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On the effect of Kirkendall voids on solder joint reliability

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A model for the theoretical description of KIRKENDALL voiding is presented based on vacancy diffusion and plastic deformation of spherical voids. We start with a phenomenological explanation of the KIRKENDALL phenomenon and discuss its consequences on microelectronic reliability. After that a constitutive model for void growth is introduced, which, for instances, can be used in order to predict the temporal development of a certain void distribution. We end this paper with exemplary numerical studies.

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1 Introduction

Today's lead free solder materials (*e.g.*, SnAgCu, SnAg, SnCu) used in microelectronic packaging show a wide range of microstructural effects. A phenomenon, which considerably determines the joining capability between the functional unit and the circuit board, is the formation and growth of InterMetallic Compounds (IMCs) in the interface region between the solder and the copper pad (*cf.*, Fig. 1). Here we typically find *two* kinds of IMCs: **(a)** a thin layer of Cu_3Sn on the Cu-pad side followed by **(b)** Cu_6Sn_5 scallops on the solder-bulk side, *cf.*, Fig. 1. These compounds grow due to an interfacial reaction between Cu and Sn enabled by migration of Cu from the pad into the solder bulk.

In contrast to the solder, which is usually a highly *ductile* material with a relatively small Young's modulus, the IMCs are *brittle* and extremely stiff. Consequently, in these regions considerable stresses are induced due to the inherent mismatch of thermal expansion during thermal cycling. 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 invers diffusion of Sn through the Cu_6Sn_5/Cu_3 interface, [2]. As a consequence vacancies on the lattice sides remain within the Cu_3Sn IMC, which coalesce to *macroscopic* voids due to vacancy diffusion. Moreover, primarily initiated by stress peaks in the vicinity of the voids further void growth and micro crack formation is observed, which may proceed failure.

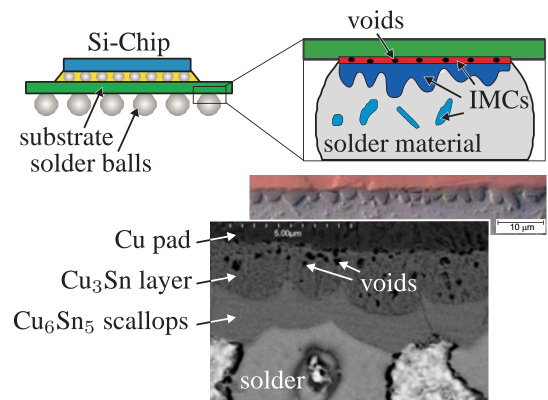

Fig. 1 KIRKENDALL voiding in microelectronic packaging, micrograph courtesy of [1].

2 Constitutive Model for Void Nucleation and Growth

In what follows we distinct between void *nucleation* and ∼*growth*. Here nucleation is associated, beyond the mechanism of vacancy formation on 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 because of diffusion. In addition, local mechanical stresses or surface energy effects promote void growth and coalescence.

2.1 Void Nucleation

First of all the following assumptions are established which are, in part, adopted from the well-established LSW theory, [3]: (*i*) the voids are spherical with radius a, *cf.*, Fig. 2, and (*ii*) are surrounded by a supersaturated spherical matrix of radius b characterized by the background concentration c_b, (*iii*) the diffusion coefficient D is constant and isotropic, and (*iv*) we assume stationary vacancy diffusion, *i.e.*, $\partial c_{\text{vac}}/\partial t \ll \partial J_{\text{vac}}/\partial x$. The following boundary value problem results for the vacancy volume concentration c presuming that $b/a \to \infty$:

$$\frac{\partial}{\partial r}\left(r^2\frac{\partial c}{\partial r}\right)=0 \quad \text{with} \quad c(r=a)=c_a=c_0\exp\left(\frac{2\gamma V_v}{akT}\right)\ ,\ c(r=b)=c_b \quad \Rightarrow \quad c(r)=c_b-(c_b-c_a)\frac{a}{r}\ , \quad (1)$$

with $c_0=\exp[-E_v/kT]$, γ: surface tension, E_v: vacancy formation energy, k: BOLTZMANN constant, V_v: atomic volume.

