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Dislocation assisted diffusion: A mechanism for growth of intermetallic compounds in copper ball bonds

Maryam Gholamirad, Siavash Soltani, Panthea Sepehrband*

Department of Mechanical Engineering, Santa Clara University, 500 El Camino Real, Santa Clara, CA 95138, USA

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ABSTRACT

A combination of Finite Element Analysis (FEA), Molecular Dynamics (MD) simulation and analytical formulation is employed to predict the thickness of Intermetallic Compounds (IMCs) right after ball bonding of copper wire to an aluminum pad. The IMCs growth is related to the enhanced diffusion through the dislocations that are generated in the aluminum pad during the bonding process. Dislocation density and diffusional constants are estimated from the results of the FEA and MD simulation and used to calculate the thickness of IMCs that can form through dislocation-assisted diffusion. It is shown that dislocations have a strong effect on controlling diffusional processes that lead to IMC growth. Results are compared with independently acquired experimental data in the literature. The good agreement between the computed and experimental results supports the validity of the proposed mechanism.

1. Introduction

Ultrasonic wire bonding is one of the main technologies used for electronic chip interconnections. Trillions of ultrasonic bonds are made annually for microelectronic devices [1]. The race toward smaller form factors with complex functionality requires finer pitch Printed Circuit Boards (PCBs) and integrated semiconductor devices with more signal pins and narrower intervals of input and output pads [2]. These applications impose greater demands of quality and efficiency in ultrasonic bonding processes [3–5]. Meanwhile, the commercial microelectronic industry has rapidly transitioned from using gold to copper for economical and technological reasons. Advantages of copper wire bonding over gold wire bonding have been extensively reported [1,6–8]. However, copper is not a “drop-in” substitute for gold in bonding technology [3]. Although Cu wire is currently implemented in industry, without an understanding of the physics of bond formation and the relevant failure mechanisms, expansion of the wire bonding process for implementing new conditions and providing longer lifetimes remains limited to trial and error approaches.

An important failure cause in wire bonding is the growth of the intermetallic compounds (IMC) that form between the ball and bond pad. Although small amounts of interfacial IMC formation increase bond strength [1,6–8]; their extensive growth leads to an increase in electrical resistivity [9,10], crack initiation [11,12] and an ultimate failure. Extensive studies have been conducted on the evolution of IMCs during post bonding stages in both Au-Al (e.g. [13–16]) and Cu-Al (e.g. [8,11,17–19]). However, analysis on the process of IMC formation during bonding is rather limited. The information is scarce and inconsistent in the Cu-Al system due to the nano-size of the thin layers, which make them extremely difficult to be detected through conventional techniques [20]. While SEM analysis did not reveal Cu-Al IMCs in the as-bonded condition [3,16], high-resolution TEM analysis detected formation of nano-size IMCs [20]. Evidence for IMC formation at various areas of the bond interface has been revealed, but the thickness of the particles has been reported to be much larger than what can be predicted from bulk diffusion.

Considering dislocation generation during plastic deformation [21], this paper proposes dislocation-assisted diffusion as an enhancing mechanism for atomic movement and IMC growth. The goal is to provide a physically-based explanation for the reported deviation between diffusion based prediction and experimental observations. For this purpose a combination of Finite Element (FE) and Molecular Dynamic (MD) techniques is implemented. Dislocation density as a result of plastic deformation during bonding is calculated using Finite Element methods. Through a synergy of analytical formulation and molecular dynamics simulation, the main diffusing element and the rate of diffusion in the vicinity of dislocation is estimated. The results are used to identify the role of dislocations in IMC growth during bonding and the successive annealing stages.

* Corresponding author.
E-mail address: psepehrband@scu.edu (P. Sepehrband).

