21st European Conference on Fracture, ECF21, 20-24 June 2016, Catania, Italy

Micromechanical model for describing intergranular fatigue cracking in a lead-free solder alloy

V. N. Lea*, L. Benaboua, V. Etgensa, Q. B. Taoa

aLISV, University of Versailles Saint Quentin-en-Yvelines, 45 avenue des Etats-Unis, 78035 Versailles, France

Abstract

Solder joints possess a small thickness of the order of a few grains but they remain one of the key concerns in thermo-mechanical reliability of high-power electronic systems. Fatigue lifetime of solder joints subjected to thermal and mechanical loading cycles is generally predicted based on phenomenological and macroscopic fatigue models that use the effective material properties as inputs. Such semi-empirical models will thus only provide a gross estimation of the engineering lifetime for some specific boundary and loading conditions while ignoring the deformation mechanisms at micro-scale. Microscopic analysis of fractured solder joints points rather to crack propagation at grain boundaries. Therefore, a 3D microstructure-informed model is developed in this study for reproducing the intergranular fatigue crack in the solder joint of a power module. The submodeling technique has been applied in order to only investigate the critical zone of the solder joint. A global model of the whole module is first simulated to obtain the inputs for a submodel focused on the zone of interest where failure is expected to develop. The submodel simultaneously makes use of the cohesive zone and the crystal plasticity theories to represent decohesion at grain boundaries and plastic slips in the grains of the solder joint, respectively. The needed crystal plasticity parameters were fitted out with the help of the Berveiller-Zaoui homogenization scheme using experimental data, while the parameters for the cohesive zone model were estimated from some physical quantities. Simulations of repeated thermo-mechanical loading on the power module demonstrate how cracking occurs at grain boundaries in the solder joint of the submodel. In addition, it is shown that the crack propagation rate is almost constant during the whole loading time. This suggests an ability of the present approach to give a fatigue lifetime estimate for the entire solder joint by extrapolating some specific computed quantities from the local model.

© 2016 The Authors. Published by Elsevier B.V.
Peer-review under responsibility of the Scientific Committee of ECF21.

Keywords: Intergranular fatigue fracture; lead-free solder; crystal plasticity; cohesive zone; finite element modelling.

* Corresponding author. Tel.: +33 1 39 25 49 34.
E-mail address: vannhat.le@lisv.uvsq.fr

2452-3216 © 2016 The Authors. Published by Elsevier B.V.
Peer-review under responsibility of the Scientific Committee of ECF21.
1. Introduction

The Insulated-gate Bipolar Transistor (IGBT), a power electronic device, is increasingly applied to answer demands of electrical energy management in transport systems [Lu et al. (2009)]. A description of a typical IGBT power module is illustrated in Fig. 1. It can be seen that the module contains a certain number of materials with different coefficients of thermal expansion; which results in the appearance of stresses during the thermal loading and, thus, the possibility of different types of failure modes such as wire bonding fracture [Celnikier et al. (2011)], substrate delamination, chip metallization degradation, and particularly solder joints fatigue [Benabou et al. (2014)]. In this paper, we focus on the solder joint fatigue due to its key role in the thermo-mechanical reliability of electronic packages.

Fig. 1. Schematic of an IGBT power module.

To date, the Tin-Silver-Copper (SAC) alloys have become the dominant choice in power module industries for replacing the former Tin-Lead alloys due to potential environmental concerns associated with the toxicity of lead. Prediction of fatigue lifetime of the newly-developed alloys is extremely difficult due to the complexity of their microstructure. Under passive thermal cycling (variation of ambient temperature), the substrate-to-baseplate joint turns out to be the “weak link” in the power module because the mismatch in thermal expansion between the joined materials is the highest at this location, coupled with the fact that this particular solder joint has the largest dimensions [Benabou et al. (2014)]. Observations show that the SAC solder experiences a brittle fracture mode with occurrence of an intergranular cracking path [Gong (2008)]. Although several previous studies dealt with solder joint fatigue lifetime predictions, this subject still needs to be developed. Several phenomenological models of fatigue already exist and are simply fitted to match experimental thermal/mechanical cyclic test data. A detailed review of solder joint fatigue models is found [Lee et al. (2000)]. The weakness of such semi-empirical approaches is that they are strongly related to the specific conditions of material characterization (size of samples, testing conditions, etc.) and that they are limited to a mere macroscopic description by completely ignoring issues like the scale at which the solder alloys are used in the microelectronic packages, namely in the form of extremely thin layers of the order of a few grains. Therefore, constitutive macroscopic laws, such as that of Anand (1985), do not possess the ability to describe the microscopic anisotropy of the alloys at this small scale and, thus, can prove very limited for the design of solder joints against fatigue.