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Note that $c_b > c_a$ must hold for void growth. Hence, there exists a critical nucleation radius, a_0, with the condition $c_b > c_0 \exp[2\gamma V_v / a_0 kT]$. However, following the strategy explained in [4] one can derive an evolution equation in form of an ODE for $a(t)$ and a diffusion rate potential Φ, namely:

$$\dot{a} = \frac{D}{a}\left[c_b - c_0 \exp\left(\frac{2\gamma V_v}{akT}\right)\right] \quad \text{and} \quad \Phi(\dot{a}, a) = \frac{E_v \dot{a}^2}{2D} - \frac{E_v \dot{a}}{a}(c_b - c_a)\ . \tag{2}$$

2.2 Void Growth

In [5] the authors developed a model for void growth in *visco-plastic* metals, which can be applied in a similar manner to the case of KIRKENDALL voiding incorporating, additionally, the diffusion rate potential of Eq. $(2)_2$. Furthermore we assume that the power density of the external load $\dot{p}$ is completely consumed by the power density required for (**a**) internal (elastic-) plastic deformations $\dot{w}$, (**b**) the storage of surface energy at the interface void/matrix $\dot{s}$ and (**c**) diffusion processes Φ, *viz.*:

$$\frac{\mathrm{d}p(t)}{\mathrm{d}t} = \frac{\mathrm{d}\,(w+s)}{\mathrm{d}t} + \Phi\ . \tag{3}$$

Here the "pressure" results from thermal cycling and can be calculated by the relation $p(t) = 3\kappa(a)\alpha[T_0 - T(t)]$ with the thermal expansion coefficient α and the (effective) bulk modulus κ. The surface contribution is given by $s = 4\pi a^2 \gamma$ and the deformation energy reads, *cf.*, [5], $w = \int \sigma_y \dot{\epsilon}_p(t)\mathrm{d}t$ with the plastic strains $\epsilon_p = \frac{\sigma_0(T)}{E(T)}(\frac{\sigma}{\sigma_0})^n$, (RAMBERG-OSGOOD power law). Eqs. (2-3) in combination with kinematical assumptions for spherical voids, *cf.*, Fig. 2 and [5], and a straightforward calculation yields the following ODE for $a(t)$:

Fig. 2 Illustration of the vacancy diffusion and of the spherical shell model, [5].

$$0 = -4\pi p(t) a^2 \dot{a} + \frac{8\pi}{3}\sigma_0 a^2 \dot{a} \log\left(\frac{b_0^3 - a_0^3 + a^3}{a^3}\right) + 8\pi a \gamma \dot{a} + \frac{E_V \dot{a}^2}{D_V} - \frac{E_V \dot{a}}{a}(c_b - c_a)\ , \tag{4}$$

which can be solved with appropriate initial conditions $a(t=0) = a_0$ and $b(t=0) = b_0$.

3 Exemplary Results & Concluding Remarks

Fig. 3 shows selected results obtained from numerical studies using the parameters of Table 1. Here $a(t)$ increases and stagnates at a limit value. Furthermore the oscillating character of r due to the cycling deformation is temporally shifted, which indicates that the expansion of small void regimes is driven by diffusion. Nevertheless the maximum radius grows monotonically and is bound due to the amplitude of thermal cycling. However, by means of the presented model one can now investigate a void regime consisting of different initial radii, [5]. The resulting temporal evolution for the void distribution function can, in turn, be used in order to define suitable mean values of material data or for a the definition of a damage parameter, *cf.*, [5].

D [m^2/s]	c_0	c_b	$2\gamma V_v/kT$	γ [N/m]
10^{-17}	10^{-6}	10^{-4}	$5 \cdot 10^{-6}$	1
E [GPa]	κ [GPa]	μ [GPa]	σ_0 [MPa]	α [1/K]
100	80	50	450	$19 \cdot 10^{-6}$

Table 1 Parameter used in the simulations.

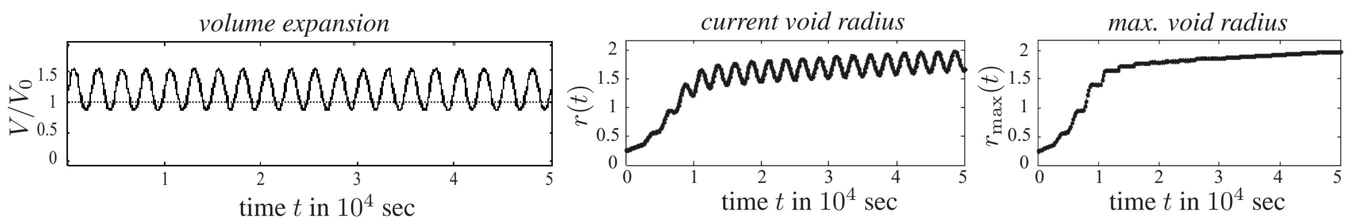

Fig. 3 Numerically results obtained for the volume expansion due to thermal cycling and for the different void radii in 10^{-5} mm.

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