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Monte Carlo Method Applied to the ABV Model of an Interconnect Alloy

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Abstract. A Monte Carlo (MC) simulation of a 2D microscopic ABV (metal A, metal B and void V) Ising model of an interconnect alloy is performed by taking into account results of Finite Element methods (FEM) calculations on correlated void-thermal effects. The evolution of a homogeneous structure of a binary alloy containing a small percentage of voids is studied with temperature cycling. The diffusion of voids and segregation of A type or B type metals is a function of the relative interaction energy of the different pairs AA, BB, AB, AV and BV, the initial concentrations of A, B and V and local heating effect due to the presence of clusters of voids. Voids segregates in a matrix of A type, of B type or AB type and form large localized clusters or smaller delocalized ones of different shapes.

1. Introduction

This work focuses on the physics of failure which is at the heart of the degradation observed in the interconnecting alloys (ICA) used as solder joints in mechatronic devices. The presence of intermetallics, voids, delamination at adjacent boundaries in a power mechatronics module [1] reduces the reliability of these devices. The analysis of the root cause of the failures can either be performed from experimentation or from simulation. The purpose of this work is to investigate how the results of Monte Carlo's simulation in the frame of the Ising ABV model [2] may provide a solution to the design of reliable mechatronic devices. Simulation is a means to drive the designer towards the best possible reliable design solutions when the model is used within the reliability based design optimization (RBDO) method [3] which combines design and reliability optimization. RBDO which leads to more efficient design and a rigorous monitoring of the design is then able to predict and detect failure modes of the designed system. Different types of innovative materials to meet regulations about hazardous substances are assembled in a power mechatronics module. The active silicon based

transistor chip that is interconnected to a copper busbar through lead alloy solder joints acts as a switch that controls the electronic current density within the chip. Although the copper busbar is cooled from the bottom by an aluminium cooling water case through an electrical insulating ceramic layer, the joule heating give rise to a thermal gradient in assemblies. As a result delamination and propagation of cracks enhanced by the differences in the coefficient of thermal expansion (CTE) of the materials in contact reduces the reliability of the device. Ageing of interconnections (solder, wire bonding …) and bulk materials (copper busbar, silicon chip, insulating ceramic …) occurs through repeated current density cycling. Figure 1 a) and b) shows the defects that are present in interconnect alloys before and after thermal shocks.

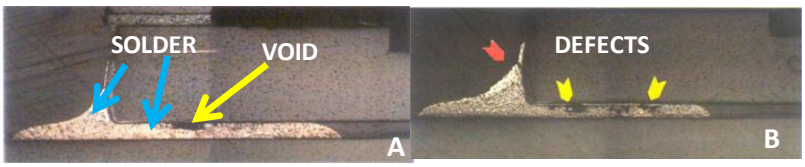

Figure 1: a) Cross-section after solder paste thermal reflow b) Cross-section after 1000 thermal shocks test -40°C/140 °C 1h/1h

2. Finite element methods to model the thermal effect of voids

In Figure 2, the x-ray tomography image of a component soldered on a FR4 substrate [4], shows the air bubbles on the thickness of the lead-free solder ICA. These defects can occupy between 10% and 60% of the surface and throughout the thickness of the solder.

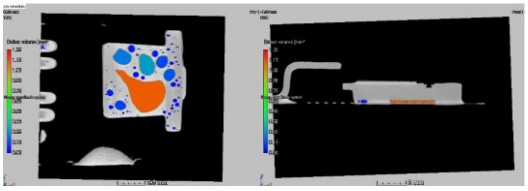

Figure 2: *x-ray tomography image of an electronic component soldered on a FR4 substrate, showing air bubbles on the thickness of the lead-free solder*

Thermal effects in the ICA in the presence porosities were modeled and simulated by FEM. Results are shown in figure 3. The main results are that the increase in the temperature of the silicon chip is a function of the spatial distribution and size of defects, with a maximum temperature localized above the larger defect. A study based on the shape of the defects had also shown similar results in the evolution and mapping of temperature. These defects behave as heat traps that cause local temperature rise [5]. If the defects are uniformly distributed the risk of lift off of the chip is more likely to occur.