With the present-day availability of cheaper and powerful computational performance, crystal plasticity (CP) theory has been implemented in many finite element codes as user subroutine for predicting the mechanisms of deformation at the grain scale, as well as for studying the solder joint reliability [Gong (2008), Bilier and Telang (2009)]. Concerning the intergranular cracking that is observed in tin-based solder joints due to their polycrystalline microstructure [Subramanian (2007), Erinc et al. (2008)], this constitutes a key issue for the fatigue behavior and failure description of these materials. The cohesive zone modeling (CZM) approach is widely known and used for evaluating the intergranular fracture in polycrystalline materials [Benedetti and Aliabadi (2013), Benabou and Sun (2014)]. For example, an analytic homogenization model, including a description of the grain boundaries behavior through the CZM approach, has recently been reported by Benabou and Sun (2014, 2015) for studying the intergranular fracture in a Cu-Ni-Si alloy.

The objective of this paper is to provide a numerical methodology for reproducing initiation and propagation of intergranular fatigue cracking in a solder joint embedded in a global model of a power module. A micromechanical finite element model, coupling CP with CZM, is developed to account for the anisotropy and plastic slips in the grain
structure on the one hand, and failure at grain boundaries on the other. Due to excessive computational requirements for simulating the whole polycrystalline microstructure of the solder layer, the sub-modeling technique has been employed in order to only investigate the critical zone of the solder joint. The global model of the power module has been first modeled, using bulk elements with the corresponding macroscopic constitutive laws, to find the joint critical zone, as well as the boundary conditions needed for the submodel. The identified critical zone is then refined in the submodel by being reconstructed with its crystalline microstructure including grains and grain boundaries. In this step, both CP and CZM constitutive laws are used for describing the behavior of the polycrystalline alloy under fatigue fracture. In addition, viscous regularization is applied to improve the convergence of the CZM.

2. Crystal plasticity model

2.1. Constitutive equations

The initial CP model of Asaro (1983) gives the ability to follow the most active slip systems, calculate the shear rate for each one of them, and obtain the total plastic deformation. The plastic slip rate can be expressed as follows [Hutchinson (1976)]:

\[
\dot{\gamma}^{(\alpha)} = \dot{\gamma}_0 \left( \frac{\tau^{(\alpha)}}{g^{(\alpha)}} \right)^n \text{sgn}(\tau^{(\alpha)})
\]  

(1)

where \( \dot{\gamma}_0 \) is the reference strain rate, \( n \) is the rate sensitivity exponent, and \( \tau^{(\alpha)} \) and \( g^{(\alpha)} \) are the resolved shear stress and the slip system strain hardness for the \( \alpha \)th slip system, respectively. The hardening law is given by:

\[
g^{(\alpha)} = \sum_{\beta} h_{\alpha \beta} \dot{\gamma}^{(\beta)} \quad \text{with} \quad h_{\alpha \beta} = \begin{cases} h(\gamma) = h_0 \sec h \left( \frac{h_0 \gamma}{\tau_0 - \tau_s} \right) \quad (\alpha = \beta) \\ q h_{\text{lat}} \quad (\alpha \neq \beta) \end{cases}
\]

(2)

where \( h_{\alpha \beta} \) represents self and latent hardening moduli, respectively. The parameters \( h_0 \), \( \tau_0 \), \( \tau_s \), and \( q \) are material constants.

This CP model is implemented for FCC systems into the widely used commercial FE software ABAQUS through the user-defined material subroutine (UMAT) of Huang (1991). The subroutine has been adapted in this work to the BCT system of the tin-based solder alloy.

