Void nucleation by vacancy condensation

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A computational simulation of Kirkendall voiding in metallic materials is presented. After a brief explanation of the phenomena and its consequences on the reliability of microelectronic components we introduce a constitutive model for void nucleation and growth which is based on vacancy diffusion and rate-dependent inelastic deformation. This model can be used to predict the temporal development of voids in solder during thermal cycling and/or impact loading. A numerical study illustrates the potential of the model for the failure analysis.

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1 The Problem

Solder joints of microelectronic circuit units are to an increasing extent made of tin alloys (*e.g.*, Sn-Ag or Sn-Ag-Cu). These joints hold the multi-layered unit in position and, in addition, the solder joints provide electrical conductivity between the metallic (coppered) layers of the units. "Aging" of solder, such as phase separation, coarsening or the formation of InterMetallic Compounds (IMCs), as well as the formation and growth of pores and cracks in the vicinity of heterogeneities significantly effect the life expectation of the joints and considerably influence the reliability of the whole component.

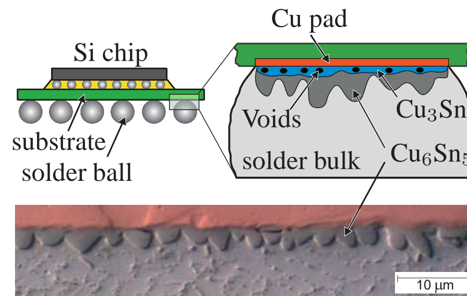

Fig. 1 Intermetallic Compounds at copper-solder interfaces in microelectronic components, micrograph courtesy of K. Müller, Neue Materialien Bayreuth, Germany, 2005.

During manufacturing the (molten) Sn-rich solder wets the copper pad and IMCs are formed due to an interfacial reaction. These IMCs are relatively stiff and considerable stresses are induced in these regions due to mismatching thermal expansion. Furthermore the IMCs show different diffusion coefficients w.r.t. Cu and, therefore, the diffusion of Cu from the pad via the interface Cu/Cu_3Sn into Cu_3Sn is much *slower* than the diffusion of Cu from Cu_3Sn into the Cu_6Sn_5 scallops, which also cannot be "corrected" by the vice versa diffusion of Sn via the Cu_6Sn_5/Cu_3 interface. As a consequence vacancies on the lattice sides remain within the Cu_3Sn compounds, which coalesce due to vacancy diffusion to *macroscopic* voids. Moreover, primarily initiated by stress peaks in the vicinity of the voids they further grow and merge to cracks, which may proceed such that failure occurs.

2 Constitutive Model for Void Nucleation and Growth

In [2, 3] the authors developed a detailed model for KIRKENDALL voiding in IMCs. The main ideas are sketched here shortly. To this end we distinct between void *nucleation* and ∼*growth*. The nucleation process is understood, beyond the atomic scale, to be the result of vacancy diffusion. The resulting vacancy "cluster" is, if a critical amount of vacancies would be reached, treated as a nucleated macroscopic void. However, these voids do not exclusively grow due to diffusion. In particular, local mechanical stresses or surface energy effects result in proceeding void growth and coalescence.

Nucleation. The following assumptions are established: (*i*) the voids are spherical with radius a, and (*ii*) surrounded by a supersaturated matrix of radius b, $b \gg a$, characterized by the background concentration c_∞, (*iii*) the tracer diffusion coefficient, D_V, is constant and isotropic, and (*iv*) we assume stationary vacancy diffusion. The resulting boundary problem for the vacancy volume concentration c is known as Ficks law (in spherical coordinates): $\frac{\partial}{\partial r}\left(r^2 \frac{\partial c}{\partial r}\right) = 0$. With $c(r = a) =$

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$c_a = c_0 \exp[a^*/a]$ we obtain $c(r) = c_\infty - (c_\infty - c_a)\frac{a}{r}$. Symbol a^* denotes a product of material constants. Note that $c_\infty > c_a$ must hold for void growth. Then follows an evolution equation in form of an ODE for $a(t)$, namely:

$$\dot{a} = \frac{D_V}{a}\left[c_b - c_0 \exp\left(\frac{a^*}{a}\right)\right]. \tag{1}$$