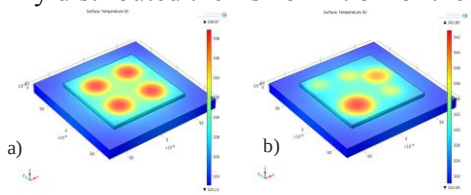

Figure 3: *Temperature mapping with circular defects distributed in the ICM: a) regularly (radius 2.2 mm, porosity 40%), b) at random (maximum radius 1.8 mm, porosity 40%)*

The position of the defect influences the maximum temperature reached (62°C). It is higher if a defect is near the center of the chip than close to the borders. In dynamic mode when the mechatronics module is subjected to power cycles, the difference in temperature will necessarily increase. Consequently, these heat trapping zones will induce thermo-mechanical stresses in the chip. Simulation results show that the maximum temperature depends on the degree of porosity. For the same degree of porosity it is localized on the defect of larger radius. One finds: T max (n = 1)> T max

(n = 2)> T max (n = 3) where n is the number of defects. There is an increase of the maximum temperature with the size of the defects as the porosity ratio increases. The maximum deformation increases with the porosity up to 21% and beyond this threshold it decreases. RBDO method can be applied to determine the thermo-mechanical properties of the materials assembled in a mechatronic device. This method takes into account the uncertainties of the physical parameters in the context of ageing of interconnections of the devices during operation, and then optimize the finite element model used to determine the elastoplastic behavior of the material. The ABV model can also be implemented in the RBDO method to simulate the properties of innovative materials and identify the different schemes along which voids and cracks develop in the alloy and thus limit the uncertainties on the thermo-mechanical parameters.

3. The ABV model

The Ising model is a generic model that can be applied to different phase transition physics as can be observed for example in Magnetic Spin Cross-Over (SCO) compounds [2], Binary alloy, Grain boundary energy (Potts model). Based on the equivalence between the Ising-lattice gas and a binary alloy, the ABV model was developed by Yaldram and Binder [6-8], where A and B stand for two different metals and V for void or a vacancy. It has been widely used to study the configurational statistics of alloys on a microscopic basis using phenomenological atomic interaction parameters or values obtained from numerical simulation [9-10]. This model has been discussed by Tafa, Puri and Kumar [11] in connection to several other models BEG, FL, PS, PG or JM as referenced in [11] in terms of phase separation in ternary mixtures leading to characteristics features of the domain growth process.

In order to get an insight in the solutions to implement to reduce observed degradation leading to failures in the interconnexion of a mechatronic module, a Monte Carlo simulation in the Metropolis scheme is applied using the ABV model. Diffusion or aggregation effects are discussed in terms of initial conditions and interaction energies between the metal atoms. To study the temperature effect on the homogeneous structure of a binary alloy of constant composition containing voids, the simulation is performed on a 2D microscopic Ising model by using the following three states Hamiltonian which can be derived from the physical configuration [11]:

$$H = H_0 - J\sum_{\langle ij\rangle}^{NN}\sigma_i\sigma_j - K\sum_{\langle ij\rangle}^{NN}\sigma_i^2\sigma_j^2 + U\sum_{\langle ij\rangle}^{NN}(\sigma_i^2\sigma_j + \sigma_i\sigma_j^2) \tag{1}$$

where σ can be set to -1, 0, 1. In equation 1, the different parameters K, J and U are defined by the following equations:

$$\begin{aligned} J &= \frac{1}{4}(2\varepsilon_{AB} - \varepsilon_{AA} - \varepsilon_{BB}) \\ K &= \varepsilon_{AV} + \varepsilon_{BV} - \varepsilon_{VV} - \frac{1}{4}(\varepsilon_{AA} + \varepsilon_{BB} + 2\varepsilon_{AB}) \\ U &= \frac{1}{4}(\varepsilon_{AA} - \varepsilon_{BB}) + \frac{1}{2}(\varepsilon_{BV} - \varepsilon_{AV}) \end{aligned} \tag{2}$$

Where ε_{ik} ($i = A, B$ or V and $k = A, B$ or V) are the interaction energy parameters between the metal atoms A, B and void V. In order to model the observed diffusion of intermetallics in interconnexion materials, the interaction parameters ε_{AA}, ε_{BB} and ε_{AB} are adjusted and the time evolution of this material pseudo-spin configuration is calculated. There are no pairwise interaction terms involving voids but phase separation is mediated by vacancies. The physical processes that enable segregation are due to vacancy atom exchanges rather than exchanges between A and B. J determines the ordering of the system. In the absence of vacancies, the systems tends to mix if J < 0 and become homogeneous (complete disorder) if J > 0, then the system tends to segregate in A and B atoms. Parameters K/J and U/J account for the order or disorder that result from one of these two possible configurations. The

results are discussed in terms of intensity of the interaction parameters, void percentage and local heating effect as modelled by FEM during cycling.

4. Results and discussion

Simulations were performed on a square containing 10000 atoms with an approximate atomic radius of 1.6 10^{-10} m on a surface area of 256 nm^2. Different cases were considered to determine the effect of the interaction energies on the segregation of A and B atoms as shown in figures 4 to 6. In figures 4 and 5, the initial conditions correspond to 20% of voids, with A and B in equal proportions (40%) on the square lattice and in figure 6, 80% of A, with B and V in equal proportions (10%) and the pair interaction are scaled with respect to $\varepsilon_{VV} = 1$ and the temperature T.

