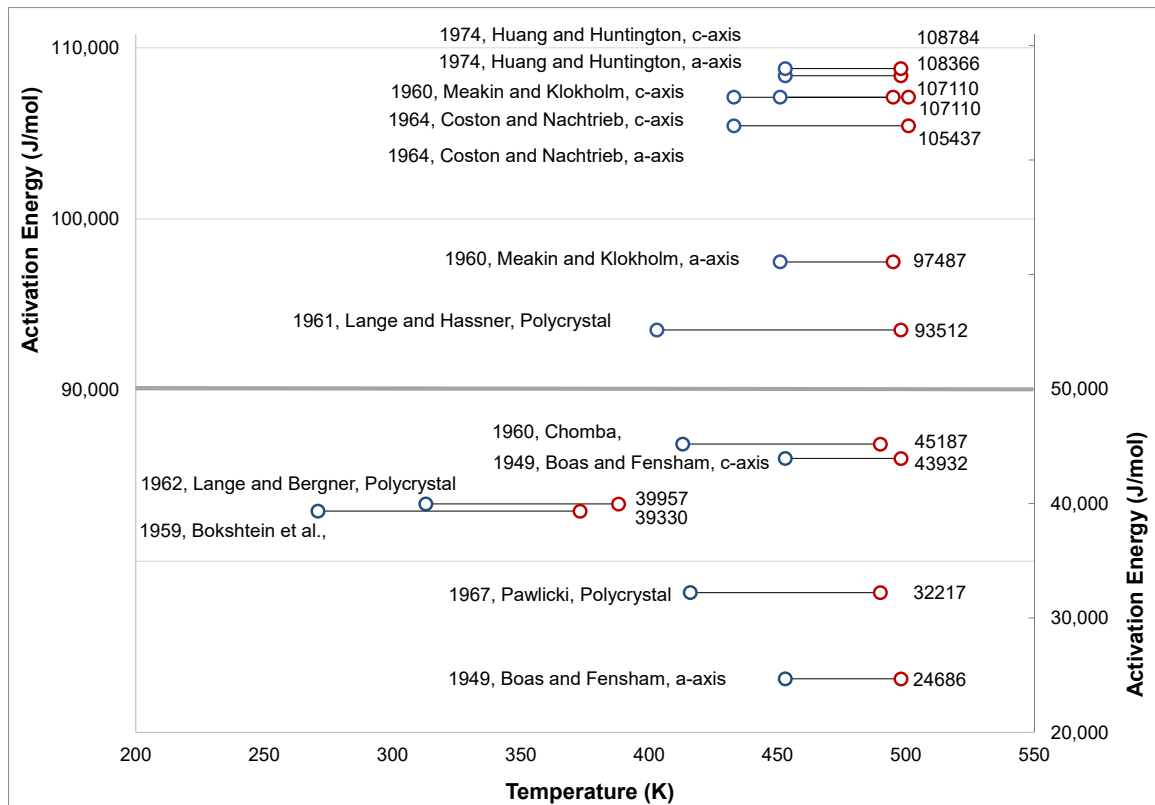


Figure 4.1 Activation energy of self-diffusion reported for Sn

Weertman and Breen (1956) conducted constant-stress creep tests on a series of single-crystal Sn specimens, with loading axis almost perpendicular to the $[0\ 0\ 1]$ direction. Measured deflections revealed the existence of two creep activation energies: 92048 J/mol at temperature above 130 °C, and 46024 J/mol at temperatures below 130 °C, corresponding to a homologous temperature of 0.8 ($=403\text{ K} / 505\text{ K}$). This suggested that two competing processes simultaneously dominate the steady-state creep of Sn, yet no consensus was reached on the type of mechanisms or the value of the diffusion energy. Later Weertman also conducted compression tests (Weertman, 1957) on specimens with c-axis parallel to the loading direction, and both the activation energy and stress exponents were comparable with their previous study. This observation is also compatible with the experimental measurements that the self-

diffusion energies in Sn along the a-axis and c-axis are also close to each other. Chu and Li (1979) conducted impression creep on single β -Sn crystal along three orientations: $[1\ 0\ 0]$, $[1\ 1\ 0]$ and $[0\ 0\ 1]$, and reported that the steady-state creep impression velocity has a power-law dependence on stress and exponential dependence on temperature. Both the activation energy and the stress exponent from impression creep tests (Yu and Li, 1997) are comparable with those obtained from conventional creep tests that generate uniform stress fields in the specimen (Weertman and Breen, 1956). Extensive analytical and numerical studies have been carried out to determine the relationship between punching stress and compressive stress, as well as the relationship between impression velocity and compressive strain rate (Yu and Li, 2013). The dependency of the impression velocity on the indenter size is commonly used to identify the possible creep mechanisms in impression creep (Li, 2002; Yu and Li, 1997). The steady-state impression velocity linearly increased with punch size, indicating the dominant mechanism in β -Sn is dislocation creep, instead of bulk or surface diffusion of vacancies. The temperature dependence of the steady-state impression velocity exhibits a knee for all three orientations, which is consistent with the findings from Weertman's tests and confirms that there are two competing creep processes, with one dominating at low temperatures and the other dominating at high temperatures. Slip line observations after the impression suggested that the low temperature process involves dislocation slip and the high temperature process involves recovery mechanisms such as diffusion-assisted dislocation climb. The two mechanisms operate in parallel and independently (Chu and Li, 1979). Although impression creep contains similar transient and steady state

stages as conventional creep tests, the stress fields are not uniform and hence numerical or analytical correlations are needed to compare impression creep test results with those from conventional creep tests.

The present work aims to model the steady-state creep of a single β -Sn crystal as a function of stress, temperature, and crystallographic orientations, on the basis of dislocation density and mobility. The selection of the creep models for the two mechanisms (dislocation climb & slip) operating in conjunction on each slip system is based on the observation and analysis of conventional and impression creep tests of single crystal specimens. This crystal viscoplasticity model is calibrated with the help of Weertman's test results, and its predictions are compared with the overall conclusions obtained from impression creep tests. After calibration, this crystal viscoplasticity model is used as a virtual testing method in this paper to determine the model constants for anisotropic continuum representation of viscoplasticity of single-crystal β -Sn. It is parametrically applied along different crystal orientations to estimate the model constants for an anisotropic continuum creep constitutive representation of the observed steady-state creep behavior. The anisotropic steady-state continuum creep model selected for this study is a Hill-Norton model, where the constants for Hill's potential describe the state of crystal anisotropy and constants for Norton's power-law describe the resulting creep deformation rates as a function of stress, at a given temperature. Future work will extend this approach to other temperatures, using an Arrhenius temperature dependence.

4.2 Crystal viscoplasticity model for anisotropic steady-state creep based on dislocation mechanics

Steady-state creep of single β -Sn crystal, as a balance state between work-hardening and recovery, is modeled as a consequence of a stable saturated density of dislocations moving with constant velocities. Strain rate is first obtained along each slip system, as a function of resolved shear stress and saturated dislocation density, and then rotated back to the crystalline coordinate. After being calibrated with Weertman's tests on single β -Sn crystals, this modeling approach is used as a virtual testing method to determine the Hill's constants, and Norton power-law constants, which are used in a constitutive law for anisotropic steady-state creep.

4.2.1 Dislocation-based model for anisotropic steady-state creep deformation

Movement of dislocations along facile slip systems is believed to be the dominant deformation mechanism in β -Sn at the stress and temperature levels considered in this paper (Adeva et al., 1995). β -Sn is expected to have multiple families of possible slip systems. $\mathbf{m}^{(k)}$ and $\mathbf{n}^{(k)}$ represent unit vectors normal to the slip plane and along the slip direction, respectively, and the superscript (k) denotes the k^{th} slip system. When the crystal is subjected to stress state $\boldsymbol{\sigma}$, the resolved shear stress $\tau_{re}^{(k)}$ along the slip direction is defined as (Hutchinson, 1970):

$$\tau_{re}^{(k)} = \boldsymbol{\sigma} \boldsymbol{\mu} = \sigma_{ij} \mu_{ij}^{(k)} \quad (\text{Eq. 1})$$

where Schmid tensor $\boldsymbol{\mu}^{(k)}$ is determined from the mutually orthogonal vectors $\mathbf{m}^{(k)}$ and $\mathbf{n}^{(k)}$:

$$\mu_{ij}^{(k)} = \frac{1}{2} \left(m_i^{(k)} n_j^{(k)} + m_j^{(k)} n_i^{(k)} \right) \quad (\text{Eq. 2})$$

Once stress σ is applied on a crystal, the macroscopic strain rate is dependent on the density and velocity of mobile dislocations within it. A model describing the evolution of mobile dislocation density under given stress was proposed by (Alexander and Haasen, 1969):

$$\dot{\rho}^{(k)}(t) = \rho^{(k)}(t) \cdot v^{(k)}(t) \cdot \delta^{(k)}(t) \quad (\text{Eq. 3})$$

$\rho^{(k)}(t)$, $v^{(k)}(t)$ and $\delta^{(k)}(t)$ denote the time-dependent density, velocity, and multiplication rate, respectively, of dislocations moving in the k^{th} system at time t . Both the velocity and multiplication rate are assumed to be proportional to the difference between the resolved stress $\tau_{re}^{(k)}$ and a mean internal back-stress $\alpha G^{(k)} b^{(k)} \sqrt{\rho^{(k)}(t)}$, which results from statistically stored dislocations:

$$v^{(k)}(t) = v_0^{(k)} \left(\tau_{re}^{(k)} - k_3^{(k)} \sqrt{\rho^{(k)}(t)} \right) \quad (\text{Eq. 4})$$

$$\delta^{(k)}(t) = k_2 \left(\tau_{re}^{(k)} - k_1^{(k)} \sqrt{\rho^{(k)}(t)} \right) \quad (\text{Eq. 5})$$

where $k_1^{(k)} = \alpha G^{(k)} b^{(k)}$, $k_3^{(k)} = 0.9 k_1^{(k)}$ and k_2 is a constant (Brehm and Glatzel, 1999; Preußner et al., 2009). $b^{(k)}$ is the Burgers vector of the k^{th} system and shear modulus $G^{(k)}$ is determined by elastic compliance S_{ijkl} and unit vectors $\mathbf{m}^{(k)}$ and $\mathbf{n}^{(k)}$ (Ting, 2005):

$$1/G(\mathbf{n}, \mathbf{m}) = 4S_{ijkl}n_i m_j n_k m_l \quad (\text{Eq. 6})$$

The 4th order elastic compliance tensor S_{ijkl} is calculated from the six engineering elastic constants, as expressed in Table 1 in Voigt's reduced notation (Rayne and Chandrasekhar, 1960).

Table 4-1 Elastic constants of β -Sn crystal (Unit: 10^{10} Pa)

C_{11}	C_{33}	C_{44}	C_{66}	C_{12}	C_{13}
7.23	8.84	2.203	2.4	5.94	3.58

The matrix of stiffness constants to which the BCT β -Sn belongs is

$$\mathbf{C} = \begin{bmatrix} C_{11} & C_{12} & C_{13} & 0 & 0 & 0 \\ C_{12} & C_{11} & C_{13} & 0 & 0 & 0 \\ C_{13} & C_{13} & C_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{66} \end{bmatrix}$$

The initial reference velocity $v_0^{(k)}$ is defined as (Kumar and Kumble, 1969):

$$v_0^{(k)} = c_0 \frac{\tau_{re}^{(k)} b^{(k)}}{B^{(k)}} \quad (\text{Eq. 7})$$

The drag coefficient $B^{(k)}$ is used to describe the overall viscous damping effect contributed by phonons, electrons and magnons. The drag mechanism here is assumed to be dominated by phonons, since magnons exist only in ferromagnets, ferrimagnets and antiferromagnets, and the influence of electron drag is very limited at high temperature ($T \gg T_\theta$, where T_θ , the Debye temperature is 200 K for β -Sn). Although multiple mechanisms affect phonon drag, the drag coefficient is approximated with a simple method at temperatures of interest (Alshits, 1992; Nadgorny, 1988):

$$B \approx B_{ph} = \frac{3k_B T}{b^{(k)^2} C_t^{(k)}} \quad (\text{Eq. 8})$$

where $C_t^{(k)}$ is the transverse sound velocity for each slip system ($C_t^{(k)} = \sqrt{G^{(k)}/\rho_m}$) (Hirth et al., 1983), k_B is Boltzmann's constant and ρ_m is the mass density of Sn.

Considering the mutual interaction of dislocations among different glide systems, both dislocation velocity and multiplication rate in k^{th} slip system are coupled with dislocations in the other systems. Eq. (3) is thus updated as follows, using Eqns. (9-11) (Preußner et al., 2009):

$$v^{(k)}(t) = v_0^{(k)} \left(\tau_{re}^{(k)} - k_3^{(k)} \sum_{l=1}^N \sqrt{c_{kl} \rho^{(l)}(t)} \right) \quad (\text{Eq. 9})$$

$$\delta^{(k)}(t) = k_2 \left(\tau_{re}^{(k)} - k_1^{(k)} \sum_{l=1}^N \sqrt{c_{kl} \rho^{(l)}(t)} \right) \quad (\text{Eq. 10})$$

$$\begin{aligned} \dot{\rho}^{(k)}(t) = & \sqrt{\rho^{(k)}(t)} \cdot \sqrt{\sum_{l=1}^N \rho^{(l)}(t)} \cdot v_0^{(k)} \left(\tau_{re}^{(k)} - k_3^{(k)} \sum_{l=1}^N \sqrt{c_{kl} \rho^{(l)}(t)} \right) \\ & \cdot k_2 \left(\tau_{re}^{(k)} - k_1^{(k)} \sum_{l=1}^N \sqrt{c_{kl} \rho^{(l)}(t)} \right) \end{aligned} \quad (\text{Eq. 11})$$

N denotes the total number of slip systems considered, and component c_{kl} in the interaction matrix representing the influence of l^{th} slip system on the dislocation density of k^{th} slip system. The instantaneous dislocation density in the k^{th} slip system is updated after each time increment:

$$\rho^{(k)}(t + \Delta t) = \rho^{(k)}(t) + \dot{\rho}^{(k)}(t) \cdot \Delta t \quad (\text{Eq. 12})$$

A similar approach has been previously used by this group, to assess transient creep rates of Sn-based solders (Mukherjee et al., 2016). In the present study, this recursive incremental calculation is continued until both the multiplication rates and dislocation density rates of all slip systems reduce to zero, thus allowing the number and velocity of all moving dislocations to asymptotically saturate at constant values.

At a macroscopic scale, the crystal now deforms at a constant rate, resulting in steady-state creep deformation. A similar approach was also used by this group to study steady-state creep of Sn-based solders (Mukherjee et al., 2015).

Steady-state creep is commonly considered as a balance state between work-hardening and recovery under given conditions. The semi-logarithmic plot of strain rate vs temperature showed a transition in slopes, for both conventional creep tests (Chu and Li, 1979; Weertman, 1957; Weertman and Breen, 1956) and impression creep tests (Chu and Li, 1979) on β -Sn single crystals. The transition revealed the existence of two activation energies within the range of testing temperatures. This indicates that there are at least two simultaneous competing creep mechanisms taking place within the β -Sn single crystal.

Two recovery mechanisms are considered in the current work (Mukherjee et al., 2016; Poirier, 1976): (i) below the transition temperature, steady-state creep rate is dominated by the cross-slip of screw dislocations ($\dot{\gamma}_{CS}^{(k)}$ in Eq.13); and (ii) above the transition temperature, the steady-state creep rate is controlled by the climb of edge dislocations ($\dot{\gamma}_{CL}^{(k)}$ in Eq. 14). Since the two mechanisms operates in parallel and independently (Chu and Li, 1979), the overall strain rate along the k^{th} slip system $\dot{\gamma}^{(k)}$ is the sum of both mechanisms (i) and (ii), as shown in Eq. 15:

$$\dot{\gamma}_{CS}^{(k)} = A_{CS}^{(k)} \left(\frac{b^{(k)}}{\lambda^{(k)}} \right)^2 \left(\frac{\tau_{re}^{(k)}}{G^{(k)}} \right)^2 \exp \left(-\frac{Q_{CS}}{RT} \right) \quad (\text{Eq. 13})$$

$$\dot{\gamma}_{CL}^{(k)} = \frac{A_{CL}^{(k)} G^{(k)}}{k_B T} \left(\frac{b^{(k)}}{\lambda^{(k)}} \right)^2 \left(\frac{\tau_{re}^{(k)}}{G^{(k)}} \right)^3 \exp \left(-\frac{Q_{CL}}{RT} \right) \quad (\text{Eq. 14})$$

$$\dot{\gamma}^{(k)} = \dot{\gamma}_{CS}^{(k)} + \dot{\gamma}_{CL}^{(k)} \quad (\text{Eq. 15})$$

Where, $\lambda^{(k)}$ is a geometrical parameter, which is inversely proportional to the square root of the saturated dislocation density. R is the universal gas constant. $A_{CS}^{(k)}$ and $A_{CL}^{(k)}$ are model constants to be determined by comparison with experiments. Q_{CS} and Q_{CL} represent the creep activation energy of cross-slip and climb mechanisms respectively, which are determined based on creep tests of single crystal specimens. Under constant tensile stress (in loading coordinates), Weertman and Breen (1956) determined that the activation energy is 92 kJ/mol at temperatures above 403 K and 46 kJ/mol at temperatures below 403 K. The corresponding values they reported in compression creep tests, are 102.5 kJ/mol, and 50.2 kJ/mol, above and below 393 K, respectively. The activation energy obtained from the impression creep test is 104.7-108.9 kJ/mol at high temperatures and about 40 kJ/mol at low temperatures. The measured results for both types of creep tests are comparable to each other. The activation energy used in this work is from Weertman and Breen (1956), as shown in Table 3. The higher activation energy is ascribed to the dislocation climb mechanism. In comparison, the deformation due to Harper-Dorn creep mechanism is assumed to be negligible, at the stress levels considered here.

The total strain rate in the crystalline coordinate system is approximated as the sum of the contributions $\dot{\gamma}^{(k)}$ from all n facile slip systems as shown above in Eq. 15, after rotating them to the principal crystallographic coordinate system, using the Schmid tensor, as shown in Eq. (16).

$$\dot{\epsilon}_{ij} = \sum_{k=1}^n \dot{\gamma}^{(k)} \mu_{ij}^{(k)} \quad (\text{Eq. 16})$$

4.2.2 Calibration of crystal viscoplasticity model for anisotropic creep

As discussed in Section 1, the rate-dependence of steady-state creep is governed by diffusion-assisted recovery from obstructions on the families of facile slip systems. Different operating slip systems were observed in prior work in the literature (Yang and Li, 2007), based on the slip lines identified after tests. Considering the variations in loading condition, crystal orientation and temperature among those studies, the prevailing slip systems might change from test to test. A total of 10 possible slip families and 32 slip systems (Zhou et al., 2009) were considered in this paper, as shown in Table 2. The contribution of each slip system, at a given condition, depends on the dislocation mobility and the resolved shear stress along the slip direction. Weertman conducted constant-stress creep tests on β -Sn single crystal specimens of known orientations: Crystals J, K, B, A, E were wire specimens subjected to axial tensile loads, while Crystals 3 and 4 were cubes subjected to compressive loads. Tests were conducted at various homologous temperatures between $0.60T_m$ and $0.99T_m$ (melting temperature $T_m=505$ K) and under applied stresses ranging from 0.3 to 12 MPa. Specimens extracted from the same source are assumed to have identical crystal orientations.

In the present work, each experimental result is used as one training sample in this scenario to calibrate the dislocation-based creep model proposed above. Uniaxial loading is first transformed into crystal coordinates and then resolved along the slip direction of each slip system. After the dislocation densities reach saturation, the calculated strain rates on different slip systems are summed in crystal coordinates and finally converted back to the sample structural coordinates. The component along the

loading direction, as one of the model outputs, is fitted by experimental measurements to determine the value of constants $A_{CL}^{(k)}$ and $A_{CS}^{(k)}$. $A_{CL}^{(k)}$ and $A_{CS}^{(k)}$ are unified parameters, representing the combined effect of self-diffusion, the length swept, respectively, by the edge and screw dislocations, the statistical distribution of dislocations, etc. Although $A_{CL}^{(k)}$ and $A_{CS}^{(k)}$ should depend on the slip systems, we currently do not have sufficient test results to obtain unique values for all slip systems considered here. The 32 dominant slip systems are divided into two categories, according to the value of component $\mu_{33}^{(k)}$ in their Schmid tensor. Creep rates on slip systems 1-20 are expected to not be affected by extensional stress σ_{33} along the stiff direction of the crystal, since the Schmid tensor component $\mu_{33}^{(k)} = 0$ for these slip systems. In contrast, in slip systems 21-32, $\mu_{33}^{(k)} \neq 0$, and creep strain rates are therefore expected to depend on σ_{33} stresses along the crystal stiff direction. The values of $A_{CL}^{(k)}$ and $A_{CS}^{(k)}$ are approximated to be different for each of these two categories and applicable to all slip systems belonging to each category. Their values are determined from reported experiments (Weertman, 1957; Weertman and Breen, 1956) using a curve fitting process. The values of all model parameters used in this study are summarized in Table 3.

The correlation between the experimental data and predictions of analytical model is illustrated on a log-log scale in Fig. 2, where the strain rates measured by Weertman are plotted against those from the dislocation-based crystal-viscoplasticity model, for Crystals J, K, B, A, E, 3 and 4. The scatter of different crystalline orientations, which cover a wide range of strain rates from 10^{-8} to 10^{-2} s^{-1} , are

grouped by shapes. Considering the variabilities and potential uncertainties among measurements, the calibrated analytical model is considered to be in reasonable agreement with the experiments. Most of the single-crystal tests were performed at stresses between 0.6 to 9 MPa, with only two exceptions: one was performed at a stress of 12 MPa, and the other one was performed at a stress of 0.3 MPa. Due to the small number of tests at the extreme limits of the stress range, the fitting result is better at intermediate stress levels, and the most significant outlier case occurs at the high stresses. Considering this limitation, subsequent simulations of both analytical model and FEA, were performed at stresses below 10 MPa.

Table 4-2 Ten Families of Slip Systems (Zhou et al., 2009) in β -Sn and the magnitude of the corresponding Burgers Vector

No.	SS	Slip System	Magnitude of Burgers Vector (Å)	No.	SS	Slip System	Magnitude of Burgers Vector (Å)
1	1	(1 0 0) [0 0 1]	3.18	17	7	(0 0 1) [1 0 0]	5.83
2		(0 1 0) [0 0 1]	3.18	18		(0 0 1) [0 1 0]	5.83
3	2	(1 1 0) [0 0 1]	3.18	19	8	(0 0 1) [1 1 0]	8.24
4		(1 $\bar{1}$ 0) [0 0 1]	3.18	20		(0 0 1) [1 $\bar{1}$ 0]	8.24
5	3	(1 0 0) [0 1 0]	5.83	21	9	(1 0 1) [1 0 $\bar{1}$]	6.64
6		(0 1 0) [1 0 0]	5.83	22		(1 0 $\bar{1}$) [1 0 1]	6.64
7	4	(1 1 0) [1 $\bar{1}$ 1]/2	4.42	23		(0 1 1) [0 1 $\bar{1}$]	6.64
8		(1 1 0) [$\bar{1}$ 1 1]/2	4.42	24		(0 1 $\bar{1}$) [0 1 1]	6.64
9		(1 $\bar{1}$ 0) [1 1 1]/2	4.42	25	10	(1 2 1) [$\bar{1}$ 0 1]	6.64
10		(1 $\bar{1}$ 0) [$\bar{1}$ $\bar{1}$ 1]/2	4.42	26		(1 $\bar{2}$ 1) [$\bar{1}$ 0 1]	6.64
11	5	(1 1 0) [1 $\bar{1}$ 0]	8.24	27		($\bar{1}$ 2 1) [1 0 1]	6.64
12		(1 $\bar{1}$ 0) [1 1 0]	8.24	28		($\bar{1}$ $\bar{2}$ 1) [1 0 1]	6.64
13	6	(0 1 0) [1 0 1]	6.64	29		(2 1 1) [0 $\bar{1}$ 1]	6.64
14		(0 1 0) [1 0 $\bar{1}$]	6.64	30		($\bar{2}$ 1 1) [0 $\bar{1}$ 1]	6.64
15		(1 0 0) [0 1 1]	6.64	31		($\bar{2}$ $\bar{1}$ 1) [0 1 1]	6.64
16		(1 0 0) [0 1 $\bar{1}$]	6.64	32		(2 $\bar{1}$ 1) [0 1 1]	6.64

Table 4-3 Model Parameters used for β -Sn crystal viscoplasticity modeling

Name	Symbol	Value	Unit	Reference
Boltzmann Constant	k_B	1.38e-23	$\text{m}^2\text{kgs}^{-2}\text{K}^{-1}$	-
Universal Gas Constant	R	8.314	$\text{JK}^{-1}\text{mol}^{-1}$	-
Mass density of Sn	$\rho_{m(\text{Sn})}$	7287	kgm^{-3}	-
Factor for initial dislocation velocity	c_0	1e-16	-	Current study
Geometrical factor	α	0.2	-	(Preu ß ner et al., 2009)
constant	k_1	$\alpha G^{(k)} b^{(k)}$	-	(Preu ß ner et al., 2009)
Dislocation multiplication constant	k_2	10	-	(Preu ß ner et al., 2009)
Dislocation velocity constant	k_3	$0.9k_1$	-	(Preu ß ner et al., 2009)
Dislocation interaction coefficients	c_{ii}	1	-	(Preu ß ner et al., 2009)
Dislocation interaction coefficients	$c_{ij} (i \neq j)$	1e-8	-	Current study
Activation Energy	Q_{CL}	92048	Jmol^{-1}	(Weertman and Breen, 1956)
Activation Energy	Q_{CS}	46024	Jmol^{-1}	(Weertman and Breen, 1956)
Constant for dislocation climb	$A_{CL}^{(k=1-20)}$	6.72 E-06	-	Current study
	$A_{CL}^{(k=21-32)}$	2.24 E-07		Current study
Constant for dislocation cross slip	$A_{CS}^{(k=1-20)}$	4.92 E+15	-	Current study
	$A_{CS}^{(k=21-32)}$	1.64 E+14		Current study

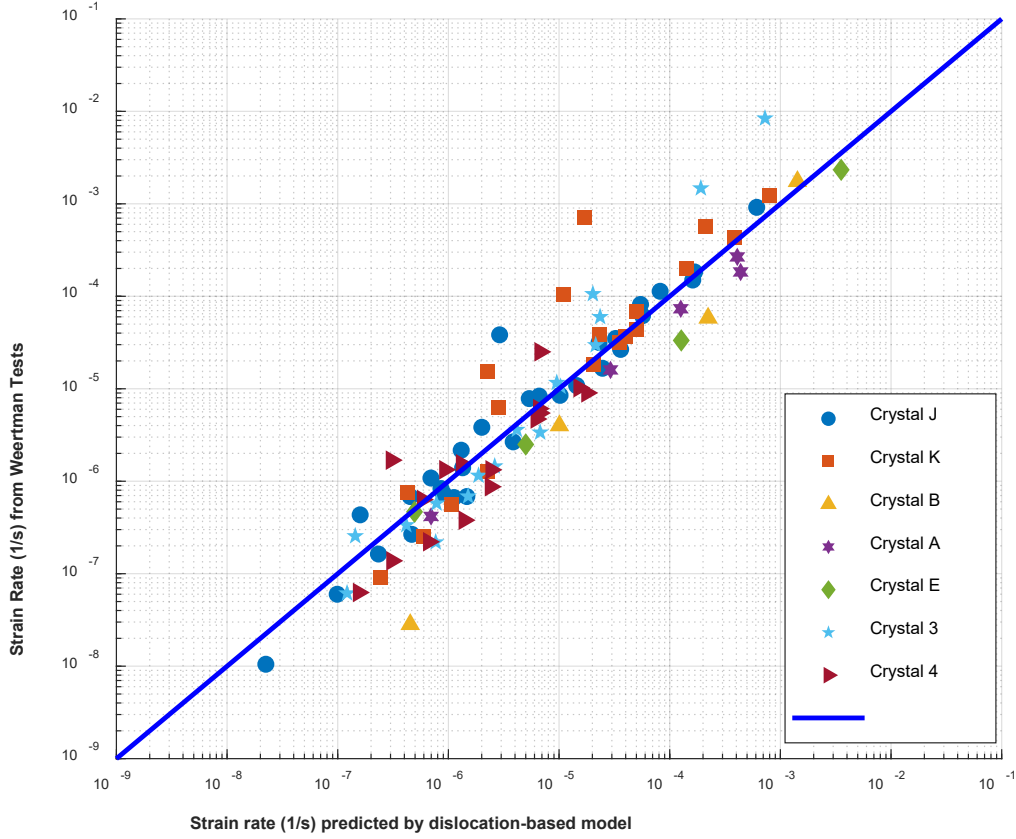


Figure 4.2 Crystal-viscoplasticity anisotropic creep model calibrated with Weertman's creep tests

4.3 Homogenized anisotropic steady-state creep constitutive model

The dislocation-based crystal-viscoplasticity model presented above in Section 2 has been implemented in a computational code, to simulate the evolution of dislocation density, dislocation movement and resulting creep rate for given loading conditions. While this approach can be coded directly into crystal-FEA codes for computational analysis of grain-scale structures, in this section we provide an alternate simplified continuum-scale, homogenized constitutive modeling approach instead, by using this dislocation-based method to derive the corresponding model constants for single-crystal anisotropic creep constitutive models. In this paper, we

focus only on steady-state creep since the dislocation model used to derive the model constant considers the saturated dislocation density instead of modeling the entire dislocation evolution history. The continuum homogenized anisotropic viscoplastic behavior is represented in this paper with a Hill-Norton model where Hill's potential (Hill, 1948) is used to represent the crystallographic anisotropy caused by the orientations of the dominant facile slip systems, while Norton's power-law model (Norton, 1929) is used to represent the creep rates caused collectively by the saturated dislocation density and mobility on all relevant slip systems. The models are briefly summarized in Sections 4.3.1 and 4.3.2, while the extraction of the model constants is described in Section 4.3.3.