2.2. Microstructure of the solder alloy

Lead-free solders contains mostly tin, usually more than 95%. Therefore, the behavior of the alloy depends mainly on the properties of tin crystals. For the sake of simplicity, the solder material is assumed in the simulation to be only made of tin grains. Previous investigations [Darbandi et al. (2014)], showed that the anisotropy of tin is characterized by six independent elastic moduli presented in Table 1.

| Table 1. Elastic constants (GPa) of Tin used in numerical analysis [Darbandi et al. (2014)]. |
|-----------------|---------|---------|---------|---------|---------|---------|
| \( C_{11} \)    | \( C_{12} \) | \( C_{13} \) | \( C_{33} \) | \( C_{44} \) | \( C_{66} \) |
| 72.3            | 59.4    | 35.8    | 88.4    | 22.0    | 24.0    |
The system of tin is defined by a body centered tetragonal crystal structure with the ratio of lattice parameters $a/c=0.5632/0.3182$ at $25^\circ$C, as shown in Fig. 2. The slip systems can be divided in 10 slip families corresponding to 32 slip systems [Zhou (2012)].

2.3. Identification of parameters for crystal plasticity

Several mean field models, based on the theory of homogenization of polycrystalline aggregates, were developed in the past and are still widely used for parameter identification of crystal plasticity, such as the models of Berveiller-Zaoui and the $\beta$-rule, for example. The Berveiller-Zaoui model has been used in this study according to the procedure described in Benabou and Sun (2014); this model does not require any additional parameters for the adjustment of the scale transition scheme and shows a good agreement in the case of radial monotone loading. The identification process is done in 2 steps: (i) a pre-identification is first carried out by using the mean field model to fit the experimental global response of the material under uniaxial tension, (ii) a FE analysis is then conducted to validate and calibrate the material parameters of the CP model. Data used for identification are found in Motalab et al. (2012) (tensile tests at three different levels of strain rate: $10^{-3}$ s$^{-1}$, $10^{-4}$ s$^{-1}$ and $10^{-5}$ s$^{-1}$). For the calibration process carried out with the software Matlab, an isotropic distribution of 100 crystallographic orientations was generated arbitrarily since the material presents no texture. The calibrated parameters are reported in Table 2 and are found to be in good agreement with recent results on lead-free solder characterization [Bieler and Telang (2009), Darbandi et al (2014)].

Table 2. Identified values of the crystal plasticity parameters.

<table>
<thead>
<tr>
<th>Crystal plasticity parameters</th>
</tr>
</thead>
<tbody>
<tr>
<td>$h$ (MPa)</td>
</tr>
<tr>
<td>6000</td>
</tr>
</tbody>
</table>

Fig. 3. (a) Aggregate of 100 grains; (b) Simulated vs. experimental behaviors of the aggregate under different strain rates.

In order to assess the predictive capability of the mean field model used for calibration, a FE computation using the identified CP parameters is carried out on a synthetic 100-grain aggregate with random crystallographic orientations, as shown in Fig. 3a. Experimental curves, corresponding to tensile testing under 3 different strain rates,
are compared to FE results in Fig. 3b, showing that the differences between the experimental behaviors and the FE predicted ones are largely acceptable. This means that the calibrated CP parameters can be used with confidence in the following sections in order to describe plastic slips in the grains of the solder joint.

3. Modelling of decohesion at grain boundaries

3.1. Theory

The CZM approach was used in this work to represent the intergranular fatigue cracking in the solder joint. Details on the constitutive equations of the model have been discussed in a previous study [Benabou et al. (2013)], in which a global damage variable is incorporated in order to explicitly reproduce the irreversible damage under cyclic loading. Evolution of the damage variable is given as:

\[ d = \frac{(1-d)k'_n}{G'_n - G''_n} \langle \delta \rangle \langle \delta \rangle \]

where \( k'_n \) is the undamaged normal stiffness of the interface and \( \delta \) its effective opening during loading, and \( G'_n \) and \( G''_n \) are the initial mixed-mode damage threshold and the mixed-mode fracture energy, respectively. To deal with numerical convergence issues when damage occurs in the cohesive elements, the model has been complemented with a viscous regularization technique which consists in using a viscous variable \( d_v \) instead of \( d \) by applying the following rate constitutive equation:

\[ \dot{d}_v = -\frac{1}{\mu} (d - d_v) \]

where \( \mu \) is a viscosity parameter representing the relaxation time of the viscous system. Further details of this method can be found in [Benabou and Sun (2015), Simonovski and Cizelj (2013)]. The traction-separation law of the cohesive elements has been implemented in the UEL subroutine of ABAQUS.

