MICROSTRUCTURALLY BASED FINITE ELEMENT SIMULATION OF SOLDER JOINT BEHAVIOR

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ABSTRACT

The most commonly used solder for electrical interconnects in electronic packages is the near eutectic 60Sn-40Pb alloy. This alloy has a number of processing advantages (suitable melting point of 183°C and good wetting behavior). However, under conditions of cyclic strain and temperature (thermomechanical fatigue) the microstructure of this alloy undergoes a heterogeneous coarsening and failure process that makes the prediction of solder joint lifetime complex. A finite element simulation methodology to predict solder joint mechanical behavior, that includes microstructural evolution, has been developed. The mechanical constitutive behavior was incorporated into the time dependent internal state variable viscoplastic model through experimental creep tests. The microstructural evolution is incorporated through a series of mathematical relations that describe mass flow in a temperature/strain environment. The model has been found to simulate observed thermomechanical fatigue behavior in solder joints.

INTRODUCTION

The long term reliability of an electronic package is often directly related to the lifetime of the solder interconnects in the package. The solder interconnect is no longer simply an electrical conductor but is also the structural material that holds the package together. The importance of the reliability of solder interconnects increases as the trend in the electronics industry moves toward surface mount technology, smaller joints, and finer pitch.

One of the serious challenges to solder joint reliability is failures that are a result of thermomechanical fatigue. In an electronic package, the solder is typically constrained between two materials with different coefficients of thermal expansion. Fatigue failures originate as cyclic strain is applied to solder joints when the package is exposed to thermal fluctuations caused by either ambient temperature changes or by heat dissipation from the integrated circuit devices in the package. Solder joints fail under conditions of thermomechanical fatigue by the initiation and propagation of a crack through the solder. An example of a failed surface mount joint is shown in Figure 1. In order to develop an expression for the reliability, life prediction methodologies must be developed for solders.

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The solder typically used for electronic packaging applications is the near eutectic 60Sn-40Pb alloy. This is the alloy of choice for a number of reasons: a reasonably low melting temperature of 183°C, excellent wetting behavior, and, most importantly, the alloy has a long history of use in the industry. The metallurgy and time-strain-temperature behavior of this solder alloy is surprisingly complex and is an important consideration in predicting the behavior and fatigue lifetime of the solder. The 60Sn-40Pb alloy has a two phase microstructure composed of Pb-rich and Sn-rich phases, as shown in Figure 2. During solidification of the solder joint, these phases nucleate and grow in the form of lamella (a series of flat plates parallel to one another). The phases nucleate heterogeneously in the joint and grow in the form of similarly oriented cells or colonies towards one another. When two solidifying colonies intersect, a slightly coarsened region of the material forms. This structure is metastable due to the high interfacial energy that results from the large number of phase boundaries present. Under thermomechanical fatigue conditions, this microstructure evolves as described below (and more extensively elsewhere [Frear, 1992]). At the low temperature portion of the thermomechanical cycle, damage is imparted to the solder. This damage concentrates in the weakest part of the solder microstructure which, in the case of near eutectic Sn-Pb, is at the slightly coarsened cell boundaries. Under shear deformation conditions (the deformation mode most common for electronic packages) the damage accumulates at cell boundaries, parallel to the direction of imposed strain. Upon heating, the damage in the joint anneals out through mass diffusion that causes the cell boundaries to coarsen further. The strain heterogeneously concentrates at the cell boundaries with little or no damage to the rest of the solder joint. In the process of coarsening, both the phase size and grain size within the structure grow. Eventually, the grain size in the coarsened regions becomes so large that it can no longer accommodate the imposed strain and intergranular cracks initiate and propagate resulting in joint failure. Due to the microstructural evolution that results in heterogeneous coarsening and concentration of the strain in a small area of the joint, the lifetime of Sn-Pb near eutectic alloys is shortened.
A few models proposed recently have begun to predict the reliability of solders. The constitutive relations developed by Akay, et al., [1993], Pan and Winterbottom [1990], Hacke, et al., [1993], Busso, et al., [1994] and Guo, et al., [1992] incorporate materials constants that are in the form of a grain or phase size. Sandstrom, et al., [1993] also modeled the isothermal fatigue hysteresis loops of solder that used variations in the dislocation density to incorporate the inhomogeneous microstructure. These constitutive relations are then used in a finite element code to predict stress and strain in the joints. Life is then predicted using an empirical Coffin-Manson relation. Most of the models published in the literature (including those above) have adopted the Sherby-Dorn relation for inelastic strain as the constitutive relation:

\[ \dot{\gamma}^{\text{in}} = \gamma_0 \left( \frac{b}{\gamma} \frac{\tau}{\mu} \right)^m n \]  

where \( \dot{\gamma}^{\text{in}} \) is the inelastic strain rate, \( \gamma_0 \) is a scalar function of the absolute temperature, \( b \) is the Burger's vector magnitude, \( \gamma \) is a scalar measure of the deviatoric stress, \( \mu \) is the shear modulus and \( m \) and \( n \) are positive material parameters that vary in magnitude depending on the controlling deformation mechanism which depends on the temperature and stress level. This equation indicates that when the grain size increases, the inelastic strain rate decreases and the lifetime should increase according the Coffin-Manson relation (slow strain rates = longer life). However, experimental evidence indicates that during thermomechanical fatigue heterogeneous coarsening occurs and immediately precedes failure. Therefore, this relation does not fully capture the behavior of the material under thermomechanical fatigue conditions. Furthermore, the microstructure in the above models is static and there is no mechanism to include heterogeneities or microstructural evolution.

It is clearly important that the life prediction methodology that is used for near eutectic Sn-Pb solders capture the behavior of the material under conditions of thermomechanical fatigue. This paper presents such a methodology in which the microstructure, and microstructural evolution, are critical elements to the mathematical relations in a materials-based finite element methodology to predict the behavior of near eutectic Sn-Pb solders under conditions of thermomechanical fatigue.

EXPERIMENTAL PROCEDURE
The input for the materials-based finite element simulation was a result of a number of metallurgical tests. The following is a summary of the metallurgical experiments and techniques. The solder alloy used in these tests is near eutectic 60Sn-40Pb joined to copper metallization.

**Thermomechanical Fatigue Tests**

The thermomechanical fatigue tests have been performed in a simple shear orientation and provide results on microstructural evolution and solder joint lifetime. This procedure is described in greater depth elsewhere [Frear 1989, Frear, et al., 1993]. A brief summary of the test method is given below. The specimen used to test solder joints is shown in the schematic drawing in Figure 3. The specimen consists of 18 electrically isolated solder joints that, when the specimen is gripped and pushed and pulled on the ends, deform in shear. The joints have a simple truncated spherical geometry. Strain is imposed upon the solder joints by a servo-hydraulic load frame operated under strain control. Thermal fluctuations are induced by a chamber that fits around the specimen in the load frame. Compressed air is heated and cooled by a commercial heating and cooling system that circulates around the specimen. The strain and temperature are computer controlled. The temperature extremes tested were -55°C to 125°C at 10% total shear strain. The thermal cycle consisted of a ramp in strain and temperature to the elevated temperature extreme and a 3 minute hold period, a ramp down, and another 3 minute hold at the low temperature extreme. The deformation rate for this test was $2.1 \times 10^{-4} \text{s}^{-1}$. Failures were monitored electrically by monitoring spikes in resistance. The electrical data, along with load, temperature, and strain were collected and stored on a computer. To examine the microstructure of the solder joints after testing, the samples were mounted and metallographically sectioned and polished to reveal the solder microstructure.

**Creep Tests**

The time dependent deformation behavior was determined through compression creep tests on bulk solder samples. Bulk solder specimens of the solder were fabricated by casting the alloy in a split steel mold. Prior to casting, the solder was heated to 220°C and then poured directly into a chilled mold. This was done in an effort to create the fine microstructure that is typically found in actual solder joints used in electronic packages. The mechanical response of the various solder alloys was determined through a series of isothermal uniaxial compression creep tests. The test specimens were right circular cylinders 1.02 cm diameter by 2.04 cm in length. Testing was performed on a servo-hydraulic test machine fitted with an environmental chamber and a 55kN load cell. Tests were performed on the alloys at -40°C, 23°C, 75°C, and 125°C. Each specimen
was allowed to equilibrate in the environmental chamber for 30 minutes prior to testing. A compressive prestrain of approximately one percent was applied to the sample to insure contact between the specimen and the platens. Testing was performed in load control, under a variety of stress levels, using a one second linear ramp. Platen displacement was monitored as a function of time using a digital oscilloscope with data stored on disk.

**Internal State Variable Model for Solder**

This model was developed to capture the effects of isotropic and kinematic hardening similar to Miller’s [1976] internal state variable model, and the effects of grain coarsening similar to Stone and Rashid’s [1994] two-phase solder model. The development of this model is described below.

A new internal state variable model was developed for solder. In this model, a state variable is used to capture isotropic hardening and recovery. A second-order state tensor is used to capture kinematic hardening and recovery. Coarsening is expected to have a significant effect on the state of the materials, and a state variable which accounts for the reduction in flow resistance with coarsening is included in the new model.

