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Edge Effect on Nanoparticles of an Interconnect Alloy from the ABV Model

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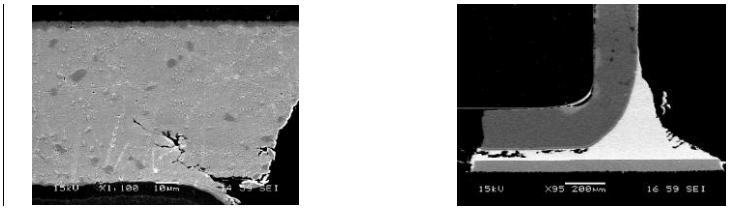
Abstract: The physical phenomena underlying crack initiation and hence failures in interconnection alloy is investigated using the ABV model [1] (Metals A and B and void V) focusing on boundary effects at the interface with the device. The Hamiltonian which is expressed as the sum of the interaction energies between A, B and V with interaction parameters E_{AA}, E_{BB}, E_{AB} , E_{AV} and E_{BV} and reformulated in terms of fictitious 3 states spins (-1, 0, +1). And new parameters J, K, and U function of the interaction energy parameters between the metal atoms A, B and void V are defined and associated to the different spin combinations of the transformed Hamiltonian. A Monte Carlo (MC) simulation of a 2D microscopic 3 states Ising model taking into account edge effects [2] at the boundary between an active chip in a photovoltaic device or a sensor and nanoparticles of an interconnect alloy is performed. The results are discussed in terms of realistic values of interaction parameters and different algorithms for fixed compositions of A, B and V.

1. Introduction

Embedded electronic systems designed for smart technology implemented in mechatronic, robotics or internet of things devices can be studied by simulation and modelling before any experimentation is performed to test its reliability. This approach makes it possible to reduce time to market and the development cost of a correct alloy. The physics of failure of the interconnecting alloys (ICA) used in mechatronics modules are related to the degradation observed as a result of the presence of intermetallics, voids, delamination at adjacent boundaries. Ageing due to current density cycling through interconnections (solder, wire bonding …) and bulk materials (copper busbar, silicon chip, insulating

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ceramic …) occurs principally because of thermal effect and the presence of voids. Figure 1 a) and b) shows the defects that are present in interconnect alloys after thermal shocks [2].



a) **b)**

Figure 1: a) Cracks and voids after thermal shocks test 1h/1h a) ASIC (683 cycles, -40/+105°C) b) Melf Resistor (1000 cycles, -40/+125°C)

The Ising model which has been developed to study phase transition physics is applied to a variety of systems not necessarily involving interacting magnetic spins in 1D, 2D or 3D configurations. A variety of models can be found: for example, the Bragg-Williams model on Binary alloys [3], the Potts model applied to Grain boundary energy [4], the Lee and Yang Lattice gas model [5] or the Magnetic Spin Cross-Over (SCO) compounds [6]. In the frame of the Ising ABV model [1], Monte Carlo simulation is performed to optimize the reliability of mechatronic devices using in their assembly innovative materials complying with regulations about hazardous substances.

2. Model For Simulation

The ABV model developed by Yaldram and Binder [1], where A and B stand for two different metals and V for void or a vacancy is based on the equivalence between the Ising-lattice gas and a binary alloy. Its application in connection to several other models, in particular the Blume-Emery-Griffths [7] has been discussed in details by Tafa, Puri and Kumar [8] with a focus on phase separation in ternary mixtures and characteristic features of the domain growth process. This model has been applied to study temperature effects and void segregation in interconnect materials using a Monte Carlo simulation (MC) in the Metropolis scheme [9]. This simulation highlighted the importance of specific temperature rise in the region of voids clusters initiating cracks and leading to delamination. The simulation work presented here in this paper, is focused on the failures observed at the interfaces of the interconnecting material of a mechatronic device. This approach is based on an ABV model which takes into account edge effects, and applies standard Metropolis Monte Carlo (MC) algorithm. The study of the edge effect is performed on the homogeneous structure of a binary alloy of constant composition containing voids. The simulation is performed on a 2D microscopic Ising model by considering a non-periodic MC application using the same three states Hamiltonian as in references [8][9] as:

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

where σ can be set to -1, 0, 1. The different parameters K, J and U are defined as :

$$J = \frac{1}{4}(2\varepsilon_{AB} - \varepsilon_{AA} - \varepsilon_{BB})$$

$$K = \varepsilon_{AV} + \varepsilon_{BV} - \varepsilon_{VV} - \frac{1}{4}(\varepsilon_{AA} + \varepsilon_{BB} + 2\varepsilon_{AB}) \quad (2)$$

$$U = \frac{1}{4}(\varepsilon_{AA} - \varepsilon_{BB}) + \frac{1}{2}(\varepsilon_{BV} - \varepsilon_{AV})$$

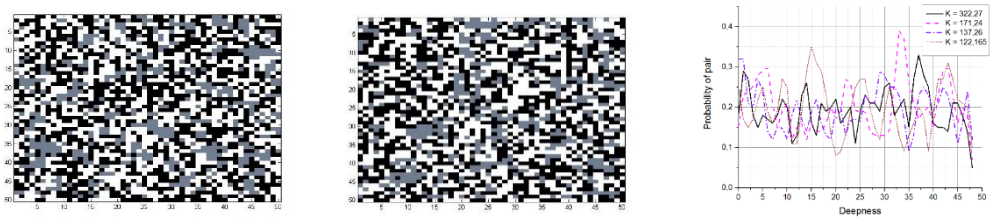
Where ε_{ik} ($i = A, B$ or V and $k = A, B$ or V) are the interaction energy parameters between the metal atoms A, B and void V. Note that phase separation is mediated by vacancies although there are no pairwise interaction terms involving voids and that segregation are due to vacancy atom exchanges rather than exchanges between A and B. In the absence of vacancies, the systems tends to mix if J < 0 (antiferromagnetic) and become homogeneous (complete disorder) if J > 0, then the system tends to segregate in A and B atoms (ferromagnetic). Parameters K/J and U/J account for the order or disorder that result from one of these two possible configurations.
In order to simulate the segregation of voids in the interconnecting material of a mechatronic module at interfaces, the interaction parameters ε_{AA}, ε_{BB} and ε_{AB} are adjusted and the spatial pseudo-spin configuration is determined. The results are discussed in terms of modifications on K and very slightly on U as a function of interaction parameters and the pair distribution function with fixed void percentage.

3. Results

To simulate the defects encountered in a mechatronics device, and precisely at interfaces as for example the active semi-conductor chip and the interconnect material, a new parameter is added to the algorithm developed for a closed system to address the problem of void clustering in an interconnect material [9]. This parameter serves to control the change in the interaction energies between atoms (A or B) and voids (ε_{AV} et ε_{BV}) at the surface at the nanometer scale under the hypothesis these values are different that at surfaces and in the bulk because the ratio of surface to bulk atoms are different. The effect of this modification is then determined by applying the standard Metropolis sampling procedure to a 2D square configuration. Two different algorithms are applied to simulate edge effects on the segregation and diffusion of voids through thermal cycling, either a clockwise search (CS) of void neighbors to mimick temperature rise effect when void clusters are formed or a search carried at random (RS), in an open system with only one external edge interface or with all the four borders. This situation is realized by breaking the symmetry in the periodic condition at the corresponding edge in the nanometer range, and replacing it by an edge of voids, which doesn't affect the total energy of the system. In the first instance, a study of the closed system i.e. when the periodic condition is verified, is performed for different values of the coefficient K.

In the results presented below, a square lattice of size 50×50, composed of atoms A and B, and voids in fixed proportion, $N_A = 40\%$; $N_B = 40\%$; $N_V = 20\%$ is used for the simulation. The interaction energies are set as: $\varepsilon_{AA} = \varepsilon_{AV} = 3{,}32\ eV$; $\varepsilon_{BB} = \varepsilon_{BV} = 3{,}19\ eV$; $\varepsilon_{AB} = 3{,}25$ eV. The initial configurations are randomly distributed in the matrix during the thermal initialization process carried at a temperature of T =300K. With U set to zero, the parameter K controls the void segregation and the results are given for different values of K. A plot of the probability of finding a pair of void as a function of the distance from the border or edge (termed deepness), allows the topology and the distribution of voids in the square lattice to be evaluated.