4.3.1 Hill's potential for modeling creep anisotropy

In this approach, a creep potential is defined in terms of the Hill effective stress σ_{Hill} , which is a generalization of the classical von Mises equivalent stress for anisotropic materials, under multiaxial stress state, as:

$$\sigma_{Hill} = \sqrt{F(\sigma_{22} - \sigma_{33})^2 + G(\sigma_{33} - \sigma_{11})^2 + H(\sigma_{11} - \sigma_{22})^2 + 2L\sigma_{23}^2 + 2M\sigma_{13}^2 + 2N\sigma_{12}^2} \quad (\text{Eq. 17})$$

where F , G , H , L , M and N are constants explicitly characterizing/specifying the state of anisotropy due to the anisotropy of effective dislocation mobility. The three mutually perpendicular axes (1, 2, 3) correspond to the material principal axes of anisotropy (crystal directions [1 0 0], [0 1 0] and [0 0 1]). The corresponding work-conjugate strain-increment tensor $\dot{\epsilon}_{ij}$ for the Hill effective stress is defined as:

$$\dot{\epsilon}_{ij} = \frac{\partial \sigma_{Hill}}{\partial \sigma_{ij}} \dot{\epsilon}_{eq} \quad (\text{Eq. 18})$$

where $\dot{\epsilon}_{eq}$ is a scalar multiplier constant (termed Hill equivalent creep strain rate in this work, as the anisotropic analog of von Mises' equivalent strain-rate in isotropic materials), and is obtained depending on the constitutive creep law adopted. Usually, Hill's dimensionless constants are empirically determined from creep experiments with simple fundamental loading conditions along selected crystal principal directions (Artzt et al., 2014; Hyde et al., 2005). In the current study, these fundamental Hill tests are simulated with 'virtual tests' conducted with the dislocation-based creep model of Section 2.1 (calibrated with Weertman's single-crystal tests). The load states used for these 'virtual tests' are uniaxial normal stress and simple shear stress along crystal principal directions.

Furthermore, as a simplifying approximation, the anisotropy in steady-state creep is assumed to be constant at a fixed temperature. In other words, Hill's constants are assumed to be temperature-dependent but independent of the magnitude of equivalent stress.

4.3.2 Norton power-law for modeling creep rate

Since the stress dependence of strain rate in Weertman's tests shows the usual power law for all crystal orientations, Norton's power law is adopted in this study to extract the constitutive steady-state anisotropic creep rates, in terms of the Hill effective stress and the corresponding work-conjugate effective strain-rate (termed Hill equivalent creep strain rate in this work). Thus, the multiplier constant $\dot{\epsilon}_{eq}$ in Eq.

(18) was replaced by Norton's model $A(T)\sigma_{Hill}^{n(T)}$ and the strain-increment tensor $\dot{\epsilon}_{ij}$ with respect to that is given by:

$$\dot{\epsilon}_{ij} = \frac{\partial \sigma_{Hill}}{\partial \sigma_{ij}} \dot{\epsilon}_{eq} = \frac{\partial \sigma_{Hill}}{\partial \sigma_{ij}} A(T) \sigma_{Hill}^{n(T)} \quad (\text{Eq. 19})$$

Although the crystal-viscoplasticity model did indicate that the stress exponent $n(T)$ increases at a stress level far beyond 10 MPa (range of current interest in this paper), this behavior is not included here due to the lack of experimental verification. In other words, the model constants presented here are suitable for modeling secondary creep behavior for stress of 10 MPa or less. As discussed below in Section 3.3, the Norton constants $A(T)$ and $n(T)$ (along with the Hill's constants) are extracted from 'virtual creep tests,' conducted with the help of the calibrated crystal-viscoplasticity model of Section 2.

4.3.3 Estimation of Hill-Norton constants

The calibration results of Section 2 (using Weertman's single-crystal test results) demonstrated that the analytical crystal-viscoplasticity model is indeed capable of effectively representing the orientation-dependent steady-state creep behavior of β -Sn crystals to a reasonable degree of accuracy. Thus, it is reasonable to utilize this model as a 'virtual testing' tool, as long as we do not extrapolate the model conditions beyond the range of stresses used in Weertman's experiments.

The values of the six Hill's constants and Norton's constants for Sn single-crystal creep behavior are next extracted from a suitable suite of 'virtual creep tests' (conducted with this calibrated crystal-viscoplasticity model), under selected fundamental stress conditions, both uniaxial and pure shear, in lieu of a corresponding

suite of physical tests. The stress matrix input to the crystal viscoplasticity model for this suite of virtual tests and the corresponding strain rate components along the loading directions, are shown in Table 4. Due to the BCT symmetry of Sn crystal structure, Directions 1 and 2 (Crystallographic Directions [100] and [010]) are equivalent to each other.

Table 4-4 Fundamental stress states applied to the crystal-viscoplasticity model of Sn single-crystal (along crystal principal directions and the corresponding strain rate components, obtained as the output of this virtual testing exercise (Directions 1 and 2 have lattice dimensions a=b, while Direction 3 has lattice dimension c)

INPUT	$\begin{bmatrix} \sigma_{11}^i & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$	$\begin{bmatrix} 0 & 0 & 0 \\ 0 & \sigma_{22}^i & 0 \\ 0 & 0 & 0 \end{bmatrix}$	$\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \sigma_{33}^i \end{bmatrix}$	$\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & \sigma_{23}^i \\ 0 & \sigma_{23}^i & 0 \end{bmatrix}$	$\begin{bmatrix} 0 & 0 & \sigma_{13}^i \\ 0 & 0 & 0 \\ \sigma_{31}^i & 0 & 0 \end{bmatrix}$	$\begin{bmatrix} 0 & \sigma_{12}^i & 0 \\ \sigma_{21}^i & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$
OUTPUT	$\dot{\epsilon}_{11}^i$	$\dot{\epsilon}_{22}^i$	$\dot{\epsilon}_{33}^i$	$\dot{\epsilon}_{23}^i$	$\dot{\epsilon}_{13}^i$	$\dot{\epsilon}_{12}^i$

To be consistent with Weertman's physical tests, the virtual test predictions are restricted to stress levels ranging from 0.2 MPa to 10 MPa and temperature levels ranging from 273 K to 498 K. The predicted strain rate components for loading along Directions 1 and 3 differ up to two orders of magnitude. Since the variation of the stress exponent under different fundamental stress conditions at the same temperature is less than 3%, it is assumed that the stress exponent is identical for all orientations at a given temperature. The values are determined as a shared parameter in power-law fitting. $n(T)$ remains almost unchanged at low temperatures, and ranges from 4 to 4.7 at temperatures from 348 K to 500 K. This result is in good agreement with the measured values (3.6 to 5.1) of both the conventional creep test and the impression creep tests for β -Sn single crystal specimens. Each stress condition is taken as a

distinct dataset and simultaneous curve fitting operations are performed on multiple datasets at a constant temperature.

The relative values of Hill's six constants (in Eqn. 17) indicate the degree of anisotropy of the material and quantify the difference in creep resistance along different directions, with a larger value indicating a higher creep resistance. The numerical values of Hill's constants are therefore usually specified on a normalized scale (normalized in the present study with respect to Hill's constant G of Eqn. 17). Thus constant G is defined to be equal to one for all conditions. These anisotropic constants are used to estimate the effective stress (σ_{Hill}) for any given state of stress in this anisotropic material. This effective Hill stress is then used to estimate the corresponding steady-state scalar equivalent creep Hill strain rate $\dot{\epsilon}_{eq}$, and the corresponding creep strain rate tensor $\dot{\epsilon}_{ij}$, using the Hill-Norton model given in Eq. (19). The values of the resulting Hill-Norton model constants are calculated for all 'virtual test' datasets, and presented in Fig. 3. The slope of the pre-exponential parameter $A(T)$ (Fig. 3 (b)) decreases with increasing temperature, which corresponds to the fact that different activation energies dominate the low and high temperatures respectively, as presented in the training result of Weertman's tests. The Hill's constant H remains unchanged at temperatures below 323 K and finally decreases by 28% when the temperature reaches 498 K. The constant M continues to decrease as the temperature increases, and its total decrease is about 18%. Unlike H and M , N has very limited change over the entire temperature range. According to the values of Hill's constants, the overall anisotropy of steady-state creep decreases with increasing temperature.

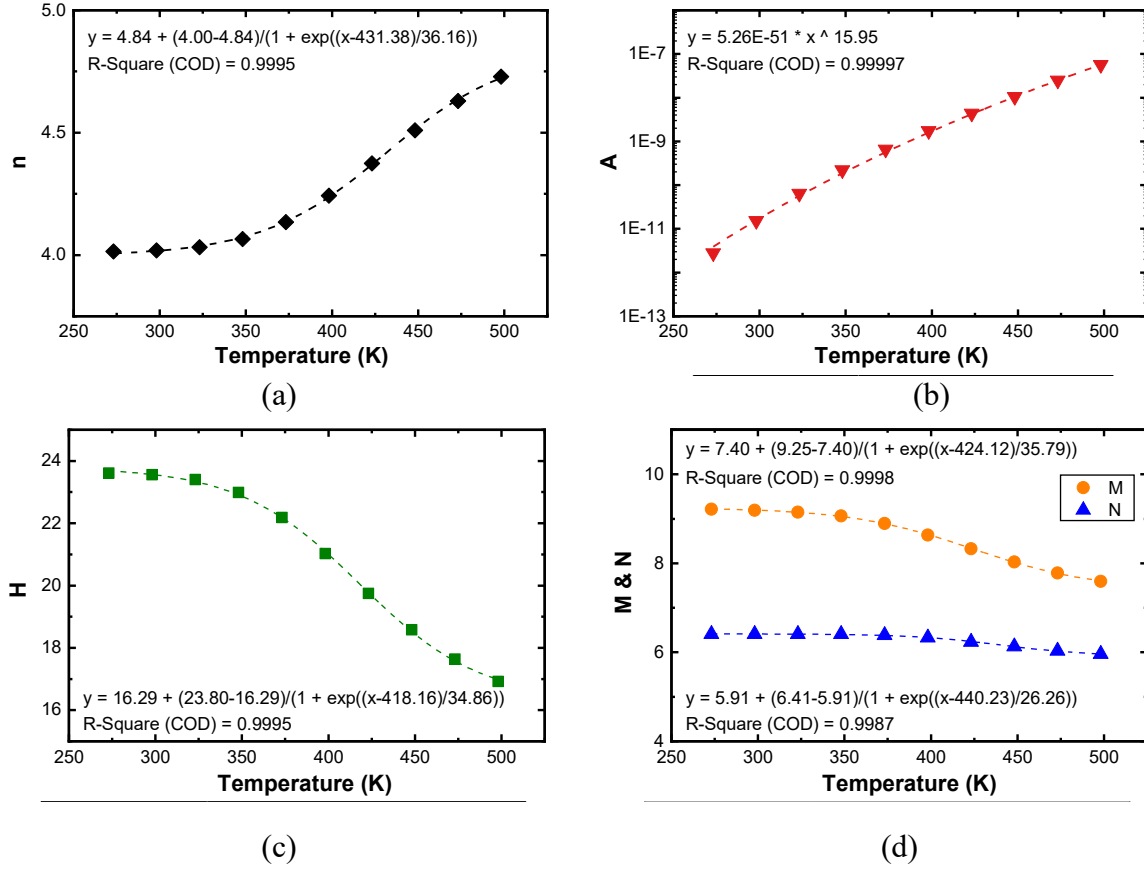


Figure 4.3 (a) Stress exponent $n(T)$, (b) pre-exponential parameter $A(T)$, (c) Hill's constant H , (d) M and N estimated from uniaxial tensile and pure shear virtual tests conducted at various temperatures with the dislocation-based crystal-viscoplasticity analytical model

4.4 Verification of Hill-Norton model constants

As a confirmation of the accuracy of the Hill-Norton constants obtained in Section 3, anisotropic finite element simulations are conducted of Weertman's single crystal creep tests and the simulation results are compared with those from the physical tests. The finite element model used to simulate Weertman's tensile creep tests (Weertman, 1957; Weertman and Breen, 1956) is shown in Fig. 4. The specimens are in the form of wires, with a diameter of 2.39 mm and an approximate length of 50.8 mm. Global coordinate indicates the overall loading direction and local

coordinate depicts the crystal's orientation. Uniform stress is applied at one end of the wire along the global Z-axis, while the opposite end is completely restrained. Two groups of creep tests are simulated with this geometry, using the Hill-Norton model constants of Section 3 for anisotropic steady-state creep. The purpose of the first set is to confirm the ability of the model constants estimated in Section 3, by comparing Crystal J creep test results in Weertman's study with FEA simulations of the tests. The loading axis is 45° , 45° and 90° from the crystal directions $[1\ 0\ 0]$, $[0\ 1\ 0]$ and $[0\ 0\ 1]$ respectively, as shown in Fig. 4 (b). This verification is reported in Section 4.4.1.

The second group of FEA simulations aims to verify the ability of the Hill-Norton FEA results to represent the crystal viscoplasticity results along many crystal orientations, other than the calibration cases along the fundamental crystal axes. This parametric study is implemented by incrementally rotating the crystal about the global X-axis between 0 and 90 degrees in small steps. The crystal's stiff direction $[0\ 0\ 1]$ initially coincides with the loading direction (global Z-axis), as illustrated in Fig. 4 (c), and is perpendicular to it after 90° rotation. This verification study is reported in Section 4.4.2.

Simple uniform stress fields are well suited for estimating constitutive model constants, and are therefore used here to calibrate the anisotropic crystal viscoplasticity model in Section 2, to calibrate the anisotropic continuum viscoplasticity model in Section 3, and to further verify the continuum viscoplasticity model in Section 4. Although the tensile bar (used from Weertman's study for model calibration purposes) is subjected to uniaxial loading in the axial direction, the crystal

is actually in a uniform multi-axial stress state in its principal material coordinates, since the material principal axes do not coincide with the loading axis.

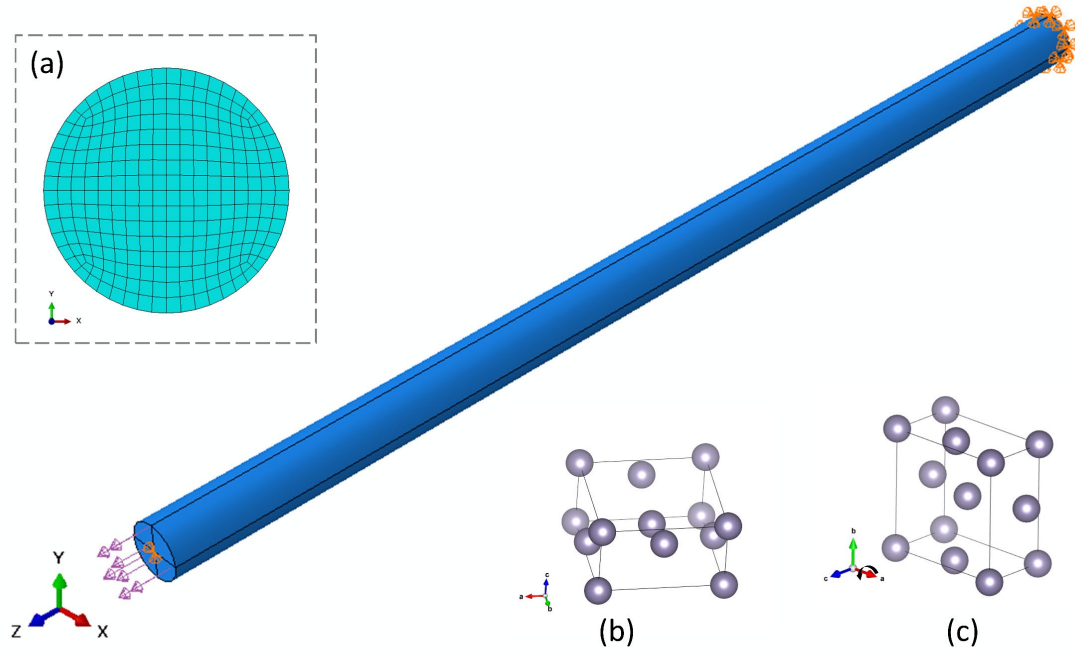


Figure 4.4 FEA model of wire specimen used in Weertman's experiments: (a) cross-section mesh; (b) local coordinate indicating the material orientation of Crystal J; (c) local coordinate indicating the initial orientation for parametric analysis

4.4.1 Model verification for Weertman's crystal J

Hill's constants and corresponding parameters in Norton's law extracted above in Section 3 are first applied to simulate all the tests conducted on Crystal J, since most of the tests among all five crystals tested by Weertman were for Crystal J. The uniaxial engineering strain rates are estimated by dividing the average deformations of all nodes on the loading surface by the total length of the wire specimen and time interval. The comparison between Weertman's results and the FEA simulations of

Crystal J are illustrated in Fig. 5 (on log-log scale), where the applied stress ranges from 0.73MPa to 9MPa and temperature varies from 303K up to 492K.

The spot size indicates the applied stress level, and the colors represent testing temperatures. Most tests on Crystal J were performed at stresses below 6 MPa, with one exception of a test at 9 MPa. The fitting results are better for intermediate stress levels, and the most discrepancy is at high stresses, which is consistent with the predictions of the analytical crystal-viscoplasticity model.

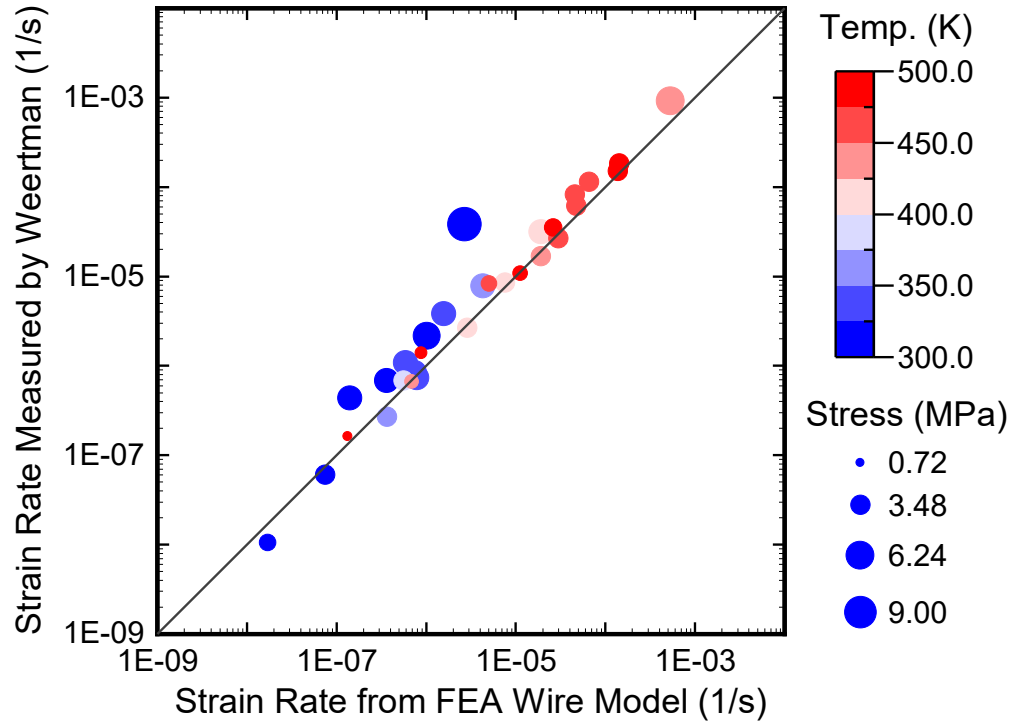


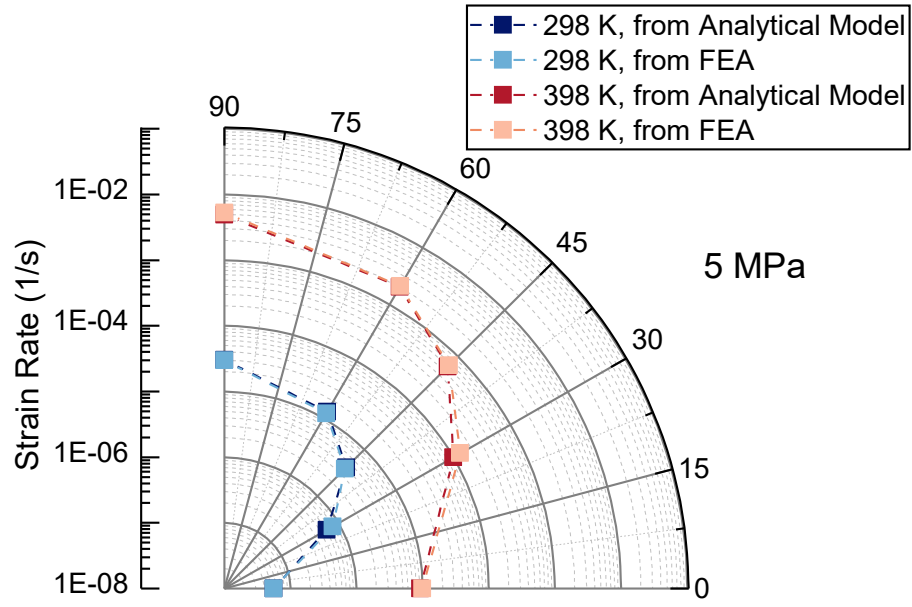
Figure 4.5 Comparison between Weertman's experimental results for Crystal J (Weertman and Breen, 1956) and corresponding FEA simulation with Hill-Norton model constants

4.4.2 Model verification for parametric variation of crystal orientation

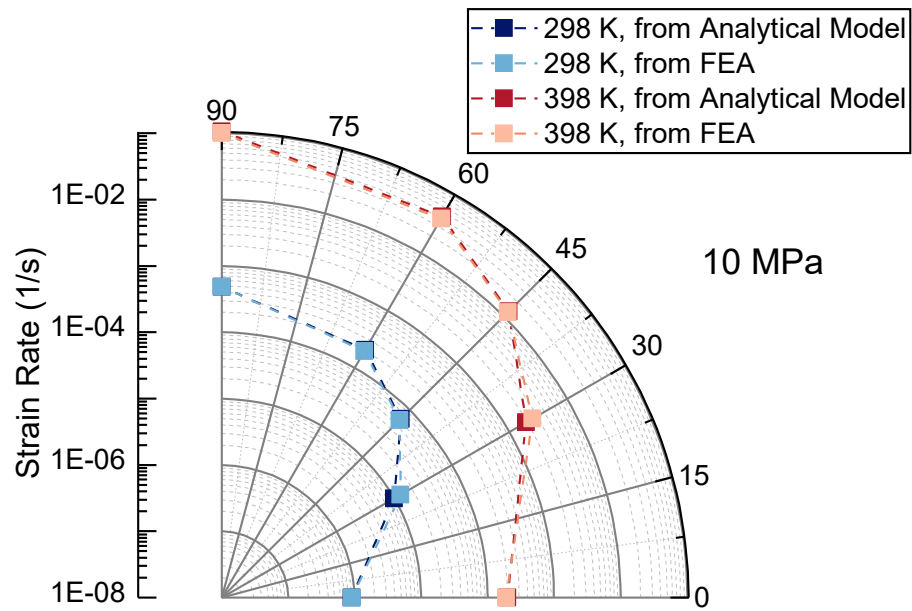
As discussed above, the purpose of this parametric study is to explore the agreement between the Hill-Norton continuum modeling approach and the crystal-

viscoplasticity analytic modeling approach for other orientations beyond the calibration cases defined for crystal principal directions. In this parametric study, the crystal direction $[0\ 1\ 0]$ (global X-axis) is held constant, and the stiffest direction $[0\ 0\ 1]$ is gradually rotated from the uniaxial loading direction to the orthogonal direction. Results of all tests performed are plotted against the rotation angle in Fig. 6. The darker markers represent outputs of analytical model and lighter ones represent corresponding FEA outputs. There is reasonable agreement between the Hill-Norton FEA model and the crystal viscoplasticity analytic model for temperatures of 298K and 398K, and applied stresses of 5 MPa and 10 MPa. Although the largest discrepancy is for 30° orientations, even for this case, simulations with directional Hill's constants can offer reasonable predictions. Since the Hill-Norton model constants have been calibrated in an average sense across different stress states, some extreme cases are overestimated, such as for 30° rotation.