3.2. Material parameters

The input parameters for the CZM includes the stiffness \( k_n \), the damage threshold energy density \( G'_n \) and the fracture energy density \( G''_n \) for each particular mode \( x \) (\( x=\text{I, II or III} \)). The initial tensile and shear stiffnesses of the cohesive elements can be derived from the elastic and shear modulus of the solder bulk material [Benabou et al. (2013)]:

\[ k_n = \frac{E}{t_{nxyz}} \quad \text{and} \quad k_i = \frac{G}{t_{ixyz}} \]

where \( E \) and \( G \) are the elastic young and shear moduli of the bulk element, and \( t_{nxyz} \) is the fictitious thickness of the cohesive element. The elastic constants of the solder, which are here assumed independent of temperature for simplicity, are \( E = 41000 \text{ MPa} \) and \( G= 15070 \text{ MPa} \) [Motulab et al. (2012)]. The damage threshold energy density, \( G'_n \), and the fracture energy density, \( G''_n \), for mode \( x \), are two decisive parameters in determining the evolution of the intergranular cracks. These fracture energies can be measured by experiments, but there is no efficient method to do this, particularly at the microstructure scale. In this paper, the grain boundary fracture energy in mode-I is determined based on the surface energy, \( \gamma_s \), and the grain boundary energy, \( \gamma_{gb} \) following an approach presented in Simonovski and Cizelj (2013). For tin element, the surface energy is taken as \( \gamma_s = 0.709 \times 10^{-3} \text{ mJ/mm}^2 \) with a ratio of \( \gamma_{gb}/\gamma_s = 0.24 \) [Vitos et al. (1998), Tyson (1977)]. Fracture energies in the tangential modes (II and III) have been assumed equal to that of mode-I, e.g. \( G''_n = G''_x = G''_y \). All the CZM parameters used in the FE analysis are reported in Table 3. With
regard to the damage threshold energy density, $G_c$, the value is expected to be very small in the case of solder alloys. Since this parameter does not significantly influence the final lifetime prediction, its value is chosen equal to 2% of the fracture energy density $G_c$.

Table 3. Estimated parameters for the CZM approach.

<table>
<thead>
<tr>
<th>$t_{cr}$ (mm)</th>
<th>$E$ (MPa)</th>
<th>$G$ (MPa)</th>
<th>$G_c^I$ (mJ/mm)</th>
<th>$G_c^{II}$ (mJ/mm)</th>
<th>$G_c^{III}$ (mJ/mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.01</td>
<td>41000</td>
<td>15070</td>
<td>0.0014</td>
<td>0.0014</td>
<td>0.0001</td>
</tr>
</tbody>
</table>

4. Finite element simulation

4.1. Numerical methodology

Simulation of the IGBT module is done according to a two-step procedure illustrated in Fig. 4. Firstly, the global model is built based on the real geometry of the power module whose components are given their distinct thermomechanical properties. Due to the symmetry in the 3D geometry, only one-fourth of the model is considered, resulting in a substantial reduction of the model size. The visco-plastic behaviour of the solder alloy is governed by the classical Anand law [Anand (1985)]. The model parameters estimated by Motalab et al. (2012) are taken in our work. Concerning the properties of the other materials used in the power module (silicon chip, copper substrate, aluminum base plate), they are assumed to behave elastically with temperature-dependent properties.

![IGBT power module](image1)

![Submodel with microstructure](image2)

![Intergranular crack propagation](image3)

Fig. 4. Numerical methodology for studying crack propagation in the solder joint.

