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Crystal plasticity finite element study of deformation behavior in commonly observed microstructures in lead free solder joints

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ABSTRACT

The anisotropy of the tin phase in a Pb-free tin based solder joint has a significant effect on heterogeneous deformation and therefore, the reliability of solder joints. In this study the ability of crystal plasticity finite element (CPFE) modeling to account for elastic and plastic anisotropy in tin based solder joints was examined using shear deformation applied on a simplified representation of a real microstructure of four specific SAC305 solder balls. Commonly observed microstructures in lead free solders are either single crystals or a particular microstructure with solidification twin relationship with about 55–65° rotations about a common [100] axis (known as beach-ball microstructure [6]). In this study two different single crystals and two different beach-ball microstructures were investigated using CPFE modeling.

Simulation results show the ability of CPFE to predict the heterogeneous deformation due to the anisotropic elastic and plastic properties of tin in lead free solder joints.

1. Introduction

Due to the requirement to eliminate lead in electronic assembly, the tin–silver–copper (SAC) family of alloys has been heavily used in electronic assembly in recent years. A significant challenge resulting from introducing these alloys is that the fracture probability differs from Sn–Pb solders because of the anisotropy of tin [1–3]. The location in the package that is most prone to failure cannot be predicted as easily as in Sn–Pb alloys, because the single crystal or large grain microstructure and the crystal orientation in lead-free solder alloys greatly affect damage initiation and evolution. Miniaturization is a very important issue in solder joints because the dimension of a joint is similar to the size of the Sn grains. The design of solder joints will increasingly require considering the grain scale anisotropy. Studies of the microstructure and Sn grain morphologies in lead-free solder joints show peculiar microstructures, such as the beach-ball morphology, in which cyclic twins form (rotations of 60° about a common [100] axis) during solidification [6], which are illustrated in several of the figures in this paper. The strongly anisotropic elastic modulus and coefficient of thermal expansion (CTE) play an important role in thermo-mechanical loading of solder joints, leading to complex heterogeneous stress states acting on joints [4]. Due to this anisotropy, crystal features such as grain size and grain morphology have significant effects on the mechanical properties and reliability of sub-mm scale joints. There are very few prior studies about modeling the real microstructure of lead free solders [5–11]. Park et al. [10] used an anisotropic linear elastic constitutive model in an FEM simulation to simulate three-dimensional elastic strains measured experimentally in lead-free solder balls. Although they could predict the location of damage near the grain boundary, the observation of plastic deformation by Bieler et al. [6] in the samples that experience thermo-mechanical loading suggests that application of more sophisticated plastic constitutive models are required for prediction of damage evolution in lead free solders that fail by ductile fracture caused by plastic deformation.

More recently, Maleki et al. [11] used a J2 plasticity constitutive model to investigate the effect of aging conditions on deformation behavior of the eutectic micro-constituent in SnAgCu lead-free solder. Although their study accurately modeled the geometry of Sn grains and intermetallic, the isotropic plasticity associated with J2 model is unrealistic and oversimplified.

Darbandi et al. [14] used a crystal plasticity model to investigate the effect of grain orientation and its relationship with morphology (grain position within a simplified geometry of solder ball microstructure). Specifically, this study investigated the complex interaction between the activity of slip systems, location of a particular grain within the solder ball and orientation of different grains.

Since the damage evolution highly depends on stress, strain, and the activity of slip systems, providing a model that can predict

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the local stress and strain state will be helpful from both a scientific and industrial point of view. Furthermore, the use of a microstructure scale FE mesh in a crystal plasticity finite element (CPFE) model is also important for interpreting experimental measurements, because at these scales the experimentally imposed boundary conditions are very difficult to measure or monitor.

In this study, a CPFE model is used to simulate deformation mechanisms and anisotropy associated with the slip phenomena in Sn to compare with corresponding experimental characterization of shear deformation, in order to assess the capability of the CPFE model to predict the kinematics of plastic deformation and evolution of microstructural features in different solder joints. Firstly, two different single crystal orientations were investigated to evaluate the capability of CPFE to predict the kinematic plastic deformation. Next, the beach-ball microstructure which is commonly observed in lead free solder was investigated, in two different samples to evaluate the reliability of CPFEM model to predict the plastic deformation in lead free solders. Thus, this work provides a basis for an integrated incremental model development strategy based upon experiments, modeling and comparative analysis.

2. Model description

The crystal plasticity model developed by Zamiri et al. [12,13] for FCC metals was used to study tin. Firstly, the existing crystal plasticity model was modified in order to account for the more complicated crystal structure of tin. Tin has a body centered tetragonal crystal structure with 32 possible slip systems. Since not much is known from the literature about the slip activity of tin slip systems, slip resistance or hardening characteristics, a modified crystal plasticity model was used to simulate the deformation of solder balls under shear loading in order to identify the likely active slip systems and hardening properties that allow comparison with experiments. The crystal plasticity model calculates shear rate for each slip system, allowing the user to identify the most active slip systems for a given increment of plastic deformation. The incremental hardening of slip systems is also a function of the magnitude of shear rates, and hardening parameters. By comparing the simulation results with microscopic and macroscopic measurements, estimates for the hardening parameters of slip systems for tin were identified [14]. Once these parameters were fitted to a set of experimental dataset, they were no longer modified when the code was used to simulate deformation of tin solder balls under different loadings. The formulation of crystal plasticity model is briefly described below showing the relationship between slip systems, shear rates, and hardening parameters with the rate of plastic deformation.