The same information is also presented as a histogram in Fig. 7, by plotting the percentage difference between the outputs of analytical crystal viscoplasticity model and the homogenized Hill-Norton FEA simulation. As expected, the best agreement is for grain orientations of 0° and 90°, since the Hill-Norton model constants were extracted (calibrated) at these fundamental loading directions. As discussed in Figure 6, the largest difference among all conditions is about 32% and occurs at 398K after a 30° rotation. Considering that strain rate varies by orders of magnitude in creep tests, the level of agreement obtained here between crystal viscoplasticity model and homogenized Hill-Norton FEA simulation is considered to be acceptable.



(a)



(b)

Figure 4.6 Comparison between results from analytical model and FEA simulation as grain orientation rotating about the global X-axis: (a) applied stress = 5 MPa, (b) applied stress = 10 MPa

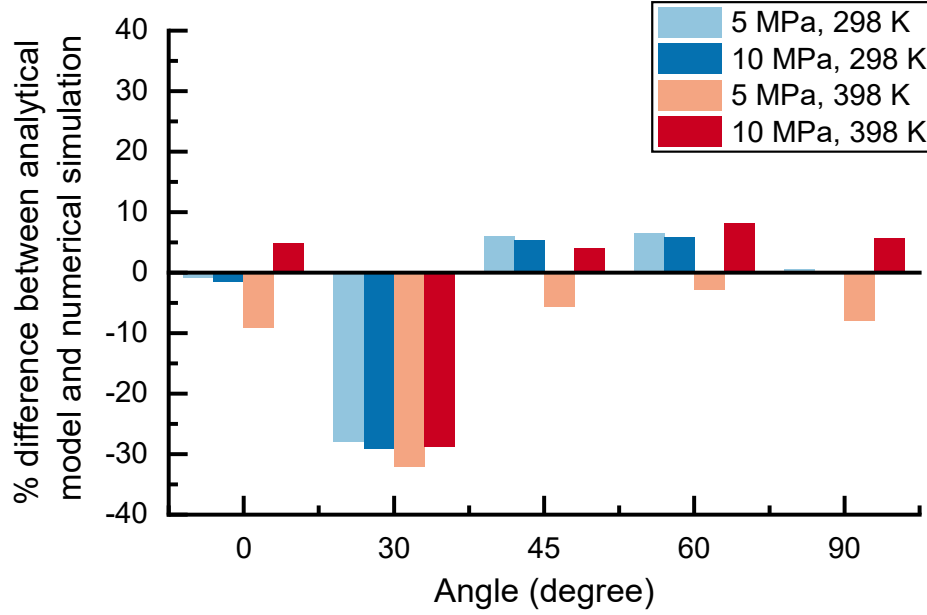


Figure 4.7 Percentage difference between analytical and numerical models

4.5 Conclusion

An analytic crystal-viscoplasticity model for calculating the steady-state creep response of anisotropic single crystal β -Sn, based on dislocation density evolution and mobility along the most facile slip systems, is proposed in the current work. This model has been calibrated using results of conventional single crystal creep tests reported in the literature. Furthermore, an anisotropic homogenized creep constitutive model is proposed for numerical FEA simulations of steady-state creep behavior. In this constitutive model, Hill's potential is used to represent the anisotropy of the creep behavior, while Norton's power-law is used to represent the steady-state creep flow rule. The temperature-dependent Hill-Norton model constants are determined from a suitable set of 'virtual creep tests' conducted using this calibrated crystal-viscoplasticity model at a specific temperature along the fundamental crystal directions. The accuracy of the Hill-Norton constitutive model is verified by first

testing its ability to provide successful FEA simulation of Weertman's creep test on Crystal J. As an additional sanity check of this constitutive model, its agreement with the crystal viscoplasticity model is explored for a wide range of grain orientations (since the Hill-Norton constants are based on calibration data that came only from loading along crystal principal directions). The FEA simulation outputs are found to agree reasonably well with both Weertman's tests and the dislocation-based crystal-viscoplasticity model.

Subsequent additional verification of this approach will be based on physical creep tests of single crystal test specimens and will be presented in future work. Since the goal in this paper is to develop single-crystal constitutive models for β -Sn (using crystal-viscoplasticity and continuum viscoplasticity), the numerical simulations (and calibration tests) use simple specimen geometry and simple loading conditions, to generate a uniform stress field throughout the sample. Future applications of the Hill-Norton anisotropic continuum viscoplasticity model will focus on more complex, non-uniform stress fields, such as those encountered in impression creep testing. This work is also a precursor to the modeling of the anisotropic steady-state creep behavior of multi-grain SnAgCu solder materials.

Chapter 5: Crystal Viscoplasticity Approach for Estimating Anisotropic Steady-state Creep Properties of Single-crystal SnAgCu Alloys

Abstract

Creep can have a significant impact on the reliability of Sn-based solder alloys even at room temperature because of their relatively low melting temperatures. SnAgCu (SAC) solder joints used in electronic packaging typically consist of only a few highly anisotropic grains, which consist of Sn dendrites embedded in a near-eutectic Sn-Ag phase. The unique grain structure of each joint leads to stochastic variations in the thermomechanical response of such joint. Therefore, grain-scale testing and modeling are recommended to better characterize the anisotropic behavior and to estimate the influence of stochastic variability of grain structure on the viscoplastic response of the joint. This work aims to investigate the anisotropic steady-state creep behavior of single-crystal SAC solder joints. The orientation-dependent viscoplastic behavior of individual SAC grains is modeled with a multi-scale crystal-viscoplasticity approach for representing the relevant dislocation mechanics. The response predicted by the crystal viscoplasticity model is then captured in an equivalent homogenized continuous-scale constitutive model (Hill-Garofalo formulation).

This modeling strategy was implemented in numerical simulations, as an illustrative example, to analyze the behavior of single-grain Ball-Grid Array (BGA) joints subjected to combined steady compression (from heat-sink clamping force) and thermal cyclic loading. The cyclic ratcheting in the presence of the steady

compressive force causes: (i) transverse expansion of the solder ball, potentially leading to eventual short circuits; and (ii) cyclic fatigue damage leading to eventual failure of the solder joint. The proposed grain-scale modeling approach is shown to be able to address the stochastic variability of both these damage mechanisms, as a function of grain orientation. The present methodology can be used to predict the behavior of solder joints based on their microstructure, and provide insights for their reliability analysis.

5.1 Introduction

Sn-based lead-free solder alloys are widely accepted as a reliable alternative to lead solders due to their reasonable price, acceptable performance, and their suitability as a direct substitute of Pb-based solders in electronic assemblies. Creep is one of the most important properties affecting the reliability of Sn-based solders because of their relatively low melting point. Even at ambient temperature, their homologous temperature is above 0.6 and creep deformation cannot be ignored. Although a great deal of work has been done to characterize the creep properties of Sn-based solder alloys, there are considerable discrepancies across different studies between experimental measurements and the model constants subsequently extracted from the test results.

One reason for this discrepancy is attributed to differences in microstructure. Functional SAC solder joints commonly exhibit oligocrystalline (up to a few grains) morphology in either discrete or interlaced structures, with stochastic distribution of grain orientations (Bieler et al., 2008; Telang and Bieler, 2005). The behavior of these individual grain-scale solder joints may be quite different from that of bulk

polycrystalline specimens (Kariya et al., 2005; Sahaym et al., 2013). More than 90% of SAC alloys are β -Sn, which is one of the most anisotropic elements due to its body-centered tetragonal (BCT) crystal structure. The intrinsic anisotropy of β -Sn promotes the formation of heterogeneous microstructures during solidification, therefore leading to complex properties and unique microstructure of each joint. In addition, there are different solidification paths in the Sn-Ag-Cu ternary system, which complicates the non-eutectic solidification and makes it very sensitive to the alloy composition, cooling rate and post-soldering thermal aging (El-Daly et al., 2013; Sungkhaphaitoon and Plookphol, 2018; Zhao et al., 2004). The effects of these microstructural features, like dendritic morphology, intermetallic compounds (IMCs) coarsening, and inter-particle spacing, and so on, are measured quantitatively (Arfaei et al., 2011; Chauhan et al., 2013; Fu et al.; Gu et al., 2021; Han et al., 2012). Moreover, the processes that lead to changes in these characteristics, such as cooling rate, isothermal aging, doping, etc., and the consequent influence on the behavior of solder joints are also investigated (Chuang et al., 2012; Darbandi et al., 2014; Lee and Huang, 2016; Maleki et al., 2014; Ochoa et al., 2004; Tsao, 2011; Yifei et al., 2008). The miniaturization of electronic circuits has further exacerbated this problem. On the one hand, the reduction in volume increases the fraction of the micro-scale joints occupied by interfacial IMC layers, changing the internal stress/strain concentration gradient (Khatibi et al., 2012; Lee et al., 2008); on the other hand, the loss of volume increases the impacts of contaminants, which are unintended elements from adjacent structures/materials, and changes the phase equilibrium and microstructure (Park et al., 2010; Wang et al., 2019; Yang et al., 2010).

Considering the inevitable influence of this heterogeneous microstructure, multiscale modeling has been proposed to better characterize the behavior of different materials, usually classified into concurrent and hierarchical approaches according to the bridging methodology (Chandra et al., 2018; de Pablo and Curtin, 2007; Groh et al., 2009; Tan et al., 2021). In the concurrent approach, methods of different length scales communicate with each other in the combined model; while in the hierarchical approach, quantities are transferred sequentially from lower to higher scales (Zeng et al., 2008). Maleki and his colleagues (Maleki et al., 2013, 2016) created statistically representative volume elements (RVEs) for SAC405 in three-dimensional finite element (FE) modeling, which preserves the characteristics of the actual microstructure obtained through tomographic images. Numerical homogenization was performed sequentially on the microscopic scale (within the eutectic mixture) and mesoscopic scale (including dendrites, surrounding eutectic phases and IMC) to extract the overall elastic-plastic behavior of the solder joint during isothermal aging. For simplicity, the anisotropy of Sn was not considered by Maleki. Mukherjee and co-authors (Mukherjee et al., 2016) proposed a mechanical model based on microstructural features and dislocation motions along the three most facile slip systems, to predict the anisotropic transient as well as steady-state creep response of SAC305 single crystals. Xu et al. (2021) focused on the effect of morphology and size of IMCs on the early-stage creep of directionally solidified SAC305 samples. In the FE analysis, RVEs representing eutectic mixtures of three different microstructures were modeled as particle-reinforced matrix composites, while the β -Sn was modeled by a dislocation-based crystal plasticity method. After

homogenization, changes in creep resistance were determined based on the microstructural evolution caused by aging.

Although the crystal plasticity method provides insight into anisotropic behavior in SAC solder joint by averaging fits to multiple slip systems, the effect of microstructural features is missing here, especially at different length scales. Multiscale modeling with the RVEs also depends on the specific sample cross-sections. Remodeling is necessary to estimate the extent of the effect of microstructural changes, which may be inefficient in time considering the stochastic and variable microstructure in SAC solder joints. Modeling strategies that provide high-quality characterization and appropriate computational efficiency are still under development. The focus of this work is to develop a comprehensive multi-scale crystal viscoplasticity method to establish microstructure-property relationships for the anisotropic steady-state creep behavior of SAC305 crystals. The crystal viscoplasticity model aims to quantify the creep deformation from a microstructural perspective and in terms of well-defined dislocation motion mechanisms. The anisotropic single-crystal response predicted by the crystal viscoplasticity approach is then captured at the continuum scale by a Hill-Garofalo formulation so that solder grains can be modeled at component scale, as a continuous homogeneous anisotropic phase. The sequential modeling strategy can not only provide insight into the effect of microstructure on steady-state creep behavior (and its stochastic variability) in applications, but can also guide the design and development of reliable materials and reliable packaging architectures, as well as guide accelerated testing procedures for product qualification.

The remainder of this manuscript is organized as follows. Section 5.2 introduces the grain-scale specimens used for mechanical testing, and for characterizing the typical microstructure of oligocrystalline SAC305 solder joints. Section 5.3 describes in detail the framework for crystal viscoplastic (CV) modeling and lists the proposed improvements/enhancements compared to other CV models reported in the literature. The determination of the constants in the homogenized continuum Hill-Garofalo model for steady-state anisotropic creep is presented in Section 5.4. Section 5.5 analyzes the effect of grain orientation on single-crystal solder joints through FE modeling. This paper concludes with a summary and conclusion in Section 5.6.

5.2 Experimental and Microstructure

Micro-scale test coupons, of the same characteristic length-scale as functional solder joints, are developed to characterize the thermo-mechanical behavior of functional SAC solder joints, as described in Section 5.2.1. These are termed grain-scale specimens since there are just a few grains throughout the solder joint (*i.e.*, the characteristic length-scale of the grains are of the same order as those of the test specimen). A description of the representative heterogeneous microstructure of SAC joints is given in Section 5.2.2.

5.2.1 Grain-scale specimens and testing

Experimental results (Kariya et al., 2005; Wiese and Wolter, 2004) show that the mechanical behavior of SAC alloys manifest clear size dependence. Microstructural analysis reveal that large bulk samples contain many grains, while modern functional solder joints are much smaller and usually contain at most a few grains. Furthermore,

the microstructural features within individual grains (e.g., dendritic and IMC morphology) are significantly different. The interactions between the grain geometry, grain boundary geometry and the finite boundaries of the joint become important determinants of the structural response of the joint. Therefore, grain-scale test coupons, that are geometrically of similar length-scales as functional joints, are recommended, in order to accurately evaluate the mechanical response of SAC solder joints.

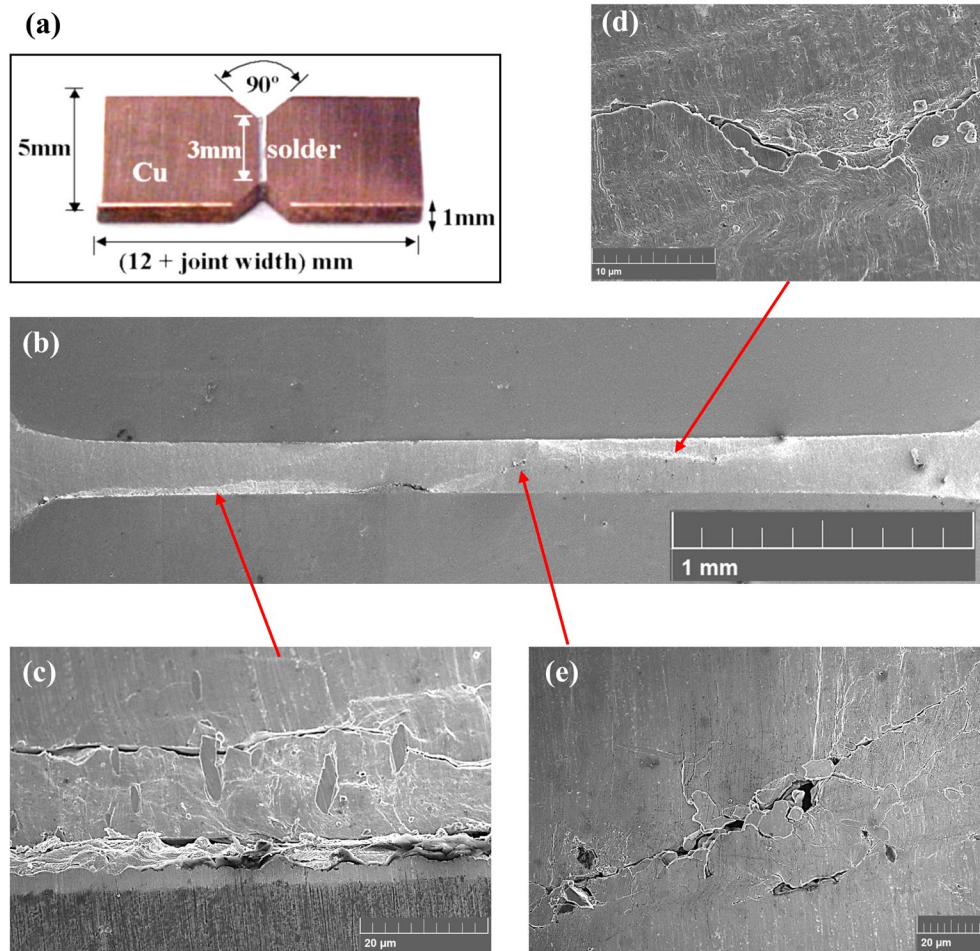


Figure 5.1 Grain-scale TMM specimen. (a) Nominal dimensions for shear specimen. (b) SEM image of one solder joint after mechanical cycling test (7% load drop). (c) Higher magnification image showing initial cracks along/near the IMCs interface. (d) and (e) Higher magnification images showing initial cracks in the bulk of solder joint

A customized thermo-mechanical-microscale (TMM) setup has been used to characterize the thermo-mechanical properties of micron-scale solder joints (Haswell, 2002). Microstructure studies have shown that TMM specimens have a oligocrystalline structure the ratio of grain size to joint size is approximately similar to that found in functional solder joints. A modified Iosipescu specimen (Haswell and Dasgupta, 2001, 2011) for pure shear loading is illustrated in Fig. 1 (a). The height of the joint is about 180-200 μm , and the 90° notches facilitate uniform stress distribution throughout the joint. Fig. 1 (b) - (e) show the SEM (scanning electron microscope) images of a TMM shear specimen, before loading and after 7% load drop. Cracks initiate either along/near the IMC interface and/or in the solder bulk (intergranular or transgranular). Even within the same joint, the degree of grain deformation varies greatly within different grains, due to different crystal orientations. In addition, the stiffest direction of $\beta\text{-Sn}$ coincides with the highest CTE direction, which implies a profound mismatch at the grain boundaries. The commonly used homogeneous isotropic material models can neither estimate the stress/strain concentrations due to grain mismatches within the solder bump nor assess the degree of variation in thermo-mechanical behavior due to microstructural differences. Grain-scale models can be used to effectively assess the influence of micromorphology on mechanical response through simulations, and anisotropic properties are necessary for this purpose.

5.2.2 Heterogenous microstructure

According to the pertinent significant length scale features, the heterogeneous microstructure of SAC solder joints is divided into multiple tiers (Mukherjee et al.,

2015), as shown in Fig. 2. Tier 3 represents the entire solder joint (not including the IMC layer), which is commonly composed of a few large anisotropic grains in discrete arrangement, as shown in BGA joints and TMM grain-scale specimens, or of three twinning orientations in interlaced arrangement. The limited number of grains, random crystal orientation, and the inherent anisotropy of β -Sn, render each joint unique in terms of its thermomechanical behavior under the same load conditions. Tier 2 focuses on the microstructure within an individual crystal in the oligocrystalline solder joints, where β -Sn exists in the form of dendritic structures and is surrounded by the eutectic Ag-Sn phase. Both 2D cross-section and 3D image are presented in Fig. 2 (b). Additional microscale intermetallic compounds of Cu_6Sn_5 rods and Ag_3Sn plates are located inside individual grains. The next lower scale, termed Tier 1, is the eutectic phase, consisting of nano-scale Ag_3Sn particles embedded in the β -Sn matrix and forming a statistically homogeneous eutectic mixture (Fig. 2 (c)). Due to the limited solubility of Ag in β -Sn, Ag_3Sn particles exist in the β -Sn matrix as a thermally stable compound. Tier 0 refers to the body-centered tetragonal (BCT) β -Sn crystal, with lattice parameters $a=b=5.83 \text{ \AA}$, $c=3.18 \text{ \AA}$. The asymmetric crystal structure leads to anisotropic physical and mechanical properties and provides the base material the heterogeneous microstructure of SAC alloys. Within each grain, the Sn crystals in both the eutectic phase and the dendritic structure have the same orientation.

Heterogeneous Microstructure of SAC Solder Joints

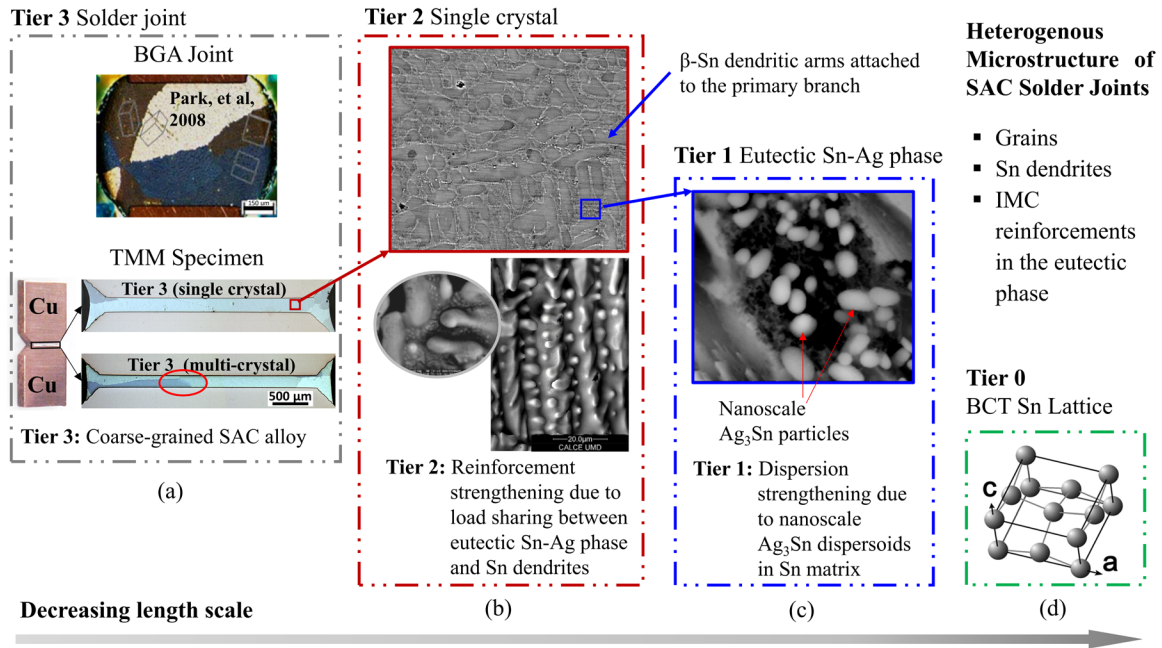


Figure 5.2 Heterogeneous microstructure of as-fabricated SAC solder joints

5.3 Crystal Viscoplasticity Model

The mechanical properties of SAC alloys are highly dependent on their microstructures, so models that can capture the complexity of the relationship between the underlying microstructure and properties are required for effective material design and material improvement. Viscoplastic deformation of SAC crystals are believed to arise predominantly from the movement of dislocations, at the stress and temperature ranges under investigation in this study. A multiscale crystal Viscoplasticity (CV) model is developed, based on the heterogeneous microstructure and different mechanisms that are believed to govern the behavior on each length scale. A hierarchical multi-tier modeling framework is developed, where the results of the lower tier (length-scale) are transferred to the next higher tier, until the steady-

state viscoplastic behavior of the SAC single crystal is fully characterized. Transient viscoplasticity is beyond the scope of the present study.

Considering the stochastic orientation of grains within the solder joints, a global coordinate frame is defined, based on the assembly or test system, and each grain contains a local coordinate whose axes are consistent with the principal directions of the crystal. The orientation of crystals in a sample can be measured by EBSD (electron backscatter diffraction). A vector $\mathbf{u}$ in the rotated system can be transformed back to $\mathbf{U}$ in the original sample system by $u_i = U_j O_{ji}$, where $\mathbf{O}$ is the rotation matrix. Under the Bunge convention (Bunge, 2013) the rotation matrix $\mathbf{O}$ can be defined in terms of three Euler angles $\boldsymbol{\varphi} = \{\varphi_1, \Phi, \varphi_2\}$, as:

$$\mathbf{O} = \begin{bmatrix} \cos\varphi_1\cos\varphi_2 - \sin\varphi_1\sin\varphi_2\cos\Phi & \sin\varphi_1\cos\varphi_2 + \cos\varphi_1\sin\varphi_2\cos\Phi & \sin\varphi_2\sin\Phi \\ -\cos\varphi_1\sin\varphi_2 - \sin\varphi_1\cos\varphi_2\cos\Phi & -\sin\varphi_1\sin\varphi_2 + \cos\varphi_1\cos\varphi_2\cos\Phi & \cos\varphi_2\sin\Phi \\ \sin\varphi_1\sin\Phi & -\cos\varphi_1\sin\Phi & \cos\Phi \end{bmatrix}$$

The conversion between the crystal coordinate and the α^{th} slip system is achieved through the rotation matrix $\mathbf{Q}^{(\alpha)} = [\mathbf{n}^{(\alpha)} \quad \mathbf{m}^{(\alpha)} \quad \mathbf{t}^{(\alpha)}]$, where $\mathbf{m}^{(\alpha)}$ and $\mathbf{n}^{(\alpha)}$ are unit vectors normal to the slip plane and in the slip direction, respectively, and $\mathbf{t}^{(\alpha)} = \mathbf{n}^{(\alpha)} \times \mathbf{m}^{(\alpha)}$. A total of 32 slips systems (belonging to 10 slip families) are considered in the current study for Tin's BCT crystal (Jiang and Dasgupta, 2021; Zhou et al., 2009).