3.1 Without edge effect



a) **b)** **c)**

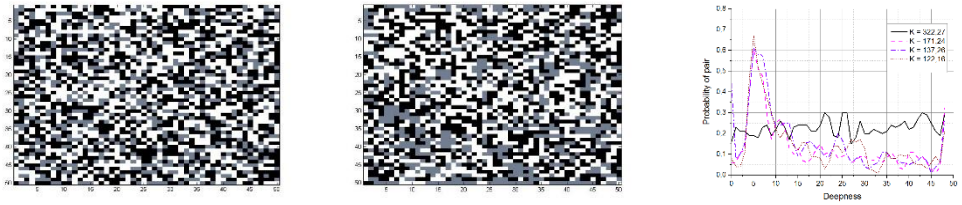
Figure 2: 2D distribution without edge effect : Topology a) and b) and c) Probability of pairs for different values of K (eV)

Topology : A White, B Dark, V Grey : (a) left : K = 122.16 eV ; (b) right : K = 322.27 eV.

As can be seen in Figure 2, there are no marked differences in the topology between the left a) and the right b) distributions for the two values of K: 122.16 eV and 322.27 eV. The only difference observed is in the random distribution of void clusters of different sizes in the lattice. In figure 2 c), the probability to find a pair of voids as a function of distance from an edge (deepness) show that voids are distributed at random whatever the deepness, such that the parameter K has no effect on this distribution when the system is closed with periodic boundaries.

3.2 With edge effect and clockwise search

3.2.1 All free edges



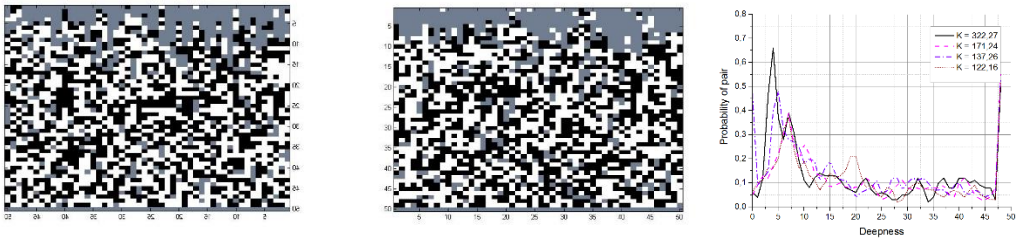
a) **b)** **c)**

Figure 3: 2D distribution with 4 free edges (CS): Topology a) and b) and c) Probability of pairs for different values of K (eV)

Topology : A White, B Dark, V Grey : (a) left : K = 122.16 eV ; (b) right : K = 171.24 eV.

Figures 3 a) and 3 b) present several differences in the void distribution, and precisely with a lower number of clusters and more voids at the borders at lower K values. At high values of K (322.17eV), void clusters increase while voids at borders decrease significantly. The pair distribution probability correlates very nicely to the analysis of the topology of voids with different values of K as shown in Figure 3 c), with a maximum in the probability of pairs for range 5 from the border and a second peak at range 25 except for K=322.27. This apparently unusual trend with no pronounced peak is attributed to the clockwise search of void neighbor algorithm as compared with the results obtained with the random search algorithm of void neighbors. This effect may be attributed to the temperature effect incorporated in the CS algorithm and which shows that voids distributes more randomly with temperature rise when K is high.

3.2.2 One free edge



a) **b)** **c)**

Figure 4: 2D distribution with 1 free edge (CS): Topology a) and b) and c) Probability of pairs for different values of K (eV)

Topology : A White, B Dark, V Grey : (a) left : K = 137.26 eV ; (b) right : K = 322.27 eV.

With only one free edge, the simulation leads to more pronounced results as shown in Figure 4. When all the edges are free, the voids tends to redistribute on the four border because they are attracted by the voids present at the boundary of the square. For the one edge case, the size of the clusters accumulating

at the border are larger because there is only one free edge which tends to attract voids. The pair distribution function of Figure 4 c) correlates to the topology presented in Figures 4 a) and 4 b) with two close maxima at range 4 and 7, the peak corresponding to K= 322.27 eV being highest. No apparent discrepancy due to the search algorithm is found in this case.

3.3 With edge effect and random search

3.3.1 All free edges



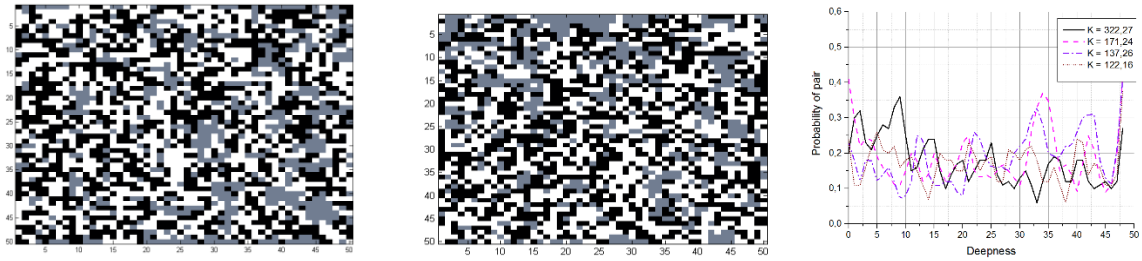
a) **b)** **c)**

Figure 5: 2D distribution with 4 free edges (RS): Topology a) and b) and c) Probability of pairs for different values of K (eV)