The global model of the IGBT module is simulated under thermal loading with cycles of 5700 seconds and temperature range from 10°C to 80°C (thermal shocks). The critical zone in the solder layer is where energy dissipation is the highest in the stabilized cycle. This region and its vicinity will be modeled more accurately in the submodel. The nodal displacements at the border of the detailed zone, obtained during the stabilized cycle, are also stored to serve as boundary conditions in the submodel.

Secondly, the submodel is generated by keeping a smaller region of the IGBT global model, comprising the critically loaded region of the solder joint and its vicinity made of the materials coming into contact with the zone of interest. The latter, located in the corner of the solder layer, is approximated by a cubic part (Fig. 4) which is modeled by a grain microstructure made of crystals and grain boundaries. The submodel is loaded during 15 thermal cycles so that intergranular cracking can occur in the polycrystalline aggregate. Fatigue behaviour of the solder joint is finally investigated using results obtained on the refined submodel, giving the ability to do extrapolation of some predicted quantities over the whole solder layer when cyclic stabilization is reached.
4.2. Results of simulation

Fig. 5 shows the grain boundary damage evolution for some of the 15 loading cycles. Most of the early damage initiates at the intersection of grain boundaries with the external surface of the model. A smaller fraction of damage initiation is found inside the model, mostly at the triple lines. This occurrence damage within the material may be explained by the increase of normal stresses in the cohesive zone elements located at the triple lines. This can be caused by the use of triangular prism cohesive elements as this is not the case when rectangular prism cohesive elements are employed [El Shawish et al. (2013)]. However, the application of rectangular prism elements is not possible here since it requires a conformal mesh between the grain boundaries and the grains. Another observation is that the dominant damage nucleation occurs in the same critical zone as where deformation is the highest in the global model. Thus, the present microscopic modeling of the solder joint has the ability to reproduce the fatigue crack initiation at the corner of the layer near the bottom interface, as well as its propagation from outside to inside by following an almost horizontal plane path. Such a numerical result is corroborated by previous experimental studies of this type of failure, as illustrated in Fig. 6 [Dupont et al. (2005), Perpina et al. (2010)].

In Fig. 7, the total number of damaged cohesive elements is plotted as function of the number of cycles. The shape of the curve shows that an interesting correlation exists between damage and the number of loading cycles, which can be approximated by a second-order polynomial evolution trend. The quadratic function, obtained by data fitting, is used to establish a fatigue criterion as follows. The cohesive element mesh size being almost uniform in the model, the average damaged area is then a linear function of the number of damaged elements. This suggests that the damaged area is a quadratic function of the number of cycles. This result is in accordance with previous studies [Pierce et al. (2008)]. Once this quadratic relation between the crack area and the number of cycles is soundly established based on longer simulations, lifetime of the whole solder joint can be predicted by a simple extrapolation of the obtained quantities in the local model.
5. Conclusions

In this work, a numerical methodology is proposed for reproducing the intergranular fatigue crack in the critical zone of the solder joint. The submodelling technique has been used to reduce the computational cost of the simulations. The global model of the power module is first simulated with the bulk material properties of all the components to find both the critical zone in the solder joint and the boundary conditions to be applied to the submodel of the module. In the submodel, the solder joint is reconstructed at grain structure level using a crystal plasticity model for the grains and cohesive elements for the grain boundaries. The parameters for crystal plasticity of the lead-free solder are calibrated using the Berveiller-Zaoui transition rule to fit tensile test data, while the cohesive zone parameters are obtained using some assumptions on the stiffness of the interface and its energy. It was demonstrated that the developed methodology could successfully reproduce the intergranular crack initiation and propagation in the solder joint during fatigue loading. Damage initiates at intersections of grain boundaries at the external surface. The dominant crack develops from the corner of the solder layer near the bottom interface and propagates towards the interior, in accordance with previous experimental observations. Another interesting result obtained in this work is the nearly stable crack propagation rate through the grain boundaries of the solder alloy during the thermal loading cycles. This suggests that the global fatigue lifetime of the solder joint can be predicted by simple extrapolation from quantities obtained in the local model.

Acknowledgements

We want to express our gratitude in particular to Jean Michel MORELLE and Philippe POU Menu from VALEO for their general advice.

References