5.3.1 Tier 0: β -Sn

The dislocation-based steady-state creep model of β -Sn phase and its calibration have been described in detail in a prior study (Jiang and Dasgupta, 2021), so only a brief summary is provided here. There are multiple slip systems in the body-center-

tetragonal (BCC) Sn lattice. The resolved shear stress causes dislocations to move along facile directions, which corresponds to macroscopic plastic and viscoplastic deformation. For a single grain subject to the Cauchy stress tensor σ , the resolved shear stress $\tau_{re}^{(\alpha)}$ in the direction of slip is defined as (Hutchinson, 1970):

$$\tau_{re}^{(\alpha)} = \sigma : \mu^{(\alpha)} \quad (\text{Eq. 1})$$

where $\mu^{(\alpha)} = 1/2 (\mathbf{m}^{(\alpha)} \otimes \mathbf{n}^{(\alpha)} + \mathbf{n}^{(\alpha)} \otimes \mathbf{m}^{(\alpha)})$ is the Schmid tensor of α^{th} slip system.

Both conventional creep tests (Weertman, 1957; Weertman and Breen, 1956) and impression creep tests (Chu and Li, 1979) of β -Sn single crystal specimens reveal that there are two parallel and independent mechanisms dominating the steady-state creep. The low temperature process is dominated by dislocation slip, and the high temperature process is dominated by dislocation climb. The steady-state creep was modeled as the result of the equilibrium state, where density-saturated dislocations move at constant velocities in facile slip systems (Brehm and Glatzel, 1999; Preu β ner et al., 2009). The total strain rate $\dot{\gamma}_{Sn}^{(\alpha)}$ in the slip direction of slip system α is equal to the sum of the contributions of dislocation slip $\dot{\gamma}_{Sn_CS}^{(\alpha)}$ and dislocation climb $\dot{\gamma}_{Sn_CL}^{(\alpha)}$, as shown below (Mukherjee et al., 2016; Poirier, 1976):

$$\dot{\gamma}_{Sn_CS}^{(\alpha)} = A_{CS}^{(\alpha)} \left(\frac{b^{(\alpha)}}{\lambda^{(\alpha)}} \right)^2 \left(\frac{\tau_{re}^{(\alpha)}}{G^{(\alpha)}} \right)^2 \exp \left(-\frac{Q_{CS}}{RT} \right) \quad (\text{Eq. 2})$$

$$\dot{\gamma}_{Sn_CL}^{(\alpha)} = \frac{A_{CL}^{(\alpha)} G^{(\alpha)}}{k_B T} \left(\frac{b^{(\alpha)}}{\lambda^{(\alpha)}} \right)^2 \left(\frac{\tau_{re}^{(\alpha)}}{G^{(\alpha)}} \right)^3 \exp \left(-\frac{Q_{CL}}{RT} \right) \quad (\text{Eq. 3})$$

$$\dot{\gamma}_{Sn}^{(\alpha)} = \dot{\gamma}_{Sn_CS}^{(\alpha)} + \dot{\gamma}_{Sn_CL}^{(\alpha)} \quad (\text{Eq. 4})$$

where $b^{(\alpha)}$ is the magnitude of the Burgers vector on slip system α , and $G^{(\alpha)}$ is the corresponding shear modulus determined by elastic compliance S_{ijkl} and orthogonal unit vectors $\mathbf{m}^{(\alpha)}$ and $\mathbf{n}^{(\alpha)}$ (Ting, 2005):

$$1/G(\mathbf{n}, \mathbf{m}) = 4S_{ijkl}n_in_jn_kn_l \quad (\text{Eq. 5})$$

Q_{CS} and Q_{CL} represent the creep activation energy of the two mechanisms respectively, which are obtained from Weertman's conventional creep tests. $\lambda^{(\alpha)}$ is a geometrical parameter, proportional to the reciprocal square root of the saturated dislocation density. $A_{CS}^{(k)}$ and $A_{CL}^{(k)}$ are model constants, representing the combined effect of self-diffusion, dislocation statistical distributions, swept length, etc., and are determined by curve fitting with the reported experiments. Detailed information about the calibration and verification of this model has been demonstrated in previous work (Jiang and Dasgupta, 2021).

The stress and the strain rate in slip system α can be related as $\mathbf{m}_{Sn}^{(\alpha)} : \boldsymbol{\sigma}_{Sn}^{(\alpha)} = \dot{\boldsymbol{\epsilon}}_{Sn}^{(\alpha)}$, where $\mathbf{m}_{Sn}^{(\alpha)}$ is the effective mobility of the selected systems. Since the shear rate $\dot{\gamma}^{(\alpha)}$ is dependent on the resolved shear stress $\tau_{re}^{(\alpha)}$ and not affected by other stress components, it is assumed that only the element $m_{Sn}^{(\alpha)}(1,2,1,2)$ or $(m_{Sn}^{(\alpha)})_{1212}$ and its symmetrical counterparts of the mobility tensor $\mathbf{m}_{Sn}^{(\alpha)}$ are non-zero.

5.3.2 Tier 1: Ag-Sn eutectic phase

The nano-scale Ag_3Sn particles embedded in the Sn matrix in the eutectic phase (Tier 1) effectively retard the movement of dislocations. Consequently, the creep resistance of the eutectic mixture is significantly increased, compared with that of the

pure β -Sn phase. The macroscopic viscoplastic deformation rate slows down since the dislocations arrested by the hard dispersoids need a certain amount of time to recover sufficient mobility. The possible mechanisms that dominate in dispersion-strengthened alloys has been extensively studied (Arzt, 1991; Arzt et al., 2001; McLean, 1985). The dependence of steady-state strain rate on stress is categorized into three distinct regions, based on the sensitivity (slope on a log-log plot) (Arzt et al., 2001), as illustrated in Fig. 3. In the low-stress Region III, the creep resistance of the dispersion strengthened is several orders of magnitude lower than that of the matrix, and various models have been proposed to explain the dislocation bypass process. As the stress increases, the stress-sensitivity of the strain rate sharply increases in Region II. At even higher stress levels (Region I), the dispersoids eventually lose their ability to obstruct the movement of dislocations, and the overall creep resistance of the alloy approaches that of the dispersion-free matrix. Due to insufficient experimental results, study of Region I is beyond the scope of this work.

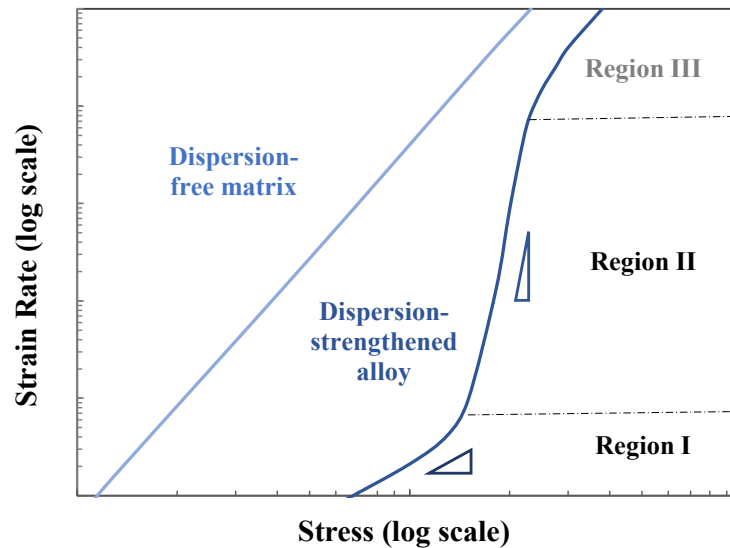


Figure 5.3 Schematic diagram of steady-state creep rate vs. applied stress in dispersion-strengthening alloys

The degree of dispersion strengthening in the Ag-Sn eutectic phase is modeled as the combined result of two competing governing recovery mechanisms (Sidhu et al., 2008): dislocation climb (Clegg and Martin, 1982) and dislocation detachment (Rösler and Arzt, 1990), as shown in Fig. 4. The overall creep rate $\dot{\gamma}_{Eut}^{(\alpha)}$ is assumed to be the sum of the two mechanisms (Ashby and Verrall, 1973), and is dominated by the higher one:

$$\dot{\gamma}_{Eut}^{(\alpha)} = \dot{\gamma}_{Eut_climb}^{(\alpha)} + \dot{\gamma}_{Eut_Detach}^{(\alpha)} \quad (\text{Eq. 6})$$

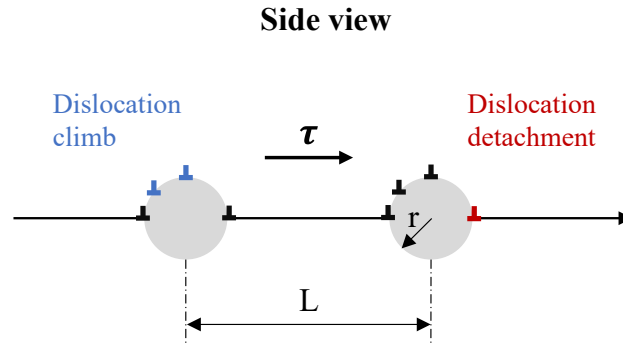


Figure 5.4 Schematic diagram of dislocation mechanisms in the Ag-Sn eutectic phase

The former mechanism assumes that the strain rate $\dot{\gamma}_{Eut_Climb}^{(\alpha)}$ is controlled by the climb of dislocations around particles:

$$\dot{\gamma}_{Eut_Climb}^{(\alpha)} = \gamma_1 \pi \rho_{sat}^{(\alpha)} L^2 \cdot \frac{G^{(\alpha)} b^{(\alpha)} D}{k_B T} \cdot \frac{b^{(\alpha)}}{r} \cdot \left(\frac{\tau_{re}^{(\alpha)}}{G^{(\alpha)}} \right)^2 \quad (\text{Eq. 7})$$

The latter is developed based on TEM (transmission electron microscopy) observations in some dispersion-strengthened alloys, where dislocations are trapped on the detachment side of the particle-matrix interface. The detachment threshold is

modeled as the governing dislocation barrier (strengthening mechanism) and the time taken for dislocations to move between particles is considered to be negligible. Since the detachment process is thermally activated, the strain rate $\dot{\gamma}_{Eut_Detach}^{(\alpha)}$ takes the form of the Arrhenius formula:

$$\dot{\gamma}_{Eut_Detach}^{(\alpha)} = \gamma_2 \cdot \frac{L\rho_{sat}^{(\alpha)}D}{b^{(\alpha)}} \cdot \exp\left(-\frac{G^{(\alpha)}(b^{(\alpha)})^2 r \left[(1-\kappa) \left(1 - \frac{\tau_{re}^{(\alpha)}}{\tau_d^{(\alpha)}} \right) \right]^{3/2}}{k_B T}\right) \quad (\text{Eq. 8})$$

The terms in the above equations are defined in the remainder of this section. r represents the average radius of nanoscale Ag_3Sn particles (~ 25 nm), based on image processing. $L = 2r\sqrt{\pi/6f_{\text{Ag}_3\text{Sn}}}$ is the mean planar spacing between Ag_3Sn particles (assuming a square lattice arrangement), where $f_{\text{Ag}_3\text{Sn}}$ is the volume fraction of Ag_3Sn particles in the eutectic phase. κ is a dislocation ‘relaxation parameter’ discussed later. The effective diffusivity D is given by:

$$D = D_0 \left[\exp\left(\frac{-Q_L}{RT}\right) + \exp\left(\frac{-Q_H}{RT}\right) \right] \quad (\text{Eq. 9})$$

where D_0 is a diffusivity constant (property of Sn); Q_L ($=31\text{kJ/mol/K}$) and Q_H ($=69\text{kJ/mol/K}$) represent the diffusion activation energy at low and high stress levels, respectively (Cuddalorepatta and Dasgupta, 2010). R is the universal gas constant, k_B is the Boltzmann constant and T is the temperature in Kelvin scale.

$\rho_{sat}^{(\alpha)}$ is the saturation dislocation density of the α -th slip system for steady state creep deformation, and is estimated as follows The evolution of mobile dislocation density in the eutectic phase is expressed as (Alexander and Haasen, 1969):

$$\dot{\rho}^{(k)}(t) = \rho^{(k)}(t) \cdot v^{(k)}(t) \cdot \delta^{(k)}(t) \quad (\text{Eq. 10})$$

$\rho^{(k)}(t)$, $v^{(k)}(t)$ and $\delta^{(k)}(t)$ are the instantaneous dislocation density, velocity, and multiplication rate at time t , respectively. It is assumed that $v^{(k)}(t)$ and $\delta^{(k)}(t)$ are linearly dependent on the difference between the resolved shear $\tau_{re}^{(k)}$ and the internal back stress (generated by the competitive process of dislocation impediment and recovery) (Mukherjee et al., 2016).

$$v^{(k)}(t) = v_0^{(k)} \left(\tau_{re}^{(k)} - k_3 \frac{G^{(\alpha)} b^{(\alpha)} N^{(\alpha)}}{L} \right) \quad (\text{Eq. 11})$$

$$\delta^{(k)}(t) = k_2 \left(\tau_{re}^{(k)} - k_1 \frac{G^{(\alpha)} b^{(\alpha)} N^{(\alpha)}}{L} \right) \quad (\text{Eq. 12})$$

where $k_1 = (1 - \beta)\zeta$, β and ζ are parameters describing the fraction of dislocations getting trapped during precipitate hardening and the fraction regaining mobility by recovery mechanisms; $k_3 = 0.9k_1$, and k_2 is a constant related to dislocation multiplication (Preußner et al., 2009). $N^{(\alpha)} = (1 - f_{Ag_3Sn})(\pi/6f_{Ag_3Sn})^{(2/3)} \rho^{(\alpha)}(t)L^2$ denotes the instantaneous number of dislocations pinned by Ag_3Sn dispersoids. The dislocation density finally saturates as $\dot{\rho}^{(k)}(t)$ approaches zero and the dislocations move at constant speeds, resulting in steady-state creep deformation at the macroscale.

The relaxation parameter κ ($0 \leq \kappa \leq 1$) in Eq. (8) describes the degree of attractive interaction between particles and dislocations, and is determined as a fitting parameter. The athermal detachment stress $\tau_d^{(\alpha)} = c\tau_{or}^{(\alpha)}\sqrt{1 - \kappa^2}$ in Eq. (8) represents the stress required for the dislocation to detach itself from the particle without the aid of thermal activation, and $\tau_{or}^{(\alpha)}$ is the Orowan stress in shear (Arzt and Göhring, 1998):

$$\tau_{Or}^{(\alpha)} = \frac{G^{(\alpha)}b^{(\alpha)}}{L-2r} \quad (\text{Eq. 13})$$

γ_1 and γ_2 are material constants to be determined through experiments. Although the best way to calibrate the proposed model within this length scale is to perform creep tests directly on this eutectic mixture, the experimental results are not yet available. Therefore, the Tier 2 model results are passed on to the next higher level (Tier 2) and finally calibrated based on the measured creep behavior of single crystal SAC solder. Similar to the β -Sn phase (Tier 0), the effective mobility tensor of the eutectic phase $\mathbf{m}_{Eut}^{(\alpha)}$ is determined for each slip system.

5.3.3 Tier 2: Homogenization in single crystal

In order to evaluate the overall creep resistance of a single SAC crystal, the load-sharing between the pro-eutectic β -Sn dendrite phase and the surrounding Ag-Sn eutectic phase is estimated. The pro-eutectic β -Sn dendrites are approximated as ellipsoidal inclusions embedded in the anisotropic Ag-Sn eutectic mixture. Therefore, Tier 2 is simplified to a two-phase composite material, where the contribution of the microscale intermetallic compounds of Cu_6Sn_5 rods is negligible. Although this assumption causes some loss of accuracy, results show that it is an acceptable approximation and can well capture the anisotropic creep response.

The effective mobility tensors $\mathbf{m}_{Sn}^{(\alpha)}$ and $\mathbf{m}_{Eut}^{(\alpha)}$ of each slip system are converted back to the crystal coordinate by the rotation matrix $\mathbf{Q}^{(\alpha)}$, and then added together for the β -Sn and eutectic phases, respectively:

$$\mathbf{m}_{Sn}^{xtal} = \sum \mathbf{m}_{Sn}^{xtal-\alpha} \quad (\text{Eq. 14})$$

$$\mathbf{m}_{Eut}^{Xtal} = \sum \mathbf{m}_{Eut}^{Xtal-\alpha} \quad (\text{Eq. 15})$$

The superscript “Xtal- α ” represents the variable of the slip system α in the crystal coordinate. Through Voigt’s reduced notion, the 4th order effective mobility tensors $\mathbf{m}_{Sn}^{Xtal}$ and $\mathbf{m}_{Eut}^{Xtal}$ are converted into 6*6 matrices, expressed as $\mathbf{M}_f$ and $\mathbf{M}_m$. The homogenized effective mobility $\mathbf{M}$ of the SAC crystal is then obtained by the Mori-Tanaka averaging scheme, which provides a direct evaluation in terms of individual phases and their volume fractions (Gavazzi and Lagoudas, 1990):

$$\mathbf{M} = \mathbf{M}_m + c_f(\mathbf{M}_f - \mathbf{M}_m)[-c_m \mathbf{V}_m \mathcal{S}(\mathbf{M}_f - \mathbf{M}_m) + c_m \mathbf{V}_m \mathbf{M}_f + c_f \mathbf{I}]^{-1} \quad (\text{Eq. 16})$$

where c_f and c_m are the volume fractions of inclusions (Sn dendrites) and matrix (eutectic Ag-Sn phase), and $\mathbf{V}_m$ is the effective viscosity matrix of the eutectic phase (the inverse matrix of $\mathbf{M}_m$). $\mathcal{S}$ is the Eshelby tensor, which relates the strain field in the heterogeneity (dendrite) to the eigenstrain of the equivalent inclusion (Eshelby, 1957). For ellipsoidal inclusions in anisotropic materials, the Eshelby tensor is derived through surface integral (Mura, 2013):

$$\mathcal{S}_{ijkl} = \frac{1}{8\pi} L_{0mnkl} \int_{-1}^{+1} d\zeta_3 \int_0^{2\pi} \{G_{imjn}(\bar{\xi}) + G_{jmin}(\bar{\xi})\} d\omega \quad (\text{Eq. 17})$$

where,

$$\begin{aligned} G_{ijkl}(\bar{\xi}) &= \bar{\xi}_k \bar{\xi}_l N_{ij}(\bar{\xi}) / D(\bar{\xi}), \quad \bar{\xi}_i = \zeta_i / a_i, \\ \zeta_1 &= (1 - \zeta_3^2)^{1/2} \cos \omega, \quad \zeta_2 = (1 - \zeta_3^2)^{1/2} \sin \omega, \quad \zeta_3 = \zeta_3, \\ D(\bar{\xi}) &= \varepsilon_{mnl} K_{m1} K_{n2} K_{l3}, \quad N_{ij}(\bar{\xi}) = \frac{1}{2} \varepsilon_{ikl} \varepsilon_{jmn} K_{km} K_{ln}, \quad K_{ik} = \\ &L_{0ijkl} \bar{\xi}_j \bar{\xi}_l, \end{aligned}$$

The value of $\mathcal{S}_{ijkl}$ is estimated numerically by the Gaussian quadrature formula (Gavazzi and Lagoudas, 1990), as shown below:

$$\mathcal{S}_{ijkl} = \frac{1}{8\pi} \sum_{p=1}^M \sum_{q=1}^N L_{0mnkl} \left\{ G_{imjn}(\omega_q, \zeta_{3p}) + G_{jmin}(\omega_q, \zeta_{3p}) \right\} W_{pq} \quad (\text{Eq. 18})$$

5.3.4 Calibration of CV model constants with single-crystal experiment

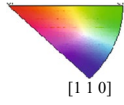
The total strain rate in the crystal coordinates is first calculated from the homogenized effective mobility matrix $\mathbf{M}$ and the stress tensor $\boldsymbol{\sigma}$ applied to the crystal. The strain rate is then transferred back to specimen global coordinates through the Euler angle rotation matrix $\mathbf{O}$. The room temperature TMM test result of a single-grain SAC sample (Cuddalorepatta et al., 2010) is modeled by the above-mentioned crystal viscoplasticity approach and used to determine the model constants. Parameters used in the crystal viscoplasticity method are summarized in Table 5-1.

Fig. 5 provides the EBSD image of the TMM specimen used for calibration and the average Euler angles of the grain that occupied almost the entire joint. The specimen is assumed to be under pure shear loading, the shear stress is calculated by dividing the applied force by the cross-sectional area, and the strain rate is determined by dividing the deformation rate by the joint height. The strain rates of the calibrated Ag-Sn eutectic phase (Tier 1) along slip directions, a combined result of the two competing mechanisms, are plotted in Fig. 6. The difference between slip systems is up to 7 orders of magnitude, depending on the applied stress state and the facileness of the slip system itself. The calibration is indeed deficient, both in terms of number of specimens and testing conditions. Additional single-grain specimens are currently being prepared and are planned to be tested at different temperatures, which falls

within the scope of future work. However, since the main purpose of this work is to formulate this multiscale modeling strategy and to verify its applicability to microscale solder joints made of SAC alloys, the current calibration results are accepted as a precursor in this regard. Detailed calibration results will be provided later, after sufficient new data have been collected.

Table 5-1 Model parameters used for crystal viscoplasticity modeling

Symbol	Value	Unit	Meaning	Reference
R	8.314	$\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$	Universal gas constant	-
k_B	1.38E-23	$\text{J}\cdot\text{K}^{-1}$	Boltzmann constant	-
r	25	nm	Average radius of Ag_3Sn particles	(Cuddalorepatta and Dasgupta, 2010)
$f_{\text{Ag}_3\text{Sn}}$	0.05		Volume fraction of Ag_3Sn particles in the eutectic phase	(Cuddalorepatta and Dasgupta, 2010)
D_0	1E-4	$\text{m}^2\cdot\text{s}^{-1}$	Diffusivity constant	(Cuddalorepatta and Dasgupta, 2010)
β	0.5		Dislocation recovery parameter	(Mukherjee et al., 2015)
ζ	0.1		Precipitate hardening parameter	(Mukherjee et al., 2016)
c	1.5		Geometric factor	Current work
κ	0.976		Relaxation parameter	Current work
γ_1	1.6E-12		Constant for dislocation climb	Current work
γ_2	1.98E-7		Constant for dislocation detachment	Current work
c_f	0.55		Volume fraction of Sn dendrites	(Mukherjee et al., 2016)
c_m	$1 - c_f$		Volume fraction of eutectic phase	-



Average Euler angles $\{\varphi_1 = 52.69^\circ, \Phi = 50.38^\circ, \varphi_2 = 24.78^\circ\}$

Figure 5.5 EBSD inverse pole figure map of the single-grain TMM specimen used for calibration

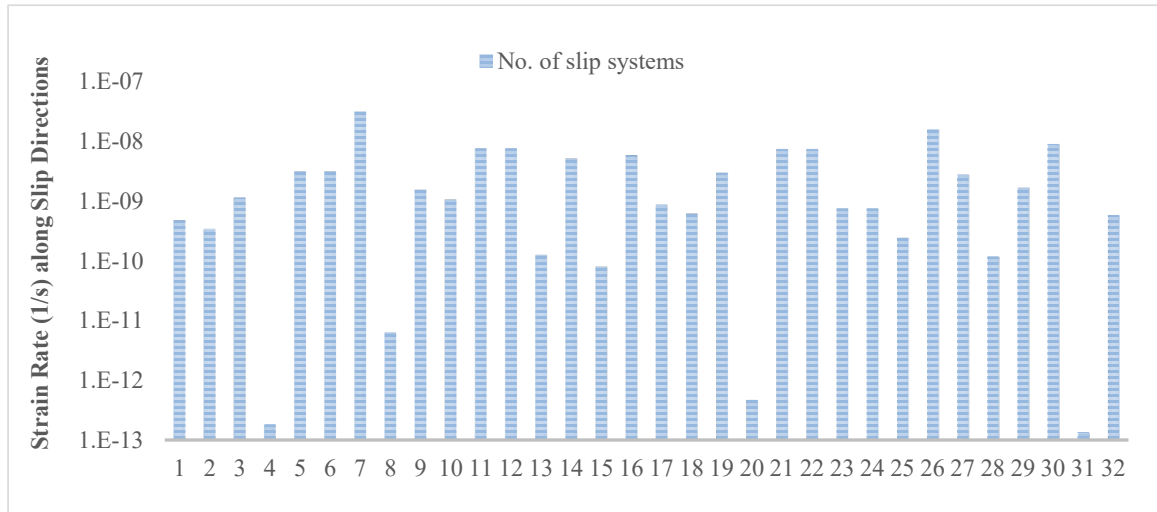


Figure 5.6 The overall strain rate of Tier 1 ($\dot{\gamma}_{Eut}^{(\alpha)}$) along the slip system

5.4 Continuum Creep-constitutive Model

Having derived the crystal-viscoplasticity model for SAC single crystals, this hierarchical modeling framework can be implemented in numerical simulations as it directly relates the steady-state strain rate to a given stress state and temperature, based on the dislocation motion on facile slip systems. This behavior of a SAC grain can then be represented in anisotropic continuum formulations, as an effective homogenized anisotropic material with principal mechanical axes coinciding with the crystal principal axes. This representation allows 3D computational analysis (e.g., with Finite element analysis) for engineering grain-scale analysis. The Hill's potential is used to represent the crystallographic anisotropy of creep resistance, while the Garofalo model is used to describe the general flow-rule between the steady-state effective strain rate and the effective stress state. The advantage of the Garofalo model is that it allows modeling of multiple deformation regimes (and mechanisms) where the stress sensitivity of the strain-rate gradually transitions from a lower sensitivity to a higher sensitivity. The identification of the associated model constants for the anisotropic potential and creep flow rule are achieved by using the crystal-viscoplasticity model of Section 5.3 as a virtual test capability.