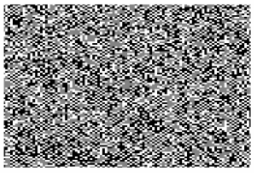

Figure 4 a). Start (1 Mc cycle)**,** A: white, B: black, V: grey (A=B = 40%, V= 20%, $\varepsilon_{AA}=\varepsilon_{AB}=\varepsilon_{AV}=0.6$; $\varepsilon_{BB}=\varepsilon_{BV}=0.4$)

Figure 4b). Segregation (300 Mc cycles)**,** A: white, B: black, V: grey (A=B = 40%, V= 20%, $\varepsilon_{AA}=\varepsilon_{AB}=\varepsilon_{AV}=0.6$; $\varepsilon_{BB}=\varepsilon_{BV}=0.4$)

In the three figures 4 to 6, voids segregate with AV interfaces only. In figure 4 B segregates slightly with AB interfaces only and segregation is more pronounced in figure 5.

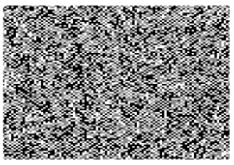

Figure 5 a). Start (1 Mc cycle)**,** A: white, B: black, V: grey (A=B = 40%, V= 20%, $\varepsilon_{AA}=\varepsilon_{AB}=\varepsilon_{AV}=\varepsilon_{BB}=0.6$; $\varepsilon_{BV}=0.4$)

Figure 5 b). Segregation (300 Mc cycles)**,** A: white, B: black, V: grey (A=B = 40%, V= 20%, $\varepsilon_{AA}=\varepsilon_{AB}=\varepsilon_{AV}=\varepsilon_{BB}=0.6$; $\varepsilon_{BV}=0.4$)

Figures 4 and 5 show no segregation of A while in figure 6, A segregates. In figure 4, voids segregates in an AB matrix and in figure 5, voids and B segregates in an A matrix.

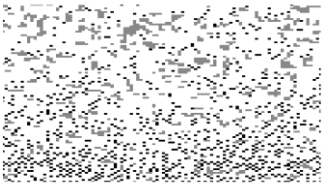

Figure 6 a). Start (1 Mc cycle)**,** A: white, B: black, V: grey (A = 80%, B=V= 10%, $\varepsilon_{AA}=\varepsilon_{AB}=\varepsilon_{AV}=0.6$; $\varepsilon_{BB}=\varepsilon_{BV}=0.4$)

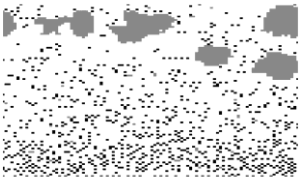

Figure 6 b). Segregation (300 Mc cycles)**,** A: white, B: black, V: grey (A = 80%, B=V= 10%, $\varepsilon_{AA}=\varepsilon_{AB}=\varepsilon_{AV}=0.6$; $\varepsilon_{BB}=\varepsilon_{BV}=0.4$)

In figure 6, voids and A segregates in a B matrix.
Different cases in interaction energies have been simulated either by changing the relative values of the interaction energies or by reproducing static temperature cycling between 300K and 600 K.
When all energies are equal, then larger size clusters of vacancies are favoured. When $\varepsilon_{AA}=\varepsilon_{AB}=\varepsilon_{AV=}$ - $0.6E_0 < \varepsilon_{BB}=\varepsilon_{BV=}$ - $0.4E_0$,then clusters of smaller sizes that spread in an AB matrix with A at the borders are simulated. When segregation by vacancies is enhanced through the reference energy E_0, vacancy clusters tend to increase in size and get localized. If $\varepsilon_{AV=}$ $-0.6E_0 < \varepsilon_{BV=}$ - $0.4E_0$, then voids drives A spatially with A at the borders of the vacancy clusters.
Cycling of temperature between 300K and 600K do not have a marked effect on the distribution of the vacancy clusters. But when local temperature rise are taken into account in the algorithm to mimic the trapping of heat by the vacancy clusters, then a 1D spreading effect of the clusters is obtained which may be interpreted as crack propagation. The results obtained show that the ABV model can be used in correlation to FEM methods to study the thermo-mechanical evolution of interconnect alloy or material during the operation of a power mechatronic device and reduce by numerical simulation the uncertainties on the coupling between thermal and mechanical parameters of materials assembled in such devices. Then RBDO method can be applied for reliability issues.

5. Conclusions

In this work, using a numerical method, the thermal effect in the presence of voids in an interconnect alloy is studied by FEM and the ABV model. Results of FEM are implemented in the ABV model.Whatever the interaction energies between the atoms of the alloy, the final configuration ends with segregation of voids. Voids segregates in a matrix of A type, of B type or AB type and form large localized clusters or smaller delocalized ones of different shapes.

Acknowledgments

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