The proposed internal state variable model for solder has the following standard constitutive relation:

\[
\dot{\sigma} = E : (d - d^{in})
\]

where \(\dot{\sigma}\) is the stress rate, \(E\) is the fourth-order elasticity tensor, \(d\) is the total strain rate and \(d^{in}\) is the inelastic strain rate. The inelastic strain rate is given by the following equation:

\[
d^{in} = \frac{\gamma}{2} n - \frac{3}{2} f \exp \left[ \frac{\lambda_0}{R \theta} \right] \frac{\sinh \left[ \frac{\tau}{\alpha (c + \hat{c})} \right]}{\left( \frac{\alpha (c + \hat{c})}{\alpha (c + \hat{c})} \right)} n
\]

where \(\gamma\) is the magnitude of the inelastic rate, \(f, p, m\) and \(Q\) are material parameters, \(R\) is the gas constant (1.987 cal/mol*K), \(\theta\) is the absolute temperature, \(\lambda\) is the current grain diameter, \(\lambda_0\) is the initial grain diameter, \(\alpha\) is a scalar function of the absolute temperature, \(c\) and \(\hat{c}\) are state variables, and \(n\) is the normalized stress difference tensor which is given by:

\[
s \cdot \frac{2B}{n} = \frac{3}{\tau}
\]

where \(s\) is the stress deviator, \(B\) is the state tensor which accounts for kinematic hardening. \(\tau\) is a scalar measure of the stress difference magnitude:

\[
\tau = \sqrt{\frac{3}{2} \left[ s \cdot \frac{2B}{3} \right] \left[ s \cdot \frac{2B}{3} \right]}
\]

Competing hardening and recovery mechanisms are captured by the evolution equations for the internal state variables. Evolution of the scalar state variable \(c\) is given by:

\[
\dot{c} = A_1 \gamma - (A_2 \gamma + A_3) (c - c_0)^2
\]

where \(c_0, A_1, A_2,\) and \(A_3\) are material parameters. Evolution of the second-order state tensor \(B\) is given by:

\[
\dot{B} = A_4 d^{in} - (A_5 \gamma + A_6) \sqrt{\frac{2B \cdot B}{3}} B
\]
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where \( A_4, A_5, \) and \( A_6 \) are material parameters. The reduction in flow resistance with grain coarsening is captured by the scalar state variable \( \tilde{C} \). The state variable \( \tilde{C} \) is related to the grain diameter, \( \lambda \), by:

\[
\tilde{C} = A_7 \left( \frac{A_0}{\lambda} \right)^{A_8}
\]

where \( A_7 \) and \( A_8 \) are positive material parameters, and \( A_0 \) is the initial grain diameter. Note that as the grain diameter, \( \lambda \), increases, \( \tilde{C} \) decreases in magnitude which has the effect of reducing the flow resistance of the material. Evolution of the grain diameter, \( \lambda \), is given by the following equation:

\[
\dot{\lambda} = A_{11} \frac{(\nu - \nu_0)}{\lambda}
\]

where \( A_{11} \) is a material parameter, \( \nu \) is the current vacancy concentration and \( \nu_0 \) is the initial vacancy concentration. Finally, evolution of the vacancy concentration is:

\[
\nu = A_9 \gamma - A_{10} \nu
\]

where \( A_9 \) and \( A_{10} \) are material parameters.

RESULTS

The data for the creep tests is in the form of viscoplastic strain as a function of time for a given temperature and stress level. These data must be transformed into a single Arrhenius-style equation to be useful as input into the finite element model. The minimum strain rate is determined from the slope of the strain-time plots and is re-plotted as a function of stress for each testing temperature. A multivariable linear regression analysis was then performed on these data to fit the Sherby-Dorn power law creep equation:

\[
\dot{\varepsilon}_{\text{min}} = A \sigma^n e^{-\frac{Q}{RT}}
\]

where: \( \dot{\varepsilon}_{\text{min}} \) is the minimum creep strain rate (sec\(^{-1}\)), \( \sigma \) is the engineering applied stress (MPa), \( R \) is the gas constant (1.987x10\(^{-3}\) kcal/mol*K), \( T \) is the absolute temperature (K), \( Q \) is the activation energy for creep (kcal/mol), and \( A \) and \( n \) are material constants. This equation worked well for the data taken above 20°C. Below this temperature, power law breakdown occurred because the minimum strain rate decreased less rapidly with decreasing stress. Therefore, a better fit to the data was found using the Garofalo sinh equation:

\[
\dot{\varepsilon}_{\text{min}} = A [\sinh(\alpha \sigma)]^n e^{-\frac{Q}{RT}}
\]

where the terms are the same as above but the stress is modified by the hyperbolic sine and the pre-exponent of the stress, \( \alpha \), has units of (MPa\(^{-1}\)). For 60Sn-40Pb this equation becomes:

\[
\dot{\varepsilon}_{\text{min}} = 1.085 \times 10^{5} [\sinh(0.0312 \sigma)]^{3.48} e^{-\frac{12,001}{RT}}
\]

with an \( r^2 \) fit of 0.917. The data, and the curve fit to the data, are shown in Figure 4.
Figure 4 Creep test results for 60Sn-40Pb solder that were used to determine the constitutive behavior of the alloy.