5.4.1 Hill-Garofalo constitutive model for anisotropic steady-state creep

As a straightforward extension of the von Mises stress for isotropic materials, the Hill effective stress σ_{Hill} for anisotropic materials in complex stress state is defined as:

$$\sigma_{Hill} = \sqrt{F(\sigma_{22} - \sigma_{33})^2 + G(\sigma_{33} - \sigma_{11})^2 + H(\sigma_{11} - \sigma_{22})^2 + 2L\sigma_{23}^2 + 2M\sigma_{13}^2 + 2N\sigma_{12}^2}$$

(Eq. 19)

where F, G, H, L, M and N are dimensionless parameters representing directional characteristics, and are usually determined experimentally for some specific loading directions (Baral et al., 2018; Hill, 1948; Khan and Liu, 2012; Park et al., 2017). Higher values indicate greater creep resistance along this direction, and the underlying isotropic state is recovered when all parameters are equal. The material principal axes (1-2-3 coordinate system) are assumed to coincide with the principal crystal directions $\{[1\ 0\ 0], [0\ 1\ 0], [0\ 0\ 1]\}$. Due to the symmetry of the crystal structure, $[1\ 0\ 0]$ and $[0\ 1\ 0]$ are equivalent to each other. Therefore, we have $F = G$ and $L = M$ for current work. This leaves only 4 independent Hill constants that require 4 sets of mechanical tests for 4 independent stress states. The corresponding work-conjugate creep strain rate is defined by the gradient of the Hill effective stress in the stress space:

$$\dot{\epsilon}_{ij} = \frac{\partial \sigma_{Hill}}{\partial \sigma_{ij}} \dot{\epsilon}_{eq} \quad (\text{Eq. 20})$$

where Hill equivalent creep strain rate $\dot{\epsilon}_{eq}$ is a scalar multiplier, analogous to the von Mises equivalent strain rate used for isotropic materials. The magnitude of $\dot{\epsilon}_{eq}$ depends on the associated flow rule, which relates the strain rate to the stress under steady-state conditions. Power-law creep is commonly observed at low stress levels, and this power-law is commonly seen to breakdown in creep testing of SAC solder joints, with a different (higher) stress exponent at above this breakdown stress level. The sine-hyperbolic Garofalo model is traditionally applied to describe the overall behavior over a wide range of stress:

$$\dot{\epsilon}_{eq} = A(\sinh(\alpha\sigma_{Hill}))^n \exp\left(-\frac{Q_G}{RT}\right) \quad (\text{Eq. 21})$$

substituting (Eq. 19) into (Eq. 20), the work-conjugate strain-rate tensor is given by:

$$\dot{\epsilon}_{ij} = \frac{\partial \sigma_{Hill}}{\partial \sigma_{ij}} \dot{\epsilon}_{eq} = \dot{\epsilon}_{eq} \cdot \frac{1}{\sigma_{Hill}} \begin{bmatrix} G(\sigma_{11} - \sigma_{33}) + H(\sigma_{11} - \sigma_{22}) \\ F(\sigma_{22} - \sigma_{33}) + H(\sigma_{22} - \sigma_{11}) \\ G(\sigma_{33} - \sigma_{11}) + F(\sigma_{33} - \sigma_{22}) \\ 2N\sigma_{12} \\ 2M\sigma_{31} \\ 2L\sigma_{23} \end{bmatrix} \quad (\text{Eq. 22})$$

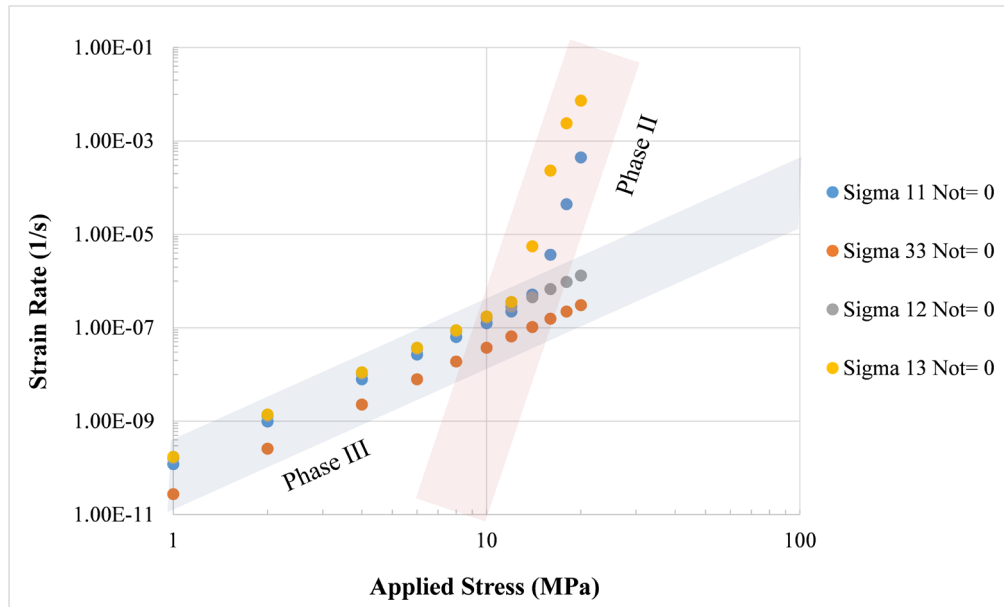
Thus, the continuum creep constitutive model can be fully defined when the 4 independent Hill constants and 3 Garofalo constants are estimated from suitable experiments under different independent stress states. Fabrication of single crystal specimens and the application of 4 independent stress states along the crystal principal coordinates is a challenging experimental task. As a convenient proxy, this paper uses the calibrated CV model as a virtual test tool.

5.4.2 Virtual testing under simple stress conditions

Since the calibrated crystal viscoplasticity model can predict the secondary creep response for a given stress condition, it offers the possibility to identify the anisotropy (Hill constants). Four fundamental stress conditions, consisting of uniaxial and pure shear loading along principal directions, are selected as input stress states. The principal loading axes $\{1,2,3\}$ are aligned with the crystal directions $\{[1\ 0\ 0], [0\ 1\ 0], [0\ 0\ 1]\}$, respectively. Fig. 7 shows the four corresponding strain rates predicted by the CV model along the loading direction, for selected stress conditions at room temperature. The secondary creep results measured from a set of TMM creep tests

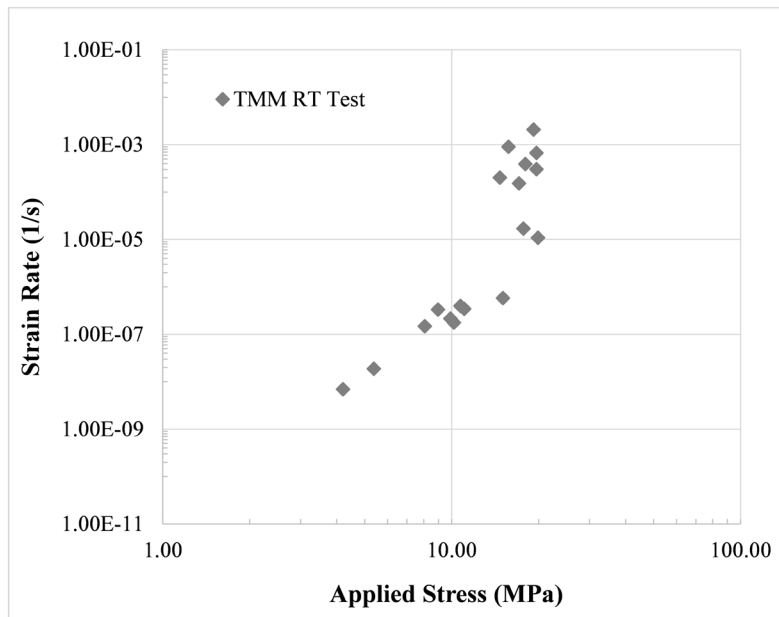
are also provided with 'x' symbols, for purposes of comparison. The condition "only $\sigma_{33} \neq 0$ " (corresponding to the uniaxial stress applied along the $[0\ 1\ 0]$ direction of the crystal) shows the highest creep resistance over the entire stress range. In the low-stress region, the predicted strain rates for the other three loading conditions are almost the same. With the increase of stress, the stress exponent for the "only $\sigma_{11} \neq 0$ " and "only $\sigma_{13} \neq 0$ " conditions increase dramatically, indicating that the dislocation detachment mechanism gradually dominates in some of the dominant slip systems. In contrast, the stress-sensitivity of the response for the other two stress conditions remains unchanged and is still governed by the dislocation climb mechanism. In the high-stress region, the strain rate difference between conditions may exceed four orders of magnitude. This reasonably explains the experimental observation that the dispersion of the data at low stresses is much smaller than that at high stresses. Not only is the strain rate extremely sensitive to the stress for dislocation detachment process, but there are also two creep mechanisms present simultaneously, depending on the grain orientation. The test data are close to or even higher than the upper limit predicted by the crystal viscoplasticity model. One possible reason is that the current predictions are for single crystals, while TMM grain-level specimens typically exhibit an oligocrystalline structure that includes deformation of grain boundaries. Another reason comes from the distribution of the grain orientation: assuming that the grain orientation is randomly distributed, the probability of the loading axis aligning parallel to the stiff crystal direction $[0\ 0\ 1]$ is smaller than the probability that it is not (Akbari et al., 2019).

Outputs of Crystal Viscoplasticity Model



(a)

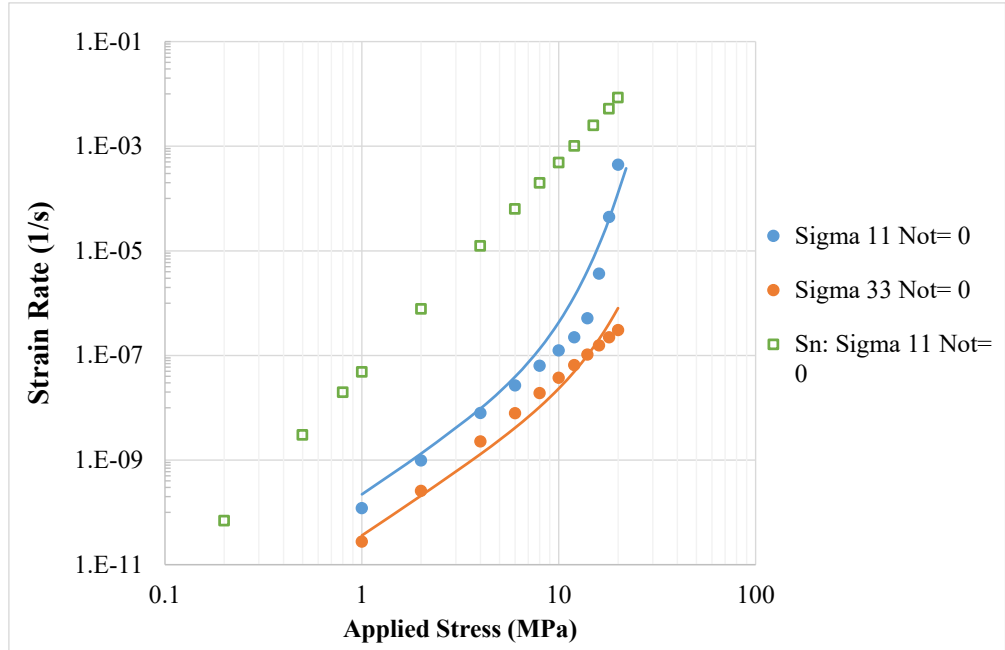
TMM Shear Tests



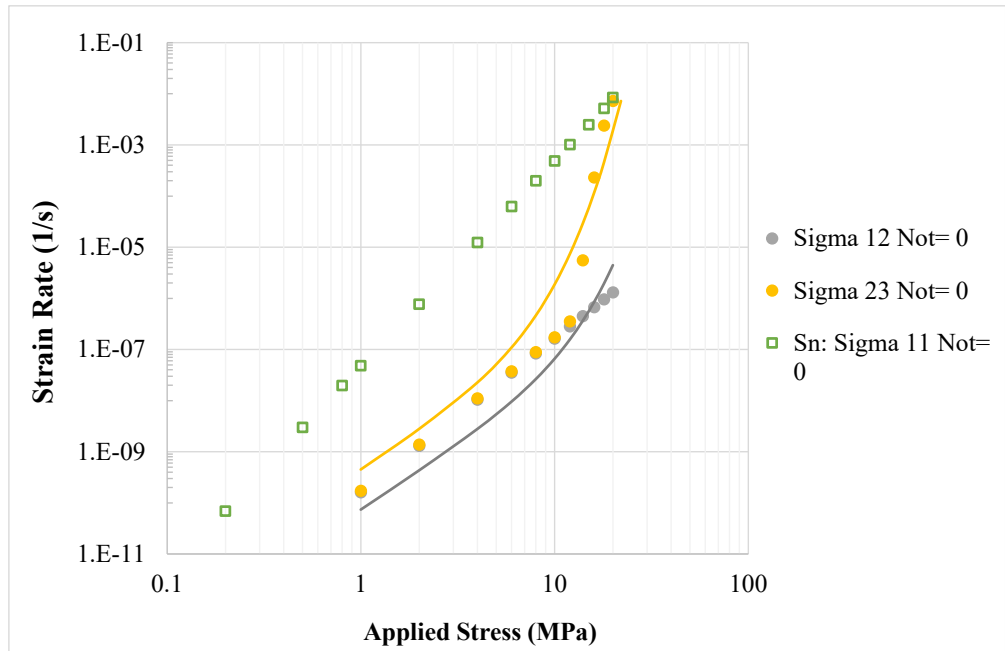
(b)

Figure 5.7 (a) Virtual testing from the crystal viscoplasticity model, strain rates along the loading directions; (b) Room temperature (RT) shear tests on grain-scale TMM specimens

The predictions discussed above can serve as a virtual testing method. Since there is only one non-zero stress component per set of tests, the creep resistance anisotropy along the principal direction is identified, in conjunction with the Garofalo creep law that regulates the overall relationship between the effective stress and the equivalent strain rate. Due to the limited tests available for the calibration of the crystal viscoplasticity model, we assume that the anisotropy of creep resistance is independent of temperature and stress level. The activation energy of the Garofalo model is adopted from a previous study (Cuddalorepatta et al., 2010). The fitting results are shown in Fig. 8 and the corresponding parameters are listed in Table 2 and 3. The fits to the "only $\sigma_{11} \neq 0$ " and "only $\sigma_{13} \neq 0$ " conditions show reasonable agreement with the virtual test results at extreme stress levels. However, in the transition region, the Garofalo formulation is unable to switch sufficiently sharply from the low stress-regime to high-stress regime, resulting in an overestimation of the strain rates (relative to the CV virtual test results). Although the current fit is not fully representative of the virtual test results over the entire stress range, as both temperature and stress levels may affect the anisotropy of creep resistance, it is still appropriate as a preliminary approximation to incorporate an anisotropic constitutive creep flow rule. Future work will focus on the variation of creep anisotropy as the dominant mechanism gradually shifts with stress and temperature.



(a)



(b)

Figure 5.8 Homogenized Hill-Garofalo fitted to virtual testing of the fundamental stress state

Table 5-2 Normalized Hill anisotropic constants

$F = G$	H	$L = M$	N
1	4.56	4.15	1.49

Table 5-3 Garofalo model constants

A	α	n	Q_G
22.75	0.09546	2.5	55793

5.5 Numerical Simulation

The Hill-Garofalo constitutive model bridges the gap between crystal viscoplasticity and numerical simulations, allowing not only for efficient parametric study, but also for modeling polycrystalline solder joints in packaging and assembly analysis. Although the exact microstructure of a particular joint is unknown prior to cross-sectioning, and it is impractical to model each joint individually based on their grain structure, parametric studies can estimate the degree of variation caused by grain orientation and arrangement, thus providing a method to quantify possible range of stochastic uncertainties in creep predictions, caused by stochastic distribution of grain structures.

As an example of the applications, the calibrated anisotropic continuum model is applied to parametrically analyze the effect of grain orientation on the deformation of a critical solder joint subjected to combined constants vertical compression (due to heat-sink clamping force) and horizontal cyclic shear (due to thermal cycling loads). The model is described in detail in Section 5.5.1. The simulation is based on two common failure modes encountered in the experiments: (i) electrical shorts caused by lateral solder bridging (Section 5.5.2) because of the vertical compression; and (ii) open circuits caused by solder fatigue damage because of the thermal cycling deformations (Section 5.5.2).

5.5.1 Finite element model of single-grain area-array joint

Solder bridging is an increasing risk in area array interconnects, as the pitch size continuously decreases due to miniaturization of electronic circuits and with the

development of 3D architectures for heterogeneous integration. This risk of shorts is exacerbated due to progressive lateral expansion of solder balls, when they experience cyclic ratcheting (due to thermal cycling deformations) in the presence of a steady out-of-plane compressive bias load (due to assembly warpage, components located above and heat-sink clamping forces).

The schematic drawing of a chip-scale package (CSP) with a heat sink above it is depicted in Figure 5.9 (a). Solder joints are subjected to both cyclic shear load and steady vertical compressive load, which are caused by the mismatch of the coefficient of thermal expansion (CTE) between adjacent materials/structures, and the heat-sink clamping force exerted for better heat dissipation, respectively. The solder joints experience significant cyclic ratcheting deformation under the action of these combined loads, resulting in progressive inelastic lateral expansion. In severe cases, the solder joints may eventually make contact with adjacent joints, leading to electrical short-circuit faults. The failure analysis (cross-section images) in Figure 5.9 (b) reveals different degrees of diameter expansion in solder joints of the same batch, resulting from the piece-to-piece variability of the SAC joints. The current study focuses on the influence of solder crystal orientation on the severity of the lateral expansion.

The critical corner joint of the CSP assembly is selected for local modeling, as illustrated in Figure 5.9 (c). Two coordinate systems are involved in this simulation: the global X-Y-Z structural coordinate system, which specifies the part positions and loading conditions for the entire domain, and the local a-b-c system, which represents the crystal principal directions $\{[1\ 0\ 0], [0\ 1\ 0], [0\ 0\ 1]\}$. To explore the limiting

extreme-case scenario, the critical solder joint is assumed to be a single-crystal with the principal directions aligned with the global coordinate system. Only half of the BGA joint is modeled due to symmetry. Both top and bottom surfaces of the joint are connected to Cu pads (colored in red in the figure).

The vertical load is simplified as a constant pressure uniformly distributed on the top Cu pad (10 MPa) and the CTE mismatch is represented by cyclic horizontal displacement of the top pad relative to the bottom pad, along the global X-axis. The magnitude of deformation is estimated based on the distance of the solder ball center to the neutral point of the CSP package. The cyclic temperature imposed on the package ranges from 233 K to 398 K, and the initial stress-free temperature is set to 398 K. The profiles of cyclic temperature and horizontal deformation are provided in Figure 5.9 (c).

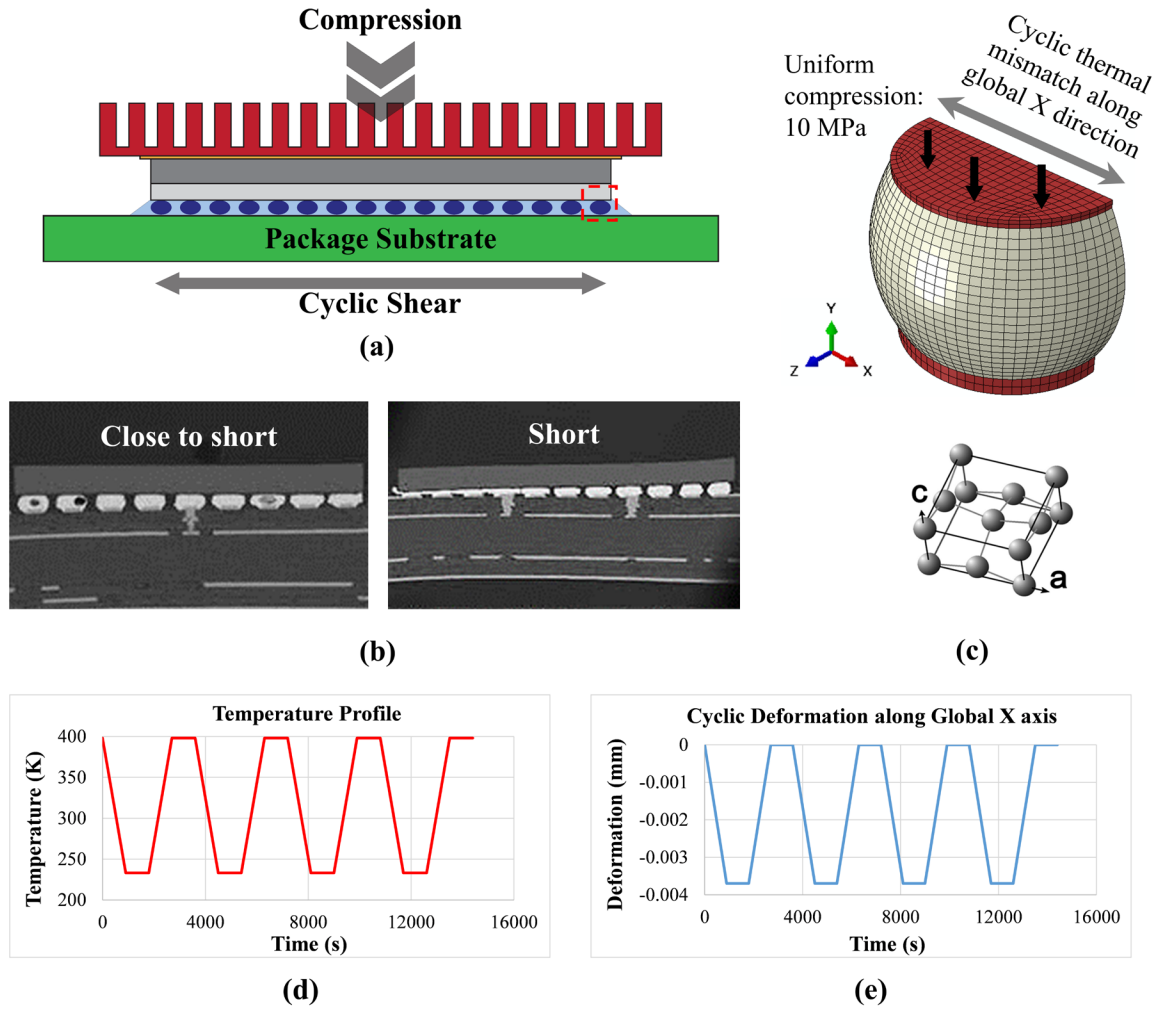


Figure 5.9 Critical BGA joint in WLCSP assembly: (a) Schematic drawing of a WLCSP; (b) Solder bridging observed in experiments; (c) Geometry and mesh of the BGA joint; (d) Profiles for temperature cycling and horizontal deformation

5.5.2 Effects of grain orientation on lateral expansion of solder ball

The initial diameter of the solder joint modeled here is 290 μm . The horizontal distance between the two outermost nodes in the cross-section (Figure 5.10 (a)) is monitored as the diameter of the deformed joint during cycling. Since the a- and b-axes of the crystal are equivalent to each other, three orthogonal grain orientations are considered in the parametric study by aligning the crystal c-axis sequentially with each of the three structural global axes, as illustrated in Figure 5.10.

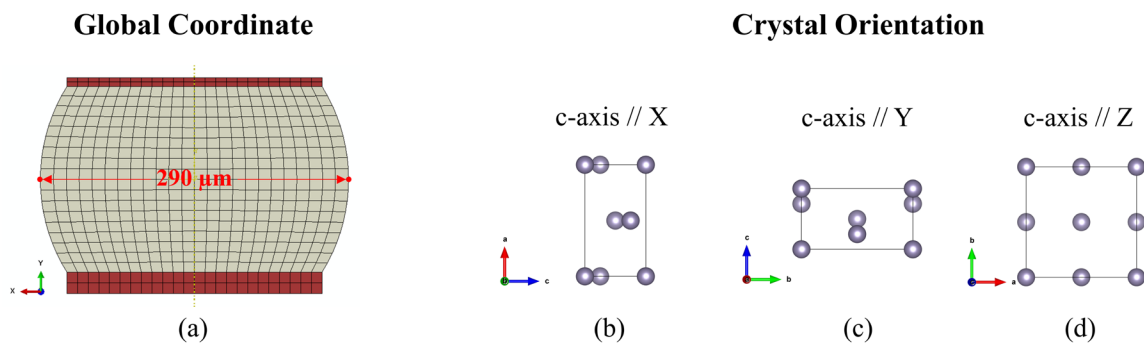


Figure 5.10 In parametric studies, the crystal orientation is sequentially aligned with respect to the global coordinates

The values and percentage of diameter change during the first four cycles are plotted in Figure 5.11. As expected, when the c-axis is parallel to global Y, the most creep-resistant direction coincides with the compressive load and the diameter expansion is minimal. Since the vertical compression deformation in this case is much smaller than in the other two cases, the expansion in the direction perpendicular to the compression load is also smaller according to the Poisson effect. For the remaining two cases with similar creep resistance to vertical compression, the diameter expansion is larger in the YZ plane when the c-axis is parallel to X. The double side arrows indicate the change in horizontal expansion due to grain

orientation, which provides the upper and lower limits of this problem. A similar approach can be used to estimate the variability in the risk of solder bridging in actual tests, under given conditions.

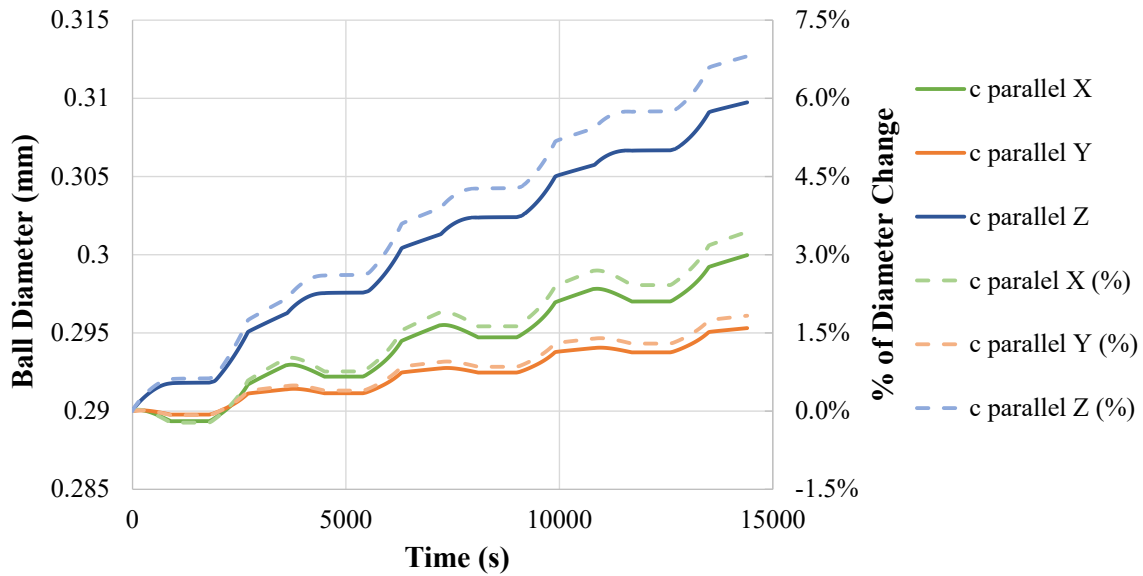


Figure 5.11 Effect of grain orientation on the diameter expansion of the critical single-grain solder joint

5.5.3 Effects of grain orientation on thermal cycling fatigue durability

Figure 5.12 shows multiple views of the contour plots of the creep dissipation energy density at the end of the 4th cycle. Although the creep energy density is mostly localized on the surface connected to the Cu pads, the maximum value occurs on the bottom surface when c-axis is parallel to global X direction, and on the top surface for the other two orientations. Since the maximum value depends on the mesh density, a local volume averaging technique is applied to the two layers of peripheral elements. The selection of elements, whether on the top or bottom surface, is based on the concentration of energy density and are highlighted with mesh in Fig. 9. The thickness of the selected double-layer elements is about 18 μm . The volume-averaged

creep dissipation energy density is plotted as a function of time in Figure 5.13. While the locations of the energy density concentrations vary considerably, the average values of the peripheral elements are fairly similar when the c-axis is parallel to X and Z. When the c-axis is parallel to Y, creep resistance is higher along the loading direction, which can effectively reduce the amount of extrusion caused by compression and minimize the overall deformation of the joint.