Growth. We postulate the existence of an energy function associated with the deformation of expanding voids and embedding material. The energy contributions result from the deformation of a void subjected to the power of a remote pressure $p(t)$. These are: *(i)* the energy of the free void surface, *(ii)* the deformation energy of the embedding material and the rate power *(iii)* of creep deformation and *(iv)* of diffusion. An action integral $I(\dot{a})$ can be formulated as sum of all rate of energy and power contributions. HAMILTON's principle then requires stationarity of the action integral $\delta I(\dot{a}) = 0$, and we obtain for growing voids in a viscous-ideal plastic material the expression

$$0 = -4\pi p(t)a^2 + \frac{8\pi}{3}\sigma_0 a^2 \log\left(\frac{b_0^3 - a_0^3 + a^3}{a^3}\right) + \frac{16\sigma_0\pi}{3\dot{\epsilon}_0}a^4\dot{a}\left(\frac{1}{a^3} - \frac{1}{b^3}\right) + 8\pi a\gamma + \frac{E_v\dot{a}}{D_V} - \frac{E_v}{a}(c_\infty - c_a)\,, \tag{2}$$

where $p(t)$ is the external pressure resulting from mismatching expansion during thermal cycling, σ_0 is the yield stress (here: 450 MPa), $\dot{\epsilon}_0$ is a reference strain rate (here: 10^{-3}s^{-1}), γ is the surface energy per unit undeformed area (here: 1 N/m). The diffusion constants are here: $E_v = 10^{-6}$ N/m , $a^* = 5 \cdot 10^{-6}$ m and $D_V = 10^{-17}$ m^2/s. Eq. (2) can be solved (numerically) for all different void sizes of interest to get the rate of void growth $\dot{a}(a)$.

3 Evolution of an Ensemble of Voids

In order to investigate an *ensemble* of voids with different initial radii we introduce a local void size distribution function $\tilde{d}(a,t)$. Then we establish for a constant number of voids a balance equation for the void size distribution and solve it for a discrete void size distribution.

$$\frac{\partial \tilde{d}(a,t)}{\partial t} + \dot{a}(a)\frac{\partial \tilde{d}(a,t)}{\partial a} = 0 \tag{3}$$

A GAUSSian distribution of 15 different initial void radii, $a = 10 \ldots 150$ nm is assumed. Within several stages of thermal cycling we obtain the temporal development of $\tilde{d}$ as illustrated in Figure 2. The initially symmetric distribution changes to an asymmetrical distribution in such a way that the fraction of smaller voids decreases and the bigger voids grow. Such results are well known from so-called LSW-theories for OSTWALD ripening, [1], where bigger "grains" grow at the expense of the smaller ones due to the GIBBS-THOMSON effect. In our model this effect also appears in the first stages of void growth, in which vacancy diffusion dominates. During proceeding growth the voids reach a size, for which the evolution is characterized primarily by elastic-plastic deformation. For such stages the distribution function considerably differs from a typical LSW distribution. In particular the number of large voids extremely exceeds the number of small voids.

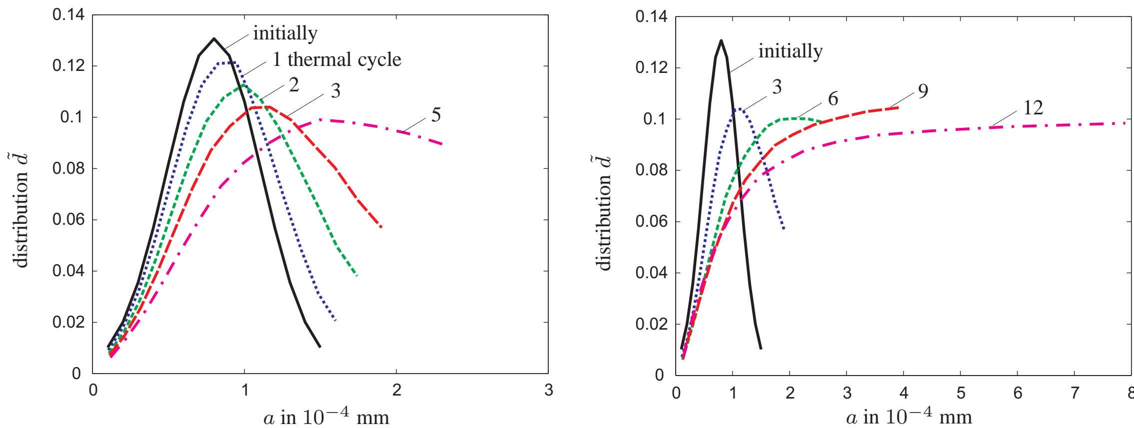

Fig. 2 Development of a GAUSSian void distribution after thermal cycling: *left*: short time behavior of $\tilde{d}$. *right*: long time behavior of $\tilde{d}$.

References

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