The microstructural evolution was qualitatively characterized in the thermomechanical fatigue tests. Microstructural evolution occurred by heterogeneous coarsening at cell boundaries parallel to the direction of imposed strain, as shown in the optical micrograph in Figure 5. This sample was thermally cycled from -55°C to 125°C for a total of 10% shear strain. Continued cycling resulted in the formation of cracks within the coarsened band that led to joint failure, Figure 6.
The time-dependent, viscoplastic, microstructurally based finite element simulation was developed and run using the creep data discussed above. The geometry of the joint tested was a three-dimensional leadless ceramic chip carrier and the mesh for this simulation is shown in Figure 7. Constants used in the model were 5x10^{-6}mm/mm°C for the substrate coefficient of thermal expansion (CTE), 6x10^{-6}mm/mm°C for the component CTE, and 25x10^{-6}mm/mm°C for the solder CTE. A plot of the hysteresis loops from the resultant load versus temperature are shown in Figure 8. In addition to the output of stresses and strains in the joint, the model predicts the evolution of the solder microstructure as shown in Figure 9. The initial condition of the microstructure in this simulation was one of uniform grain size. After thermal cycling, the microstructure heterogeneously coarsened with the darker regions representing the coarsened regions. The coarsening occurs in two regions of the joint, under the chip carrier (region B) and at the toe of the joint (region A). The location of the heterogeneous coarsening predicted in the joint is the same as that found experimentally near the interface between the solder and the metallization at the region of highest strain (Figure 5).

Figure 7 Three dimensional mesh used in the finite element simulation of a ceramic leadless chip carrier on a ceramic board with 60Sn-40Pb solder.
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Figure 8 Plot of the predicted hysteresis loops of load versus temperature.

Figure 9 Plot of microstructural grain size. Darker regions represent coarsened regions in the joint.

DISCUSSION AND CONCLUSIONS

The results of the microstructurally dependent viscoplastic model predict heterogeneous coarsening in the regions of the solder joint that were confirmed experimentally. The simulations also predict the mechanical behavior in the form of stress-temperature hysteresis loops that are the same as those found in experimental thermomechanical fatigue tests on simplified solder joints [e.g., Frear, 1989]. The basis of the microstructural evolution development is found in equations (9) and (10) and were derived from the work by Clark and Alden [1973], who modeled grain growth by relating grain size and the number and distribution of vacancies and defects. It is possible to quantify the defects that form in the near eutectic 60Sn-40Pb solder, put them in the form of the constants found in equations (9) and (10), and predict behavior with the model. The mechanical behavior of the solder is incorporated into the model in two forms. First, the constants in equations (2) - (8) are derived from the experimental creep tests. Second, the form of the equation (specifically equation (3)) was written to incorporate the constitutive behavior based upon the experimental creep tests (equations (12) and
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Therefore, the basis of the model is the fundamental mechanical behavior that was determined experimentally.

The advantages of the predictive methodology described in this paper are that it: (a) incorporates the behavior that strongly affects solder joint reliability, (b) microstructural evolution and the strain concentrations that result from the evolution are accounted for, (c) the material constants in the simulations are based upon experimental tests that are straightforward to perform, (d) extensive lifetime data are not needed to empirically predict life because the methodology is based upon fundamental microstructural behavior, and (e) the results can be easily verified experimentally. The focus for the development of this model was that it be based upon fundamental materials behavior and that the constants present in the model have a true physical significance that could be quantified experimentally.

The developmental work for this methodology is not yet complete. Quantitative lifetime prediction must still be incorporated into the model. This involves predicting crack initiation based upon grain size in the coarsened regions and determination of the crack propagation rate. Both of these efforts are experimental in nature and will result in empirical formulations that can be sequenced with the computational simulation as it now exists. The results of this work will be published at a future date.

ACKNOWLEDGMENTS

This work was performed at Sandia National Laboratories, which is supported by the U.S. Dept. of Energy under contract number DE-AC04-94AL85000.

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