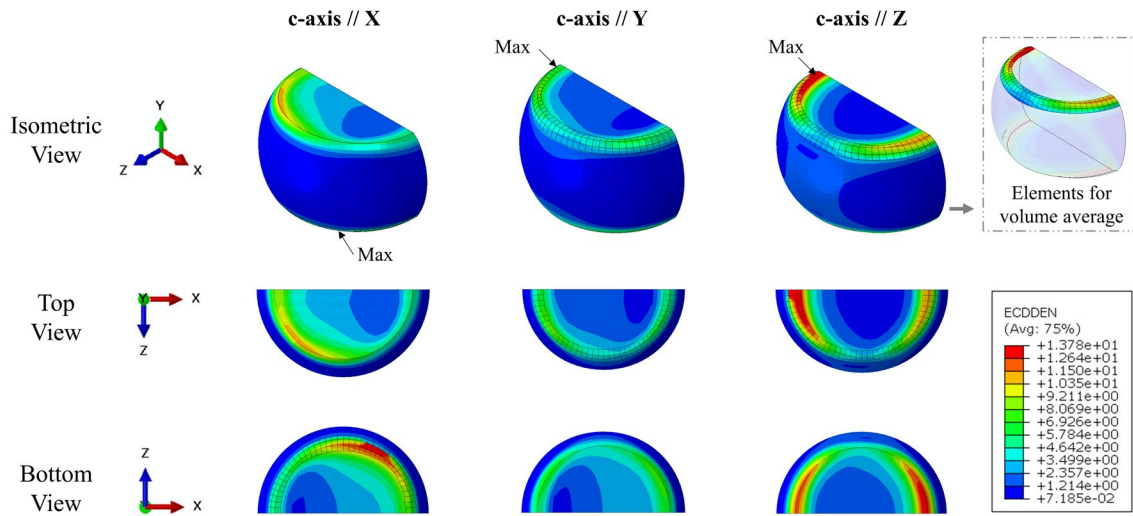


Figure 5.12 Contour plots of creep dissipation energy density at the end of the 4th cycle

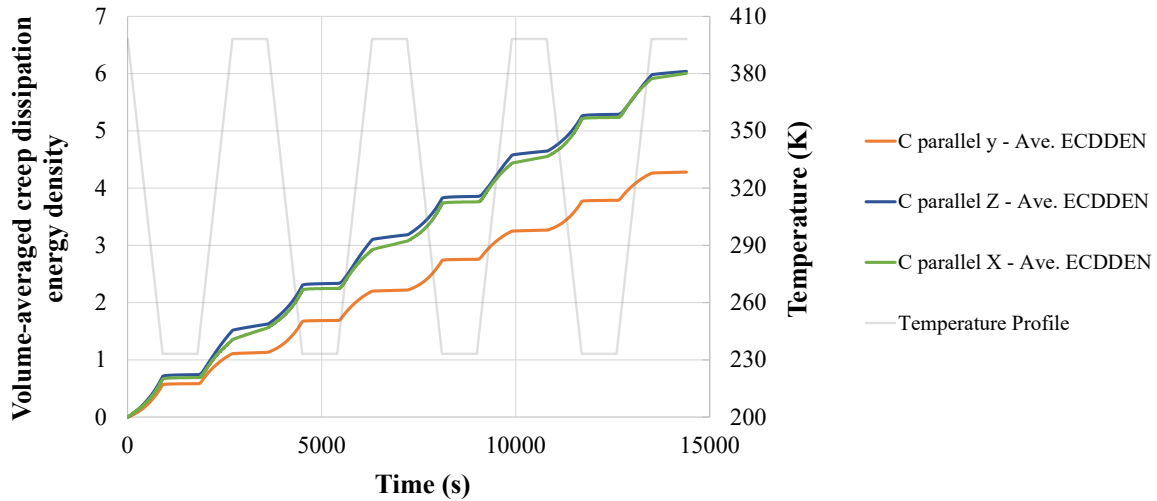


Figure 5.13 Volume-averaged creep dissipation energy density of selected double-layer peripheral elements

Various models have been proposed in the solder literature for fatigue durability assessment (Dasgupta et al., 1992; Lee et al., 2000; Syed). The fatigue durability model used here has a linear dependence on the inverse of the dissipated creep energy density (Syed). The volume-averaged creep energy density dissipated in the 4th cycle is used here to estimate the dependence of fatigue durability on the compression from the heat-sink. The predicted durability numbers are normalized to the least durable case (c-axis parallel to Z, no compression force) and summarized in Figure 5.14. In the presence of the heat sink compression, the fatigue durability is almost similar when c-axis is aligned parallel to global X and Z directions (difference is as small as 4%). When the c-axis is aligned parallel to Y, the fatigue durability increases by about 43%. When the compressive load of the heat-sink is removed, the durability decreases by approximately 8% and 6%, respectively, when the c-axis is oriented parallel to Y and Z directions, but increases by 6% when the c-axis is parallel to X. According to the parametric study, the addition of compressive force due to the heat-

sink is expected to increase the mean expected value of thermal cycling fatigue failures (average of the three orientations) by 4% and increase the stochastic variability (the largest difference between the three orientations) by 31%.

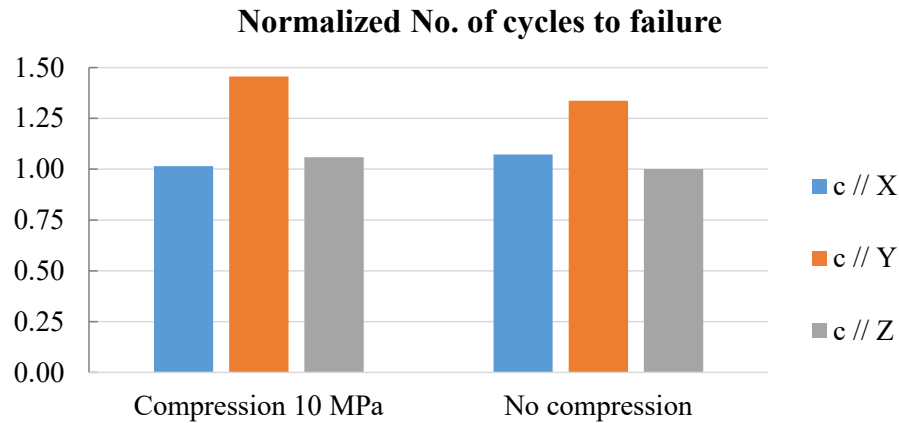


Figure 5.14 Normalized lifetime prediction by volume-averaged creep dissipation energy density in the 4th cycle, for the case with and without compression

The contours of the creep dissipation energy density are replotted in Figure 5.15, to highlight the regions of highest work dissipation ($> 3 \text{ N-m/mm}^3$). These are expected to be the regions of maximum fatigue damage. When the c-axis is parallel to X, the high damage region is predicted to be localized near the two surfaces connected to the Cu pads. However, when c-axis is parallel to Z, the high damage region also propagates into the center of the joint. These predicted damage modes appear to agree with experimental observations reported by Yu and his colleagues (Yu et al.). They identify two thermal cycling damage regions after applying vertical compression to the package, as shown in Figure 5.16: damage propagation diagonally through the height of the joint and damage propagating along the Cu pad/solder interface, either close to the component side or close to the PCB side. Needless to say, the solder joints studied by them may be oligocrystalline and may have had additional

damage mechanisms at grain boundaries. This will be the subject of a future paper where we will report on grain-scale modeling of oligocrystalline joints. In summary, current single-grain modeling based on anisotropic properties appears to provide surprisingly detailed insight into the variability of thermo-mechanical response and failure modes for SAC solder joints due to potential variability of grain orientation. Such insights are not possible from conventional modeling using isotropic properties.

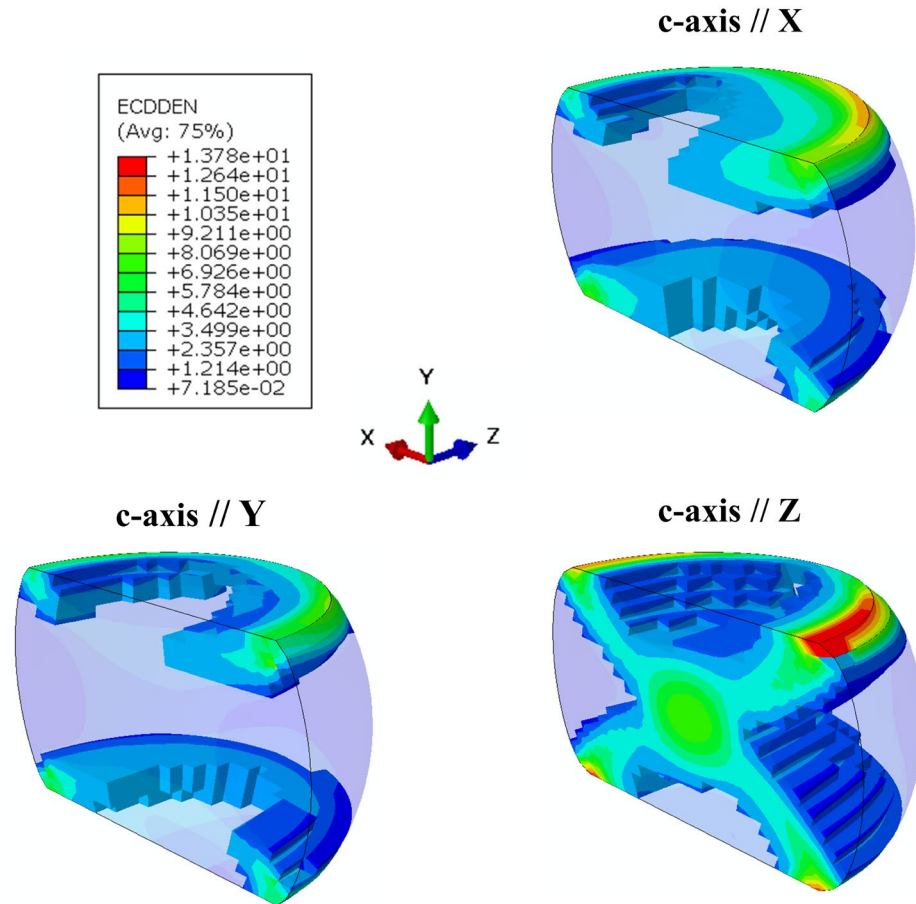


Figure 5.15 Contour plot of creep dissipation energy density at the end of the 4th cycle, elements with creep dissipation energy density less than 3 MPa are set as translucent.

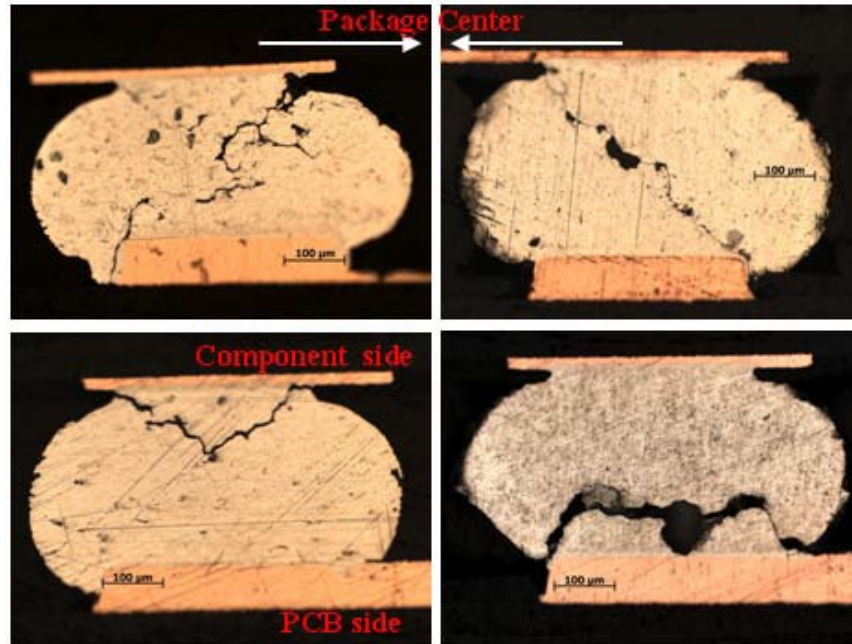
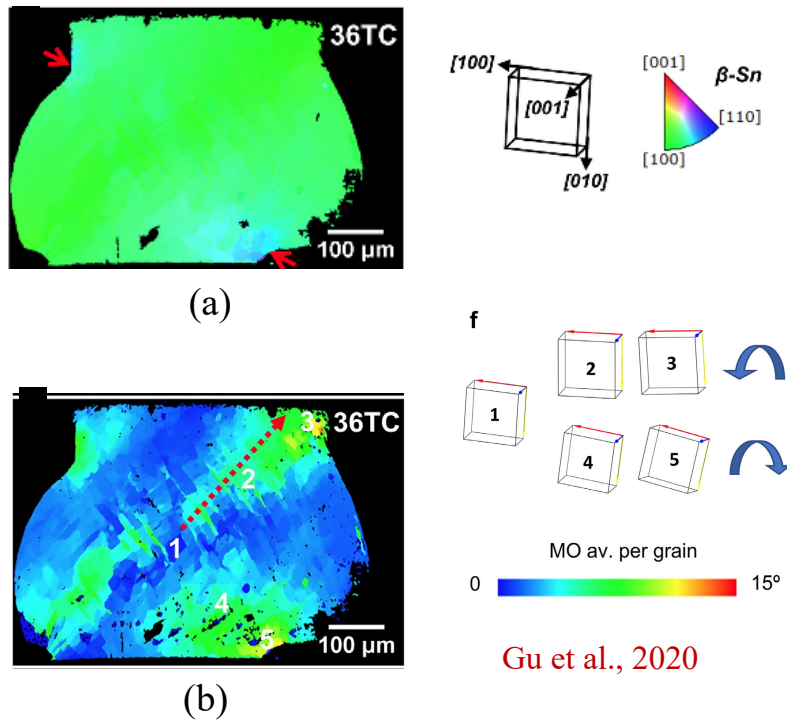


Figure 5.16 Contour plot of creep dissipation energy density at the end of the 4th cycle, elements with creep (Yu et al., 2011)

The experimental results of previous studies clearly show that solder joint damage depends on the crystal orientation. The damage path may vary considerably with the crystal stiff direction for single-crystal specimens under thermal cycling (without vertical compression). Gu and her colleagues studied a single-crystal Cu/SAC305/Cu solder joint under in-situ thermal cycling conditions using EBSD, where the c-axis is approximately 20° from the substrate plane (Gu et al., 2020). The EBSD maps demonstrate that the regions of highest amount of localized lattice rotation (precursor of sub-grain formation and recrystallization) propagates obliquely in the bulk of the joint, as shown in Figure 5.17 (a) and (b). In contrast, in the single-crystal specimen studied by Chen et al. (2011a), where the c-axis is almost vertical in the cross-sectional plane, sub-grain boundaries and recrystallization are observed to form

laterally near interface with the bonding pads, as shown in Figure 5.17 (c) and (d). Semi-quantitative similarities were found between the anisotropic single-grain simulations and experimental observations. When the stiffest direction (c-axis) is rotated from being parallel to Z to being parallel to the Y, the localization of the equivalent creep strain (CEEQ) in the solder joint under thermal cycling (without vertical compression) changes, accordingly, as shown in Figure 5.18. This dependence on orientation is clearly absent in homogeneous isotropic modeling and analysis. The similarity in localization zones within crystal provides further qualitative confidence in the simulation results.



Gu et al., 2020

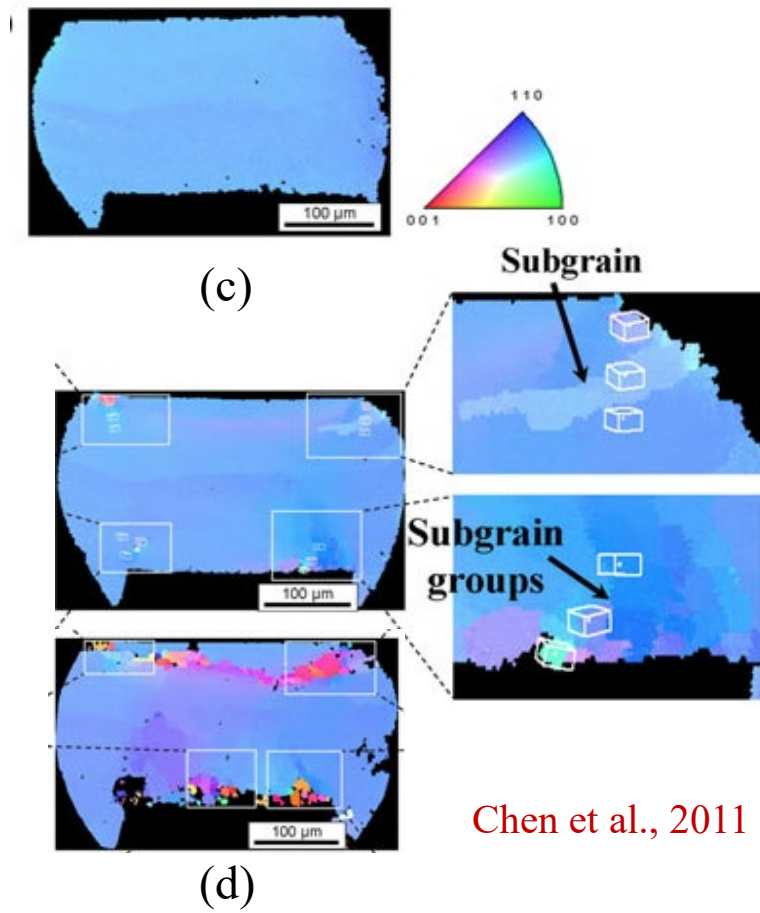
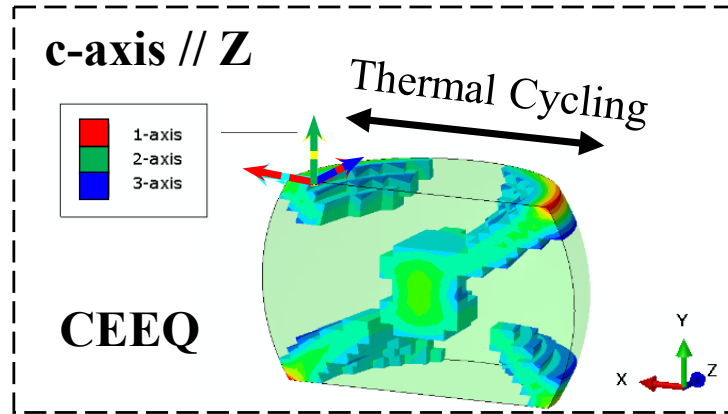
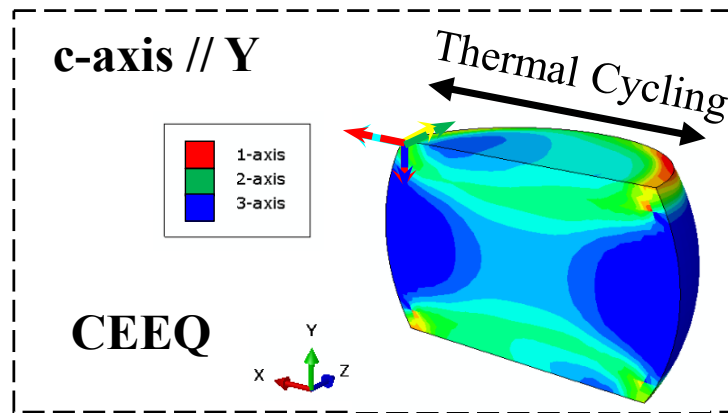


Figure 5.177 Solder joint under thermal cycling: (a) EBSD IPF-LD of a single-grain SAC305 joint, the loading direction in the map is horizontal. (b) Misorientation of (a) (Gu et al., 2020) (c) EBSD orientation map of an as-reflowed single-crystal joint.(d) After thermal cycling, orientation evolution occurred, leading to the formation of high-angle boundaries and recrystallization. (Chen et al., 2011a),



(a)



(b)

Figure 5.188 Contour of equivalent creep strain at the end of the 4th cycle for solder joint under thermal cycling: (a) c-axis is parallel to Z, (b) c-axis is parallel to Y

5.6 Summary and Conclusion

This paper focuses on a hierarchical multi-scale modeling framework for anisotropic steady-state creep of SAC crystals, from crystal viscoplasticity based on dislocation mechanics, to continuum constitutive model used in finite element (FE) analysis. The multiscale crystal viscoplasticity approach is motivated by the heterogeneous microstructure within oligocrystalline SAC solder joints, where deformations at different scales are dominated by different mechanisms. The mean effect of dislocation motion, in conjunction with microstructural features, is used to describe the effective macroscale viscoplastic flow. The selection of appropriate mechanisms is based on experimental observations and analysis, followed by calibration at the length scales for which tests are available. A continuum-scale compact anisotropic creep model, which combines Hill's anisotropic potential and Garofalo creep flow-law, is extracted from the predictions of the CV method under basic stress conditions. This methodology enables computationally-efficient FE simulations of solder joints in microelectronic assemblies and facilitates parametric sensitivity studies of different grain orientations. As one example, the corner ball in area-array assemblies subjected to compressive loading under thermal cycling is modeled a single-crystal interconnection with different grain orientations. The fatigue life prediction based on creep dissipation energy density and the estimation of horizontal expansion provide upper and lower limits for the variability of the corresponding failure modes.

Given the stochastic variation in the grain structure of SAC solder joints, grain-scale modeling with anisotropic properties is seen to provide an efficient way to

estimate the variability of thermomechanical response and helps to reduce the number of physical tests. Rather than modeling specific grain structure of specific joints, the focuses is on stochastic parametric studies to quantify the variability of solder joint behavior, caused by stochastic variability in grain orientation. the sparsity of the results and the extent of subsequent effects. In addition, since the crystal viscoplastic approach is based on explicit parameters in the microstructure (e.g. morphology of the eutectic and dendritic regions, grain orientation, etc), it can be used to predictively assess the effects of life-cycle factors that lead to microstructural changes, such as doping (alloying) and isothermal aging,. Future work aims to quantify the contribution of grain boundary deformation and eventually enable grain-scale modeling of the viscoplastic behavior of oligocrystalline SAC solder joints.

Chapter 6: Numerical Analysis of Steady-state Creep of Oligocrystalline SnAgCu Solder Joints

Abstract

Heterogeneous integration is leading to unprecedented miniaturization of solder joints, often with thousands of joints within a single package. The thermo-mechanical behavior of such SAC solder joints is critically important to assembly performance and reliability, but can be difficult to predict due to the significant joint-to-joint variability caused by the stochastic variability of the arrangement of a few highly-anisotropic grains in each joint. This study relies on grain-scale testing to characterize the mechanical behavior of such oligocrystalline solder joints, while a grain-scale modeling approach has been developed to assess the effect of microstructure that lacks statistical homogeneity. The contribution of the grain boundaries is modeled with isotropic cohesive elements and identified by an inverse iterative method that extracts material properties by comparing simulation with experimental measurements. The properties are extracted from the results of one test and validated by verifying reasonable agreement with test results from a different specimen. Equivalent creep strain variability within the same specimen and between different specimens are compared to assess typical variability due to the variability of microstructure.

Key words: Lead-free solder, anisotropic steady-state creep, Hill-Norton model, oligocrystalline finite element analysis, grain boundary creep, cohesive element

6.1 Introduction

Sn-Ag-Cu solder alloys are widely used in microelectronic packaging to provide mechanical, electrical and thermal connections between different structures/materials for proper function. Their behavior and failure mechanisms are critical to the reliability of integrated packaging systems. The development of heterogeneous integration has led to solder interconnects located in complex structures such as three-dimensional wafer-level packages, multi-die stacks, etc., and subject to quite demanding loading conditions (Lau et al., 2018). Appropriate material properties are necessary for numerical simulations in order to accurately assess their performance and reliability within the system. Extensive studies have been conducted to characterize the mechanical properties of SAC alloys, however, the results vary not only between groups but also between multiple measurements of the same group (Cuddalorepatta et al., 2010; Ma and Suhling, 2009). This is usually attributed to their stochastic microstructure, which typically consists of only a few highly anisotropic grains, in either discrete or interlaced morphology (Arfaei et al., 2013; Daszki and Gourlay, 2021). Moreover, the miniaturization of packages leads to an increase in the number of I/Os and a decrease in pitch size, which also reduces the size and volume of individual solder joints. The solder joint may be of similar length scale as the grain size, in microbumps. In view of this fact, both testing and modeling schemes should be based on such representative microstructures.

Crystal plasticity finite element (CPFE) models have been widely used to simulate anisotropic deformation of SAC solder joints at the grain scale, based on dislocations moving on preferred slip systems in accordance with phenomenological

flow models (Roters et al., 2011; Zamiri et al., 2009). To simulate the intergranular fracture observed in tin-based solder joints (Subramanian and Lee, 2004; Tian et al., 2012), the CPFE model is equipped with a cohesive zone model, in which the crack propagation is described by a traction-separation relationship (Le et al., 2017). The effect of heterogeneous microstructure on mechanical response is investigated by multiscale modeling, where three-dimensional representative volume elements (RVEs) were imported directly from tomographic images (Maleki et al., 2013, 2016) or modeled as particle matrix composites (Xu et al., 2021). However, the above-mentioned modeling approaches that incorporate anisotropic properties or/and microstructural features may be computationally expensive to some extent.