Topology : A White, B Dark, V Grey : (a) left : K = 137.26 eV ; (b) right : K = 322.27 eV.

With the random search algorithm, the accumulation of voids at the surface of the four borders is roughly the same as shown in Figures 5a) and 5b). The parameter K controls the distribution of voids, with less clusters in the bulk for higher K values. The size of clusters is enhanced with algorithm RS which limits accumulation of voids in a preferential direction. The peaks are closer to the borders with clusters in the bulk for low K values. The pair distribution curve corresponding to K=322.27 shows that voids are denser at the borders with limited clusters in the bulk.

3.3.2 One free edge



a) **b)** **c)**

Figure 6: 2D distribution with 1 free edge (RS): Topology a) and b) and c) Probability of pairs for different values of K (eV)

Topology : A White, B Dark, V Grey : (a) left : K = 137.26 eV ; (b) right : K = 322.27 eV.

With one free edge, the RS algorithm leads to results different from those obtained with the CS algorithm and looks more like results obtained with a closed system as presented in Figure 2. The voids density at the edge is not peaked as with the CS algorithm as shown in Figure 6 c). Remembering that

the CS algorithm mimicks the effect of temperature rise when clusters of voids form, then the distribution of voids depends on the competition between the K effect and the temperature effect.

4. Conclusion

Two algorithms based on the ABV model are applied to simulate by standard metropolis Monte Carlo method, edge effects on the distribution of voids in a 2D configuration of a binary alloy interconnect material. The algorithms termed CS and RS are respectively closely linked to temperature rise effect with void clustering and K effect on the void distribution. Results show that temperature effect tends to favour preferential directional spread of voids where as K effect tend to favour cluster formation in the bulk for low K values and at the border for high K values. Then, the distribution of voids resulting from temperature effect compete with the tendency of void clustering at the surface for the high K, and homogeneous spread at the lowest K value.

Acknowledgments
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References

[1] Yaldram, K. and Binder, K. Monte-Carlo simulation of phase-separation and clustering in the ABV model. 1991, *Journal of Statistical Physics*, **62**, 161. 4
[2] Dahoo P R, Alayli N, Girard A, Pougnet P, Tan K L and Morelle J M, 2010 *Mater. Res. Soc. Symp. Proc. Warrendale, PA,* **1195** 183
[3]W L Bragg and E J Williams, The effect of thermal agitation on atomic arrangement in alloys, 1934, 1934, *Proc. Roy. Soc. London*, **145A**, 699-730 (1934).
[4] Potts R.B., Some Generalized Order-Disorder Transformations, 1952, *Math. Proc. Camb. Phil. Soc*. **48**, 106-109
[5] Lee T.D. and Yang C.N., Statistical theory of Equation of States and Phase Transitions: II Lattice gas and Ising Model, 1952, *Phys. Rev. E*, **87**, 3, 410-419
[6] Linares J., Chiruta D., Jureschi C-M., Alayli Y., Turcu C.O, Dahoo P.R., "Simulations of Edge Effect in 1D Spin Crossover Compounds by Atom-Phonon Coupling Model, 2016 *Journal of Physics : Conference Series, IOP*, **738**, pp 012052
[7] Blume, M., Emery, V. J., Griffiths, R. B., Ising Model for the λ Transition and Phase Separation in He_3-He_4 Mixtures,1971, *Phys.Rev.A*, **4**(3), 1071-1077
[8] Tafa K, Puri S and Kumar D, Kinetics of phase separation in ternary mixtures, 2001, *Phys. Rev. E.*, **64**, 056139-1
[9] Dahoo P.R., Linares J, Chiruta D., Chong C., Pougnet P., Meis C. and El Hami A., Monte Carlo Method Applied to the ABV Model of an Interconnect Alloy , 2016 *Journal of Physics : Conference Series, IOP*, **738**, pp 012073