A velocity gradient in plastic deformation in the material coordinate system can be decomposed into a rate of deformation and a spin tensor:

$$L^P = D^P + W^P \tag{1}$$

An elasto-plastic problem is usually defined as a constrained optimization problem aimed at finding the optimum stress tensor and internal variables for a given strain increment. In such a problem, the objective function is defined based on the principle of maximum dissipation. This function has terms describing the incremental release of elastic strain energy and dissipation due to incremental plastic work, and the constraint is the yield function:

$$(\sigma_{j+1}, q_{j+1}) = \left\{ \begin{array}{l} Min\left[l(x) = (\sigma_{j+1}^{trial} - \sum) : C^{-1} : (\sigma_{j+1}^{trial} - \sum) + (q - q_j) : E^{-1} : (q - q_j) \right] \\ Subjected\ to : f(\sum, q) \leqslant 0 \end{array} \right\} \tag{2}$$

where $\sum$ is the design variable (stress tensor) to be found, $\boldsymbol{q}$ is a vector containing internal variables such as strain hardening and kinematic hardening parameters that need to be found, C is the material stiffness matrix, $f(\sum, q)$ is the yield function, and E is the so-called matrix of generalized hardening moduli. One of the solutions to the above problem is the following equation for the plastic rate of deformation:

$$D^{\mathrm{p}} = \lambda \frac{\partial f(\sigma, q)}{\partial \sigma} \tag{3}$$

In a crystal plasticity problem, deformation is defined by yield functions for each slip system in a crystal. Assuming the Schmid law is valid for plastic deformation of a single crystal, then for any slip system a yield function can be defined as:

$$f_\alpha(\sigma, q) = \frac{|\sigma : P^\alpha|}{\tau_{\mathrm{y}}^\alpha} - 1 \tag{4}$$

The constraints of problem (2) can be combined and replaced by an equivalent single constraint defined as:

$$f(\sigma, q) = \frac{1}{\rho} \ln \left[\sum_{i=1}^{m} \exp \left[\left(\rho \frac{|\sigma : P^\alpha|}{\tau_{\mathrm{y}}^\alpha} - 1 \right) \right] \right] \tag{5}$$

where i represents the index of summation for slip systems, $\boldsymbol{m}$ is the number of active slip systems, τ_y^α is the critical shear stress on slip plane α, and P^α is the symmetric part of the Schmid tensor, I^α, that describes the orientation of a slip system, defined as:

$$P^\alpha = \frac{1}{2}\left[(I^\alpha) + (\mathrm{I}^\alpha)^{\mathrm{T}} \right] = \frac{1}{2}\left(m^\alpha \otimes n^\alpha + (m^\alpha \otimes n^\alpha)^{\mathrm{T}} \right) \tag{6}$$

where n^α is a unit normal to the slip plane, and m^α is a unit vector denoting the slip direction.

The plastic deformation matrix can be expressed as:

$$D^{\mathrm{p}} = \sum_{i=1}^{n} \dot{\gamma} P^\alpha \tag{7}$$

where $\dot{\gamma}$ are slip rates. The spin tensor, which represents the material rotation due to slip, can be expressed as:

$$\Omega^{\mathrm{p}} = \sum_{i=1}^{n} \dot{\gamma} w^\alpha \tag{8}$$

where w^α matrix is the anti-symmetric part of $\boldsymbol{I}^\alpha$, defined as:

$$w^\alpha = \frac{1}{2}\left[(I^\alpha) - (\mathrm{I}^\alpha)^{\mathrm{T}} \right] = \frac{1}{2}\left(m^\alpha \otimes n^\alpha - (m^\alpha \otimes n^\alpha)^{\mathrm{T}} \right) \tag{9}$$

Using Eqs. (3), (5), and (7), it can be shown that during the plastic deformation of a single crystal, the slip rate on any slip system can be expressed by:

$$\dot{\gamma}^\alpha = \lambda \frac{\frac{\mathrm{sgn}(\sigma : P^\alpha)}{\tau_y^\alpha} \exp\left[\left(\frac{\rho}{m} \frac{|\sigma : P^\alpha|}{\tau_y^\alpha} - 1 \right) \right]}{\mathrm{m} \sum_{\beta=1}^{n} \exp\left[\left(\frac{\rho}{m} \frac{|\sigma : P^\alpha|}{\tau_y^\alpha} - 1 \right) \right]} \tag{10}$$

where β represents the index of summation for slip systems, $\boldsymbol{n}$ is the number of active slip systems, m and ρ are material parameters that