This paper focuses on the viscoplastic behavior of grain boundaries, an indispensable element in the grain-scale modeling of SAC solder joint. Since the steady-state creep at grain boundaries is currently difficult to measure directly, it is determined by matching simulation with experimental results as an inverse engineering problem, with the single crystal properties obtained in the previous chapter (Chapter 5). Comparison of equivalent creep strain fields shows significant differences between samples, even under similar loading states. The proposed grain-scale model, including anisotropic grains and isotropic grain boundaries, provides insight into the effect of grain structure on the steady-state creep of the joint under given conditions. Such knowledge is critical not only for achieving efficient and accurate reliability assessment of solder joints in electronic systems, but also for developing more reliable solder interconnects.

6.2 Multi-grain TMM specimen

A customized thermo-mechanical microscale (TMM) system was developed for mechanical testing of specimens with functional joint dimensions and similar coarse-grained microstructures, with the aim of minimizing the influence of factors other than grain configurations. Comprehensive details on test setup and specimen design are provided elsewhere (Cuddalorepatta et al., 2010; Deshpande et al.). In the current study, creep tests were performed on modified lap-shear specimens consisting of SAC305 solder joint and two copper platens without metallization layers. Fig.1 (a) shows a sample specimen with nominal dimensions. The specimen is nominally deformed in shear, and the 90-degree notches on both sides facilitate uniform stress distribution. The stress state of each specimen is evaluated individually, depending on the applied force and joint dimensions. Such TMM specimens usually contain only one grain, or at most a few grains and are referred to as grain-scale specimens, since the length scale of the test specimen is similar to that of individual grains. As an example, Fig. 1(b) provides an EBSD image of Sample 1, which contains four crystals. The failure patterns observed after testing (Fig. 1 (c)) indicates severe deformation discontinuity near the grain boundaries and crack propagation along the interfaces between crystals.

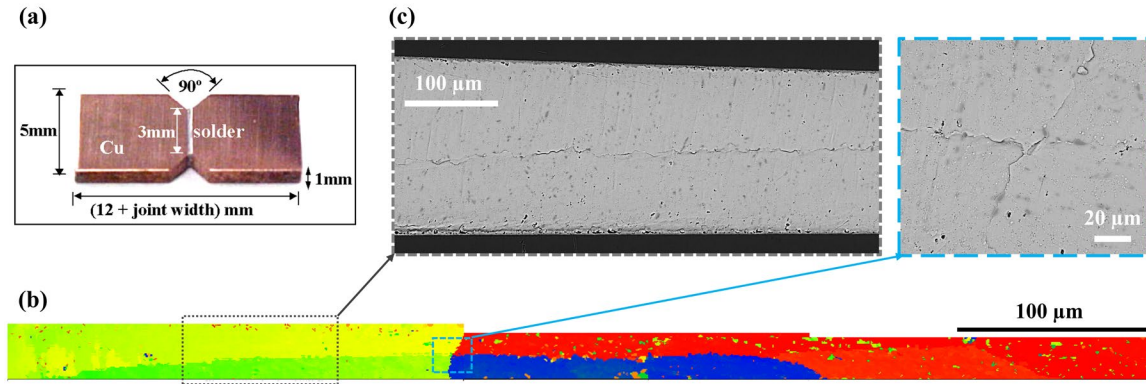


Figure 6.1 Sample 1 used in the TMM shear test: (a) nominal dimensions of modified Iosipescu shear specimens, (b) EBSD scanning of the solder joint of Sample 1, (c) ESEM images of failure patterns along the grain boundary after creep test

Grain-scale testing has been used to characterize solder properties, to gain insight into possible variabilities between specimens, and to study the effects of microstructure. Further, the test results help to understand the influence of microstructure and its correlation with mechanical response and variability, through a grain-scale modeling methodology.

6.3 Modeling Strategy

The coarse-grain microstructure, in conjunction with the anisotropy of BCT β -Sn, renders each individual microbump mechanically unique. Thus, each joint will demonstrate unique stress-strain response. A grain-scale modeling strategy is proposed to evaluate the degree of variation between joints due to microstructure at a given condition, which is achieved by the anisotropic properties of individual grains and the contribution of grain boundaries. The typical microstructure of an oligocrystalline SAC solder joint is divided into multiple Tiers depending on the critical length scales. Tier 3 refers to a general solder joint containing only one or at

most a few grains with no influence of the interfacial intermetallic compound (IMC) layer; while Tiers 0-2 are within a single grain. The modeling approach for single crystals and grain boundaries is presented in Section 6.3.1 and Section 6.3.2, respectively. Calibration of the single crystal secondary creep behavior was presented in an earlier paper. Calibration of the grain boundary model via their application to polycrystalline test specimens (Tier 3) is illustrated in Section 6.4.

6.3.1 Anisotropic single SAC crystal: crystal viscoplasticity model and Hill-Norton continuum model

A hierarchical multi-scale crystal viscoplasticity model has been proposed by the authors to capture the anisotropic steady-state creep behavior of single SAC crystal, based on key microstructure features (including Tier 2 and below) and dislocation motion (Zhou et al., 2009). The main concepts of that modeling approach are briefly reviewed here for completeness. The deformation mechanisms based on important microstructural characteristics and features at pertinent length scales is modeled using appropriate mechanisms, and then the key variables are transferred from one level to the next higher one, as the necessary basic building blocks. Tier 2 represents a single SAC crystal in which the dendritic structure of Sn is surrounded by a eutectic Ag-Sn mixture. Since the applied load is shared between these two phases, Mori-Tanaka homogenization (Gavazzi and Lagoudas, 1990) is performed to estimate the mean-field viscoplastic behavior. Tier 1 focuses on the eutectic mixture, where the statistically uniform distribution of nanoscale Ag_3Sn particles in the β -Sn matrix leads to dispersion hardening. The mobile dislocations are pinned or retarded by the dispersed precipitates, corresponding to the enhanced macroscopic creep resistance.

Based on microstructural analysis and experimental results, the bypass and recovery process for dislocations to recover from obstructions is modeled as a combination of dislocation climb and detachment mechanisms that dominate in the low and high stress regions, respectively. Tier 0 is the smallest length scale considered in the CV model and represents the anisotropic steady-state creep of the Sn phase. The presence of multiple slip systems (Zhou et al., 2009) renders the movement of dislocations along facile directions and the overall creep behavior highly dependent on the given loading conditions and grain orientation. Two creep activation energies were measured in earlier experimental studies on single-crystal Sn specimens, suggesting the existence of two competing mechanisms (Chu and Li, 1979; Weertman, 1957; Weertman and Breen, 1956). Thus, the steady-state creep of a single β -Sn crystal is modeled as dislocation climb and slip acting in conjunction (Jiang and Dasgupta, 2021).

This semi-analytical model, calibrated on length scales for which experimental results are available (single crystal β -Sn and SAC specimens), explicitly estimates the steady-state strain rate based on a given stress state, temperature, and key microstructural features. Although this model can be directly implemented for numerical analysis, an alternative approach is proposed in order to perform computationally efficient finite element simulations in microelectronic assemblies. The Hill quadratic criterion provides a user-friendly approach to characterize anisotropic behavior, analogous to the von Mises criterion used for isotropic materials. The Hill effective stress σ_{Hill} under multiaxial stress state is defined as:

$$\sigma_{Hill} = \sqrt{F(\sigma_{22} - \sigma_{33})^2 + G(\sigma_{33} - \sigma_{11})^2 + H(\sigma_{11} - \sigma_{22})^2 + 2L\sigma_{23}^2 + 2M\sigma_{13}^2 + 2N\sigma_{12}^2}$$

(Eq. 1)

where F, G, H, L, M and N are parameters that elucidate the anisotropic state, and are usually obtained experimentally at specific load directions. In isotropic materials, all of these constants default to the value 1, and thus Hill equivalent stress becomes the same as von Mises' equivalent stress in that case. The CV model described above can serve as a virtual test method to predict the strain rate under selected simple stress conditions, thus providing a method to estimate the values of Hill's constants. The subscripts 1, 2 and 3 correspond to the crystal main directions [100], [010] and [001], respectively. Therefore, SAC crystals can be simplified to an anisotropic homogeneous material in numerical simulations. The corresponding strain tensor will take the following form:

$$\dot{\epsilon}_{ij} = \frac{\partial \sigma_{Hill}}{\partial \sigma_{ij}} \dot{\epsilon}_{eq} = \dot{\epsilon}_{eq} \cdot \frac{1}{\sigma_{Hill}} \begin{bmatrix} G(\sigma_{11} - \sigma_{33}) + H(\sigma_{11} - \sigma_{22}) \\ F(\sigma_{22} - \sigma_{33}) + H(\sigma_{22} - \sigma_{11}) \\ G(\sigma_{33} - \sigma_{11}) + F(\sigma_{33} - \sigma_{22}) \\ 2N\sigma_{12} \\ 2M\sigma_{31} \\ 2L\sigma_{23} \end{bmatrix} \quad (\text{Eq. 2})$$

where $\dot{\epsilon}_{eq}$ is the Hill equivalent strain rate. It is a scalar multiplier that depends on the governing flow rule.

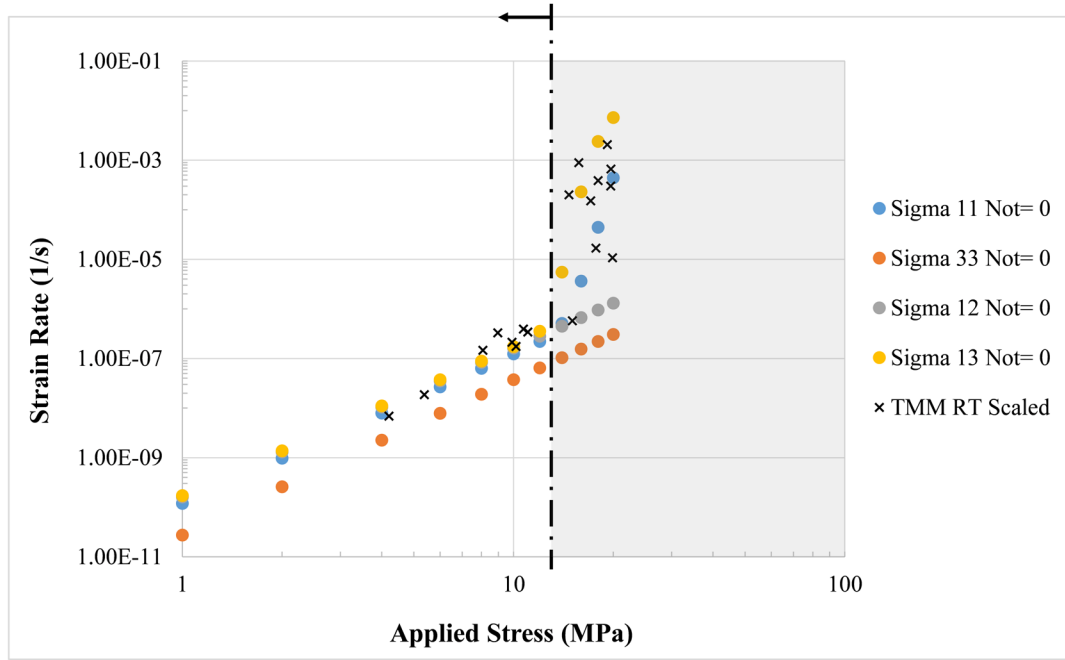


Figure 6.2 strain rates along the loading directions calculated from the CV model

Fig. 2 displays the strain rates along loading directions predicted by the CV model for selected uniaxial or pure shear loading conditions at room temperature. As modeled, creep is dominated by dislocation climb at low stresses and then shifts to be dominated by dislocation detachment mechanism as the stress increases. The dominance of these two mechanisms can be clearly discerned from the sudden increase in the stress exponent in Fig. 2. Although different stress states start to be governed by the dislocation detachment mechanism at different values, which are closely related to the slip systems activated, all stress states are dominated by the dislocation climb mechanism at stresses below 12 MPa. Thus, the steady-state creep response in the low stress region can be expressed by Norton's power law.

$$\dot{\epsilon}_{eq} = A(\sigma_{Hill})^n \quad (\text{Eq. 3})$$

Assuming that all stress conditions share an identical stress exponent at a constant temperature, the Hill-Norton parameters are extracted for low stresses (<12 MPa) from the virtual test results in Fig. 2 and summarized in Table a. Due to crystal symmetry, the crystallographic directions [100] and [010] are almost equivalent to each other, so that $F = G$ and $L = M$. F is set equal to one, and all other Hill's anisotropic constants are normalized to F . The quality of this fit is shown in Fig 3 where strain rate components estimated from the best-fit Hill-Norton formula are compared with those obtained from the CV model.

Table 6-1 Parameters for Hill-Norton models

A	n	$F = G$	H	$L = M$	N
9.51E-12	3.05	1	2.75	2.24	2.15

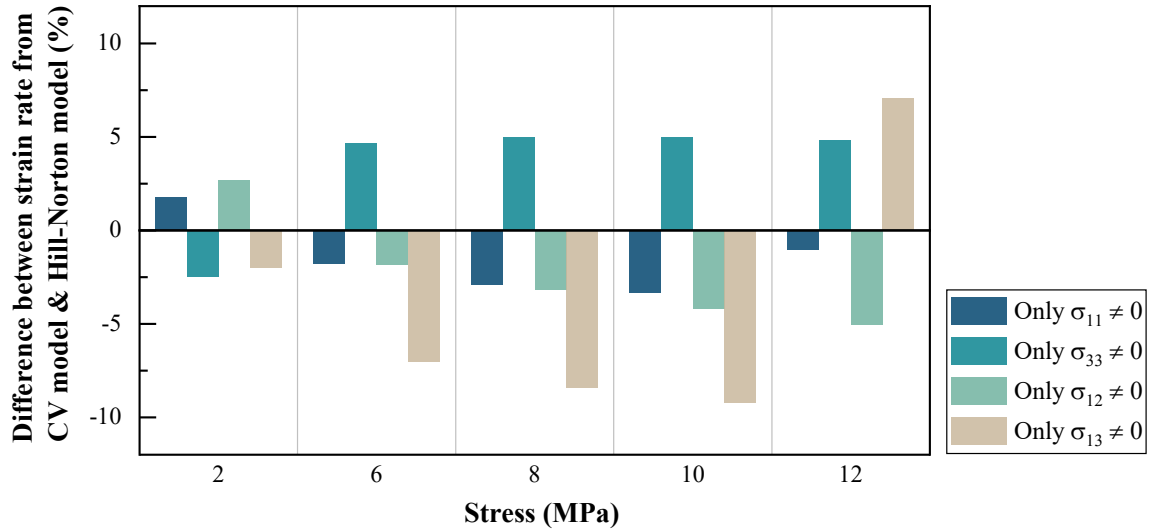


Figure 6.3 Percentage difference in strain rates along the loading directions obtained from the CV model and Hill-Norton formula in the low stress region

6.3.2 Grain boundary

Creep in polycrystalline solids is a complex process involving severe deformation of grains and accommodation of grain boundaries. Although the creep mechanisms of individual grains have been thoroughly investigated and various models have been proposed to explain that, similar studies on the viscoplastic properties of grain boundaries are still somewhat limited. To simplify the modeling, it is often assumed that the contribution of grain boundaries is either negligible or significant enough to dominate the macroscopic deformation. This leaves a dilemma for oligocrystalline materials, where neither the deformation of the grains themselves nor the deformation of the grain boundaries can be ignored. In order to quantify their viscoplastic properties, in this work, grain boundaries are modeled as isotropic materials and implemented in numerical simulations for comparison with tests.

An analytical creep model was developed (Spingarn and Nix, 1979) on the basis of dislocation climb at grain boundaries, in which shearing occurs along slip bands blocked by the grain boundaries. After a quantitative comparison with creep data of pure Sn and Sn-based alloys, the model is given in the following form

$$\dot{\epsilon}/D_{GB} \propto \left(\frac{50\delta}{b^3}\right) \left(\frac{\sigma b^3}{kT}\right) \left(\frac{Lb^3}{\lambda^4}\right) \quad (\text{Eq. 4})$$

where δ is the grain boundary thickness, usually on the scale of atomic size. L is the grain size, and λ is the slip band spacing. This model indicates that the strain rate is linearly dependent on the stress at a given temperature. A similar linear relationship $\dot{u}_{GB} = \left(\frac{\delta}{\eta_B}\right) \tau$ was used by researchers to model the relative displacement rates of grains meeting at boundaries, in the numerical analysis of non-uniform flow in

polycrystals, which are attributed to the grain boundary sliding and viscosity inside the crystals (Crossman and Ashby, 1975). η_B denotes the viscosity of grain boundary, which depends on the boundary configuration and is proportional to the temperature. Although the real grain boundary is neither flat nor uniform, it is simplified as a homogeneous isotropic material in current work, for the purpose of implementation in numerical simulations. Motivated by Eq. 4 and Crossman's numerical analysis (Crossman and Ashby, 1975), the steady-state creep rate in this study is assumed to follow a linear Newtonian isotropic viscous model, given by

$$\dot{\epsilon}_{GB} = A_{GB}\sigma \quad (\text{Eq. 5})$$

where A_{GB} is a unified parameter that represents the combined consequence of multiple factors, such as boundary configuration, thickness, diffusivity, temperature, etc. The value of A_{GB} is determined by calibrating the simulation with experimental result.

6.4 Numerical Simulations

The oligocrystalline TMM specimens are constructed in FEM based on the grain orientations obtained from the EBSD surface scanning. The effect of the grain boundaries is modeled by an ultrathin layer of cohesive elements whose viscoplasticity is identified from the inverse finite element method. Section 6.4.1 presents the determination and validation process. Further analysis of the simulation results is presented in Section 6.4.2.

6.4.1 Calibration and validation of grain boundary properties

Fig. 4 (a) shows the model construction of the middle region of the TMM specimen (loaded region spanning across the two loading grips), where the solder joint is connected to two copper platens (in green). The bottom surface is fully constrained and a uniform traction stress is applied horizontally on the top surface, so as to mimic the shear loading and boundary conditions applied in the physical shear tests. Previous studies examined both surfaces of TMM solder joints by cross-polarization microscopy and detected that the number and configuration of grains were almost invariant over the entire thickness of the specimen (Cuddalorepatta, 2010). Similar results have been observed by other groups through orientation imaging microscopy (OIM) (Telang and Bieler, 2005). Therefore, the grain orientation from the surface electron backscatter diffraction (EBSD) scan is considered to be representative of the entire volume of the joint. Sample 1 presented in Fig. 1 (Cuddalorepatta et al., 2010) is used for calibration and the grain structure is modeled accordingly (Fig. 4 (b)). There are three main grains in this specimen, separated by grain boundaries. There are two coordinate systems: the global system $\{X, Y, Z\}$ is intended to indicate the direction and position in specimen space, while the local system defines the orientation of the individual grains, where the axes $\{a, b, c\}$ correspond to the crystal principal directions $\{[100], [010], [001]\}$. Fig. 4 (c) depicts the grain orientations of Sample 1.

Each SAC grain is modeled as an anisotropic viscoplastic material, using the Hill-Norton model described in Section 3.1 and shown in in Figure 2 and Equations 1-3. The grain boundary region is discretized by a monolayer of cohesive elements with

continuum macroscopic properties. Following methods recommended in the literature, this layer is set to be flat and 1 μm thick, rather than the thickness of the real grain boundary (Crossman and Ashby, 1975). This is done for computational expedience. The 3D cohesive element formulation used in this commercial finite element analysis are capable of only three strain components defined in the local tangential-normal coordinate system: one extensional strain component in the thickness direction (along the normal to the grain-boundary surface) and two transverse shear strain components; all other strain components are assumed to be zero for the constitutive calculations. This deformation mechanism corresponds to the decohesion and sliding of grain boundaries.

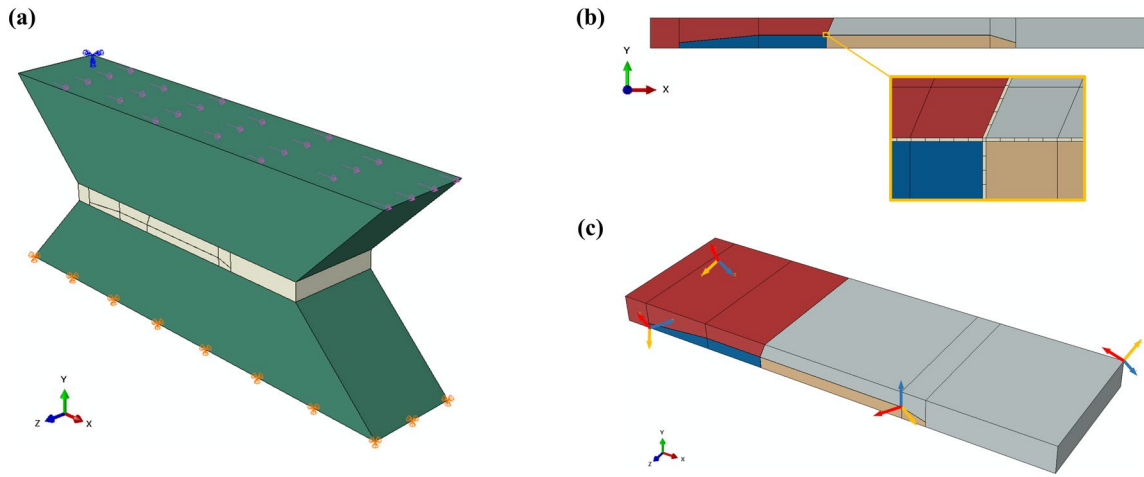


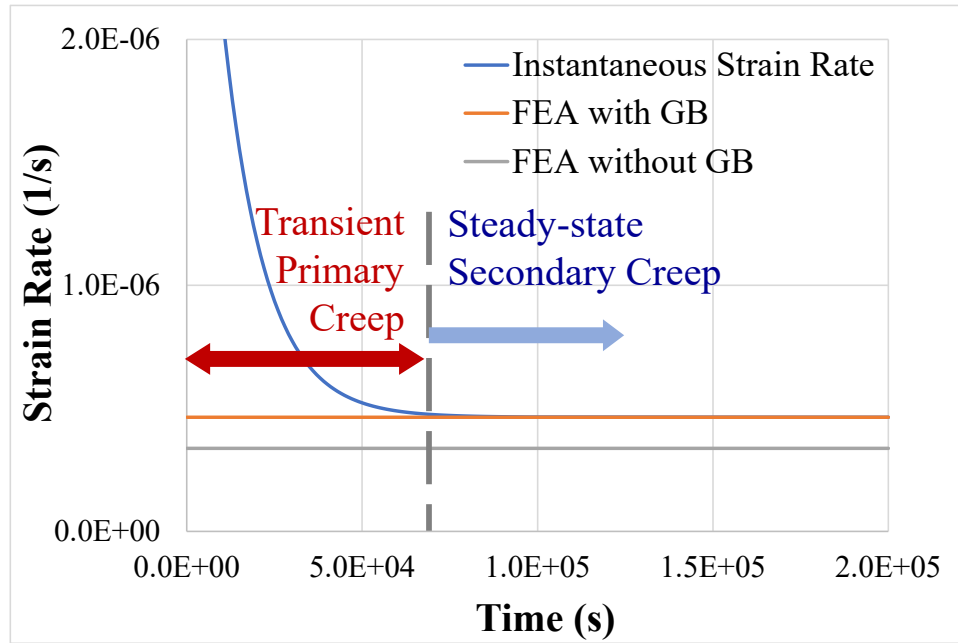
Figure 6.4 FEA model of TMM shear specimen: (1) boundary and loading conditions; (2) grain structure and grain boundary of Sample 1; (3) local coordinates indicating the direction of each grain of Sample 1

The nominal strain rate is estimated by the same procedure as in the experiment (Cuddalorepatta et al., 2010), namely, the average displacement rate along the loading direction (X) divided by the initial height of the joint, $\dot{\gamma} = \frac{\dot{U}_x}{h}$. The values of A_{GB} is adjusted until the simulated strain rate matches the measurement. The result after

calibration ($A_{GB} = 1.05E - 6$ at room temperature) is plotted against the instantaneous strain rate from the experiment, as shown in Fig. 5 (a). For comparison, strain rate without the contribution of grain boundaries is also provided, where the grain boundary is modeled as a perfectly elastic material with no viscoplasticity. For calibration purposes, experimental data of strain versus time, including primary and secondary creep regions, were fitted with the four-element Burger model (Motalab, 2013; Yang et al., 2006),

$$\varepsilon(t) = k_0 + k_1 t + k_2(1 - e^{-k_3 t}) \quad (\text{Eq. 6})$$

The instantaneous strain rate was determined as the time derivative of the fitted model. The strains are plotted versus time in Fig. 5 (b), according to the constant rates from the steady-state finite element simulations, and compared with the near steady-state region of the experimental data.



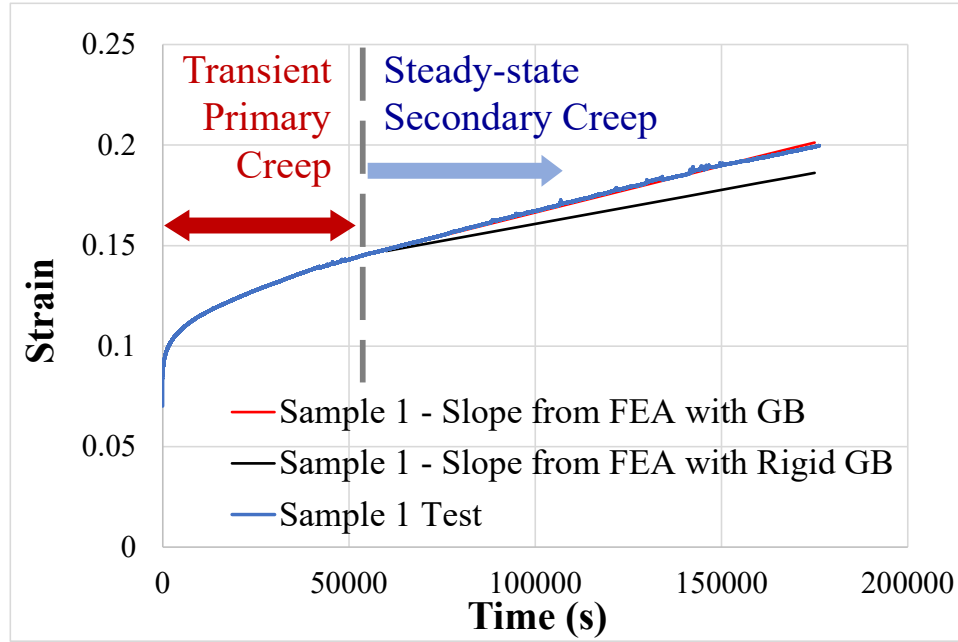


Figure 6.5 Simulation results of Sample 1 after calibration

As discussed above, this grain boundary model is next verified by modeling a second shear test specimen and comparing the prediction with experiments. The grain orientation of the oligocrystalline Sample 2 was obtained from EBSD (Fig. 6 (a)). A FEA model similar to that of Sample 1 was constructed for Sample 2, where the grain structure of the joint is shown in Fig. 6. Considering the possible issue of mesh density sensitivity (Fan et al., 2006), which arises from stress singularities, the same sizing control is applied to assign the mesh seeds. Since both tests were conducted at room temperature, A_{GB} should be identical for Sample 1 and 2. Therefore, the simulation of Sample 2 is performed with the calibrated parameter A_{GB} . Both strain rate and strain history are compared with experimental results, as illustrated in Fig. 7. This output of FEA shows good agreement with the experiment (about 2% higher).

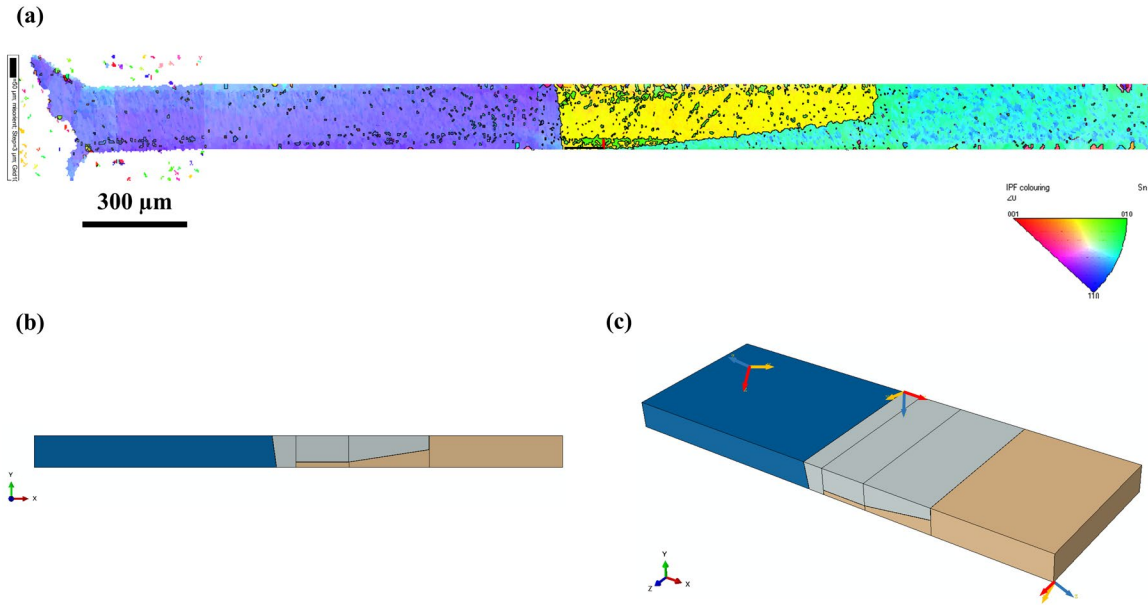
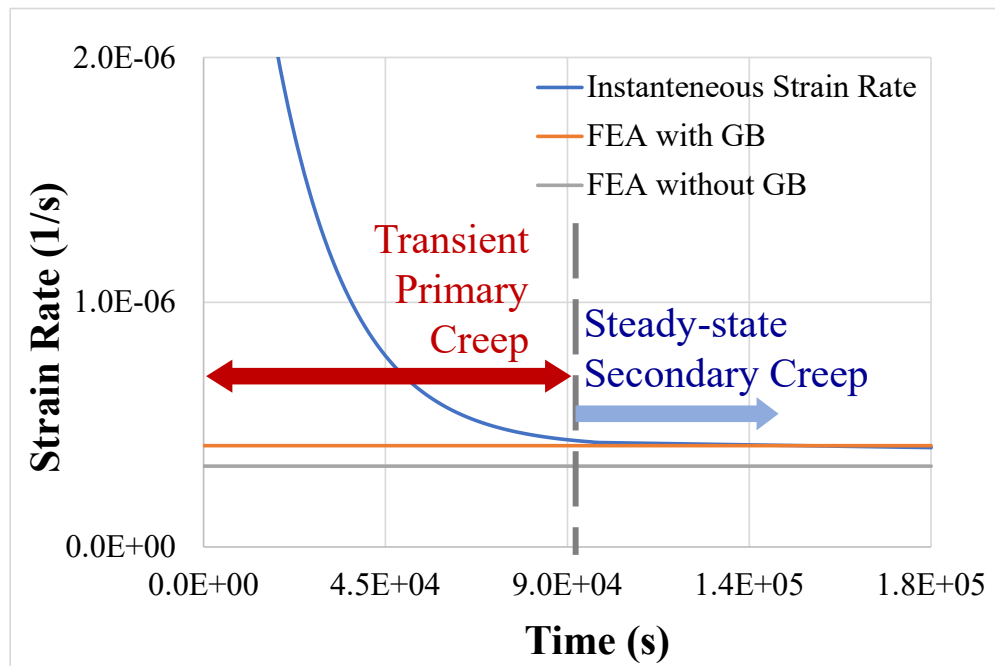


Figure 6.6 Grain structure of Sample 2: (1) EBSD image, (2) grain structure in FEA, (3) local coordinates indicating the direction of each grain of Sample 2



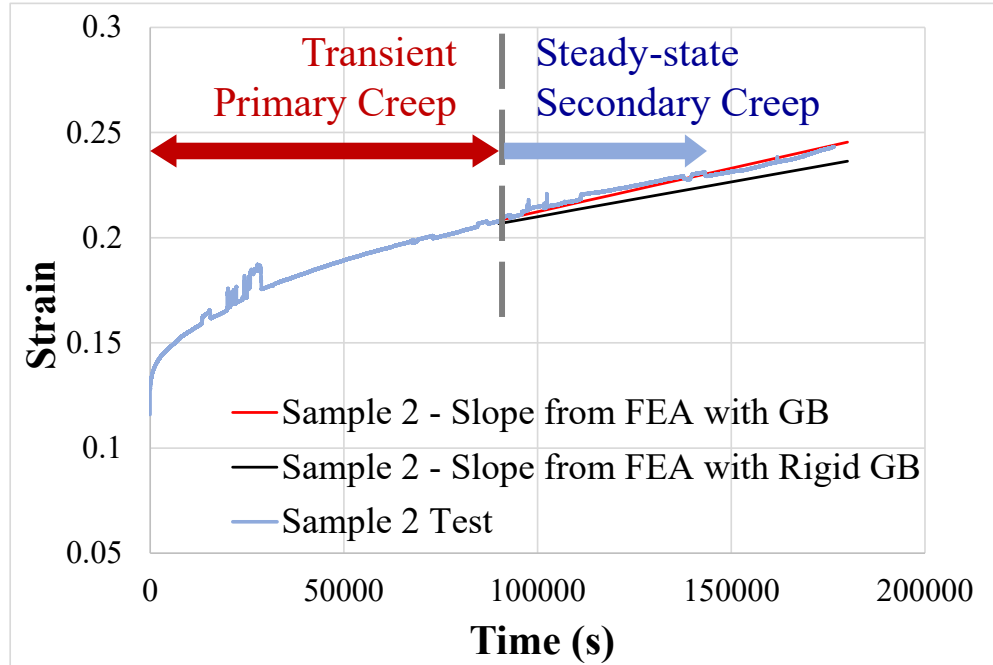


Figure 6.7 Simulation results of Sample 2

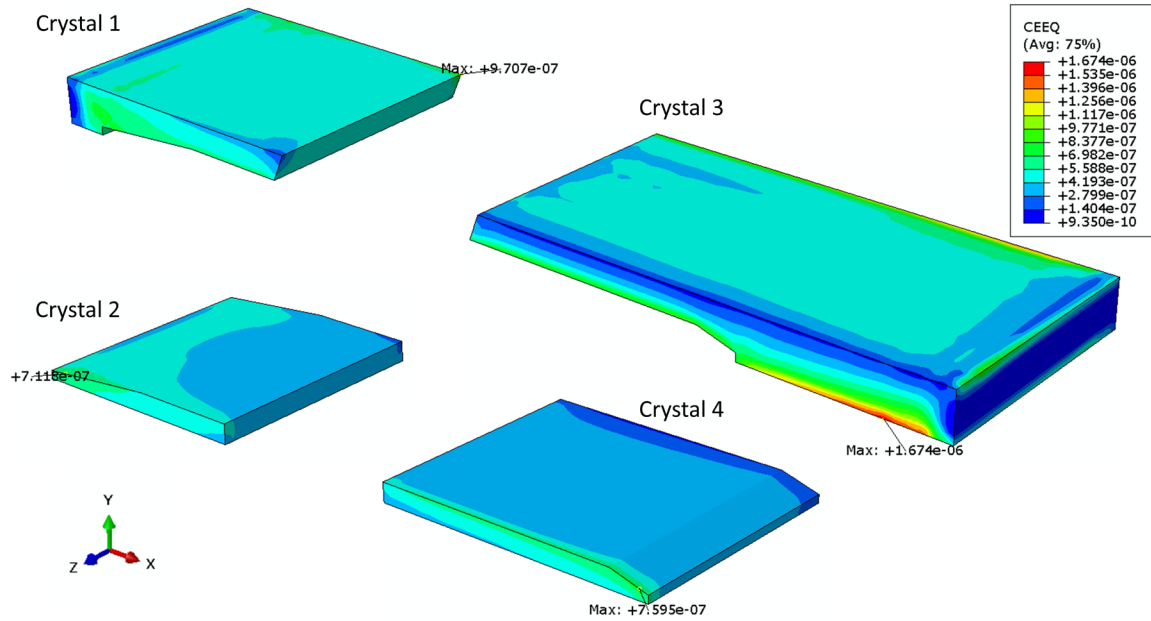
The strain rates of Samples 1 and 2, from experiments and simulations, with and without the contribution of grain boundaries, are summarized in Table 6.2. Although the volume fraction of grain boundaries is rather small compared to the entire joint, their influences on the time-dependent inelastic deformation is non-trivial. The incorporation of grain boundary regions with isotropic viscoplasticity in the finite element analysis increases the overall strain rate of Samples 1 and 2 by about 37% and 26%, respectively. Based on this result, both the deformation within individual grains and the accommodation function of grain boundaries should be considered in appropriate analysis of oligocrystalline SAC joints.

Table 6-2 Comparison of experiments and simulations for Samples 1 and 2

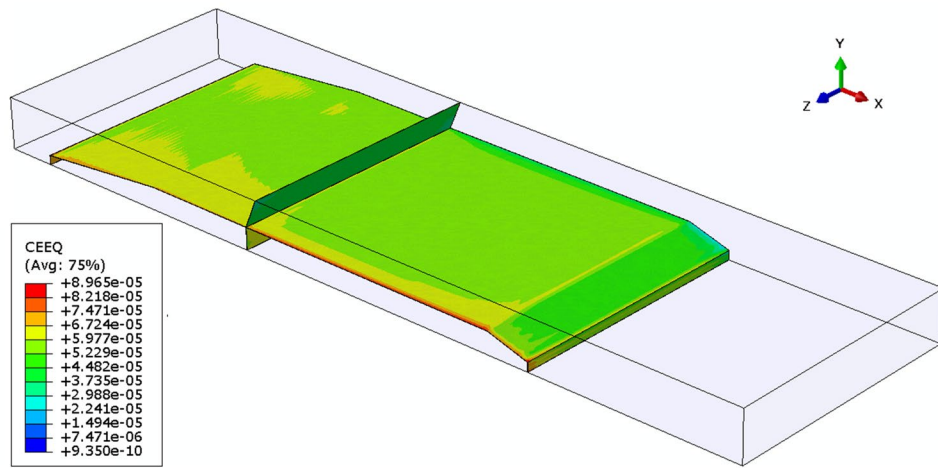
	Experiments	FEA Output		
		with Viscoplastic GB	without Viscoplastic GB	GB contribution
Sample 1 (for calibration)	4.64E-7	4.64E-7	3.38E-7	37.3%
Sample 2 (for Verification)	4.06E-7	4.14E-7	3.30E-7	25.5%

6.4.2 Results and discussion

Contours of the equivalent creep strains for Sample 1 are provided in Fig. 8. The equivalent creep strain in the grain boundary region is much higher than that in each individual grain, with a ratio of more than 50 between the maximum values. This would explain, to some extent, the observed distinct damage pattern along the grain boundaries, reported after the shear test, and shown in Fig. 1. The maximum strain for all crystals is located at the edge of Crystal 4, which is connected to the clamped Cu platen. The maximum strains in both Crystals 2 and 4 are at the edges adjacent to the cohesive elements, where they meet neighboring crystals. The presence of grain boundaries accommodates the strong mismatch between grains through limited normal traction and intensive sliding. In Crystal 3, the strain is concentrated at one vertex, which is actually the intersection point of Crystals 1, 3 and the upper Cu platen.



(a)



(b)

Figure 6.8 Equivalent creep strain contour of Sample 1 in: (a) each crystal, (b) grain boundary region

Fig. 9 displays the corresponding contours of the equivalent creep strain for Sample 2. The maximum strain ratio between the grain boundary and crystals is more than 70. The creep strain of Crystal 1 is concentrated on the side surface and near the

corner of the joint. The maximum value for Crystal 2 is located at one vertex common to Crystals 1, 2 and the bottom copper platen. In Crystal 3, the location of the peak strain is inside the grain.

Within each joint, the concentration of creep stain varies considerably from crystal to crystal, which can be attributed to its own grain orientation, the misorientation with adjacent grains, the behavior of grain boundaries and the consequent complex stress distribution, etc. This strain heterogeneity is to some extent consistent with that observed in tested failed samples: the solder joint may crack along the interfacial layer connected to other structures/materials, or through the interior of the bump. In addition, internal cracks can be either transgranular, i.e., across grains, or intergranular, i.e., decohesion or sliding along grain boundaries.

Although the nominal shear stress applied to Sample 1 is slightly lower than that of Sample 2, the creep strain field within it is much more severe. The maximum equivalent creep strain at crystals and grain boundaries for Sample 1 was 47% and 11% higher than corresponding values in Sample 2, respectively. Stress concentration is thought to be closely related to the formation of critical subgrains, the stimulation of recrystallization, and eventually the initiation of microcracks. Such a grain-scale modeling strategy provides an explicit way to quantitatively evaluate the variation between behavior of different solder joints, even those that follow identical manufacturing process and are subjected to similar loading conditions. Therefore, for a given oligocrystalline SAC joint, the effect of stochastic grain structure is accessible, which cannot be achieved by conventional isotropic homogeneous modeling. Obviously, when modeling solder joints for electronic assemblies, the grain structure

of each individual grain is not known *a priori*. Thus, it is neither possible to model each individual joint nor practical to obtain the grain structure without destroying the components. The purpose of grain-level modeling is therefore to proactively estimate the range of stochastic variation of observed mechanical behavior, through predictive parametric sensitivity studies of different grain structures, as an effective complement to physical testing. This will allow design for reliability, and significantly reduce the cost and time usually required for statistically-significant physical testing of suitable large sample size.

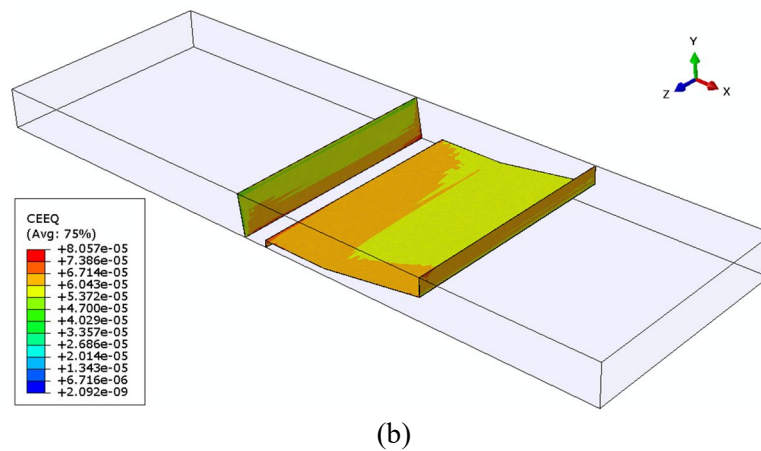
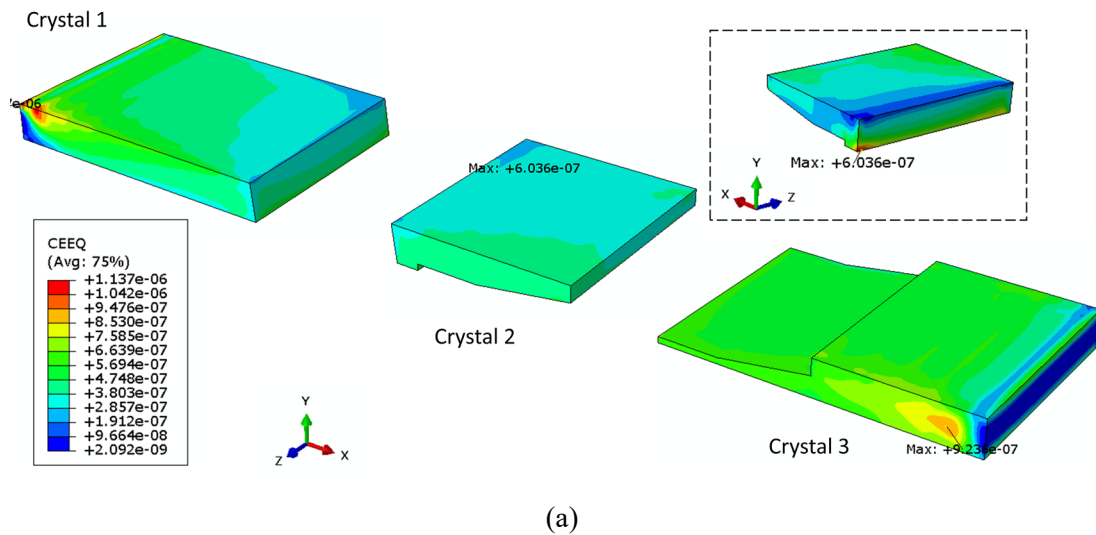


Figure 6.9 Equivalent creep strain contour of Sample 2: (a) single crystals, (b) grain boundary region

6.5 Summary and Conclusion

The purpose of this paper is to develop the capability for grain-scale viscoplastic numerical modeling of polycrystal SAC solder joints, by providing the contribution of grain boundaries to the steady-state creep of oligocrystalline SAC solder joints by an inverse fitting approach. Although SAC interconnects are usually modeled as isotropic homogeneous bodies in numerical simulations, in reality they are neither isotropic nor homogeneous. The random grain orientation and arrangement, together with the inherent anisotropic properties of each grain, renders each joint a rather stochastic microstructure resulting in unique thermomechanical response of each joint. A grain-scale modeling approach has been proposed to assess the degree of response variability caused by the stochastic variability of the grain structure. To accomplish this, properties of both individual grains and the accommodating grain boundaries are necessary. The steady-state creep behavior of single crystal has been modeled with the Hill anisotropic potential and a Norton creep-flow rule, with model constants obtained from an experimentally-calibrated crystal-viscoplastic model presented earlier by the authors. The grain boundary properties are estimated in this study from creep shear experiments conducted on selected oligocrystalline solder joint test specimens. Based on the grain structure of these test specimens, obtained from EBSD images, a grain-scale finite element model of the solder joint is developed. The grain boundaries are simulated with cohesive elements having isotropic linear viscoplastic properties. The grain boundary creep model constant is determined by matching this finite element simulation result to the experiment, and then verified on another sample. The verification exercise shows reasonable agreement. Although there is a

good quantitative match between experiments and simulations, given the limited number of samples, calibration with additional tests under various conditions is required for further analysis. The simulation results demonstrate that the strain heterogeneity within the solder bulk is susceptible to the grain structure, showing significant differences between samples.

This grain-scale modeling methodology enables user-friendly finite element numerical simulations of multi-grain solder joints in microelectronic assemblies and facilitates parametric sensitivity studies of different grain configurations. This capability will empower designers to numerically explore worst-case and best-case microstructural configurations (and associated stochastic variabilities in solder joint performance and design margins) under given loading conditions.

Chapter 7: Summary & Discussion, Contributions and Limitations & Future Work

The summary and discussion of this study are presented in Section 7.1, following the order of the chapters. The contribution and limitations & future work are discussed in Section 7.2 and 7.3, respectively.

7.1 Summary & Discussion

7.1.1 Multi-scale modeling for anisotropic elastic behavior of oligocrystalline SAC solder joints

1. The anisotropic elastic behavior of single SAC crystal is modeled based on the heterogenous multi-scale microstructure.
2. Both Ag_3Sn dispersoids and Sn dendrites are simplified as prolate spheroids, and the corresponding Eshelby's tensor is numerically estimated.
3. A parametric study was conducted to illustrate the dependence of Young's modulus on morphology of AgSn IMC particles (particle aspect ratio and prolate orientation with respect to the main axis)
4. Elastic response of few-grained solder joints is numerically predicted from the anisotropic behavior of the single crystal, by explicitly modeling the grain morphology in finite element analysis (FEA). Grain boundaries are modeled with an isotropic elastic material.
5. Preliminary elastic grain-scale analysis on oligocrystalline joints reveals that stress distribution along grain boundaries can vary up to 55% for grain structures and loading considered here.

7.1.2 Multi-scale modeling for anisotropic steady-state creep of single-crystal Sn

1. Two creep activation energies were measured in conventional creep tests and impression creep tests, indicating that two competing processes simultaneously dominate the steady-state creep of Sn crystal.
2. Crystal viscoplasticity models, based on dislocation mechanics, were applied to describe the anisotropic steady-state creep behavior of β -Sn single crystals, as a function of stress, temperature and crystallographic orientations.
3. A total of 10 possible slip families and 32 slip systems were considered and the prevailing slip systems might change from test to test, depending on the applied multiaxial stress state, crystal orientation and temperatures.
4. The proposed crystal viscoplasticity model was calibrated using constant-stress creep tests performed by Weertman on β -Sn single crystal specimens of known orientations.
5. An anisotropic homogenized creep constitutive model is proposed for numerical FEA simulations of steady-state creep behavior, where Hill's potential is used to represent the anisotropy of the creep behavior, while Norton's power-law is used to represent the steady-state creep flow rule.
6. For Sn crystals, the appropriateness of the Hill-Norton constitutive model is verified by testing its ability to provide successful FEA simulation of Weertman's creep test and the dislocation-based crystal viscoplasticity model.
7. The crystal viscoplasticity model shows that the overall anisotropy of steady-state creep in Sn decreases with increasing temperature.

7.1.3 Multi-scale anisotropic modeling for steady-state creep of oligocrystalline SAC solder joints

1. A multiscale hierarchical Crystal Viscoplasticity (CV) model is developed for SAC crystals, based on the heterogeneous microstructure and different mechanisms that are believed to govern the behavior at each length scale.
2. The improved creep resistance after homogenization can be quantified as a function of the eutectic phase volume fraction and associated microstructural features.
3. The continuum formulations with anisotropic Hill's potential allows 3D computational analysis for engineering grain-scale analysis.
4. Numerical simulations with the Hill's anisotropic potential provide estimates of the variability of the single-crystal BGA joint failure analysis for different modes: (i) transverse expansion of the solder ball, potentially leading to eventual short circuits; and (ii) cyclic fatigue damage leading to eventual failure of the solder joint.
5. The distribution of creep dissipation energy density varies significantly with different grain orientations. The strain-localization regions predicted by grain-scale analysis in single-crystal SAC joints are consistent with experimentally observed sub-grain rotation map and recrystallization map, reported in the literature.
6. The grain boundaries are simulated with cohesive elements having isotropic linear viscoplastic properties, and model constant is determined by matching this finite element simulation result to mechanical loading experiments conducted on oligocrystalline specimens with known grain structure.

7. The simulation results of oligocrystalline solder joints demonstrate that the strain non-uniformity within the solder bulk is very sensitive to the grain structure, showing significant differences between samples under identical external loading conditions. As an example, under the same nominal shear loading, the maximum equivalent creep strain at crystals and grain boundaries for Sample 1 was predicted to be 47% and 11% higher than corresponding values in Sample 2, respectively. The predicted difference in nominal strain rate in these two specimens is consistent with measured results.

7.2 Contributions

1. Multi-scale modeling of the elastic response of SAC crystal has been conducted for the first time and the influence of microstructural features (shapes & orientation) are parametrically studied.
2. Multi-scale modeling of the steady-state creep oligocrystalline SAC joints
 - Has been calibrated with conventional creep tests at different length scales, providing qualitative and confidence in applying this approach to other similar SAC solder alloys
 - Quantifies the contributions of grain microstructure features (Tier 0-2) and grain boundaries to joints' viscoplastic behavior, stress/strain heterogeneity, and associated durability/reliability issues
 - Els user-friendly computationally efficient finite element simulations for:
 - Parametric sensitivity studies of different grain configurations in microelectronic assemblies

- Worst-case and best-case microstructural configurations (and associated stochastic variabilities in solder joint performance and design margins) under given loading conditions
 - Prediction and insights into the creep behavior of joints with tailored/optimized microstructures
3. Anisotropic continuum formulations with Hill's potential are applied to represent the steady-state creep behavior of Sn and SAC grain as effective homogenized anisotropic materials

7.3 Limitation and Future Work

1. The modeling calibration of SAC single crystal and grain boundary were conducted with limited number of samples. Additional tests under various grain sizes, stress conditions and temperature levels are required for future analysis.
2. Hill's anisotropic constants are approximated to be independent of stress level. As the dominant deformation mechanism gradually changes from dislocation climb to dislocation detachment, variations in directional creep resistance are possible and should be examined in future studies.
3. Structural unit (SU) models of disordered media can later be used to analyze microstructural features and the effect of temperature on grain boundary creep. Additional micro-scale experimental results are also needed in order to improve the calibration and validation of grain-boundary deformation model.
4. Changes in creep behavior of single-grain and oligocrystalline SAC solder joints caused by isothermal aging/ cycling aging-induced microstructural

variations (Tier 1-3) can be modeled, according to the proposed modeling strategy.

5. The effect of grain size (relative to structure size), can affect the volume fraction of grain boundaries within a given joint, and should be systematically analyzed. This will provide insight into the overall degree of anisotropy as a function of numbers of grains in a joint.
6. The analysis of solder joint with interlaced morphology or recrystallized morphology should be performed with the grain-scale modeling proposed here.
7. Additional solder materials need to be characterized using the multiscale CV model and continuum model for anisotropic steady-state creep.
8. Evolution of dislocation density should be considered, to allow modeling of anisotropic transient creep

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