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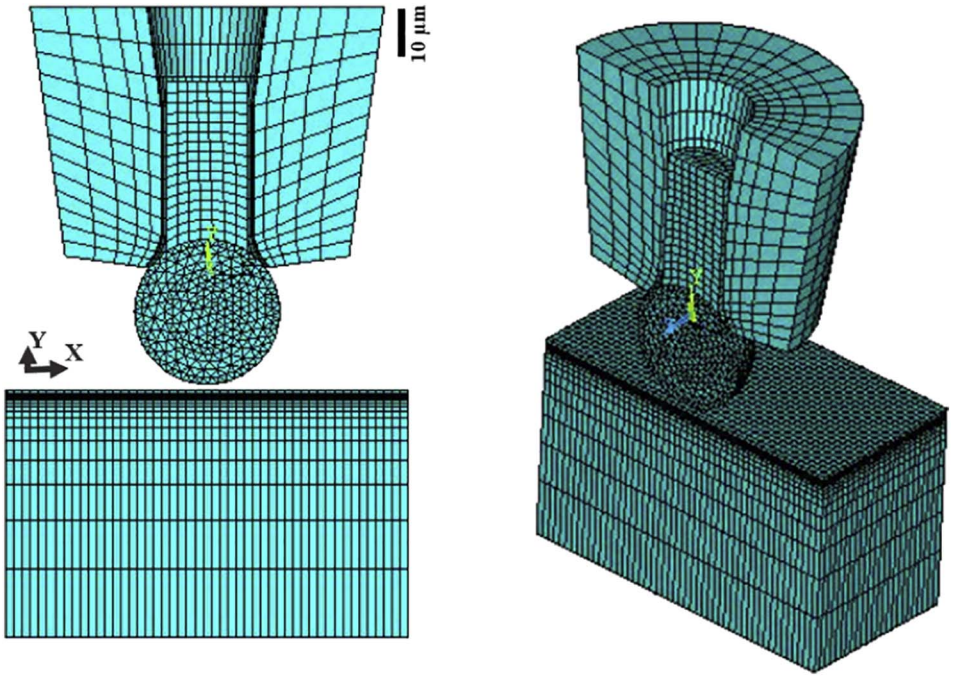

Fig. 1. 3D FEA model for the Cu-Al wire-bonding simulation. Dimensions of the silicon substrate: 100 µm × 50 µm × 60 µm.

1.1. IMC growth through dislocation assisted diffusion

Ultrasonic vibration in combination with the fast plastic deformation leads to the fracture of the thin oxide layer on the metallic pad that results in the interaction between bare metals. The combination of the bare metals contact and bonding temperature provides a favorable condition for initiation of diffusion. Using the concept of diffusion for calculation of intermetallic thickness has been heretofore challenging. The calculated values for IMCs' thickness during bonding have been found to be significantly smaller than the experimentally measured ones [22,23]. To justify this deviation between the measured and calculated sizes, various approaches such as effective temperature and effective activation energy due to mechanical deformation, have been proposed [22,23]. Instead of adopting an indirect effect of mechanical deformation through empirical approaches, in this paper we consider the effect of dislocations in enhancing diffusional mechanism. Assuming that IMC growth occurs through diffusion, growth of the IMC can be assumed to follow a parabolic law [19,20,24,25] whereby

$$x = \sqrt{Dt} \tag{1}$$

and

$$D = D_0 \exp\left(-\frac{Q}{RT}\right) \tag{2}$$

where x is the thickness of IMC (which is equal to the diffusion distance) at time t, D is the diffusivity (i.e. the growth rate constant), and D_0 is the temperature-independent pre-exponential factor. The effect of dislocation on diffusion can be considered through the effective diffusion equation given by Hart [26]:

$$D_{eff} = D_v f_v + D_c f_c \tag{3}$$

The parameter D_{eff} is the effective diffusion, D_v is the diffusion coefficient of the lattice, D_c is the diffusion coefficient of the core, f_v is the contribution from the lattice, and f_c is the contribution from the core. Eq. (3) was modified by Frost and Ashby [27] to get

$$D_{eff} = D_v\left(1 + \frac{\rho a_c D_c}{D_v}\right) \tag{4}$$

where ρ is the dislocation density and a_c is the cross-sectional area of the dislocation core. The lattice and core diffusion coefficients are given by Eq. (5) and (6), respectively:

$$D_v = D_{0v} \exp\left(-\frac{Q_v}{RT}\right) \tag{5}$$

and

$$D_c = D_{0c} \exp\left(-\frac{Q_c}{RT}\right) \tag{6}$$

where D_{0v} and D_{0c} are the pre-exponential factors, and Q_v and Q_c are the activation energies for lattice and core diffusion, respectively. The effective diffusion equation, i.e. Eq. (4) from Frost and Ashby [27] can be used along with the empirical power law for diffusion, i.e. Eq. (1) leading to:

$$x = \sqrt{D_{eff}\, t} \tag{7}$$

Rewriting it gives Eq. (8), which can be used to predict thickness of intermetallic particles as a result of dislocation-assisted diffusion.

$$x = \left[D_v\left(1 + \frac{\rho a_c D_c}{D_v}\right)t\right]^{1/2} \tag{8}$$

1.2. Finite element model

Most of the plastic deformation occurs during the impact stage of bonding. Consequently, it is assumed that compared to the impact stage, the fraction of dislocations that are generated during the ultrasonic vibration is negligible. The dislocation density, therefore, is calculated using the results of Finite Element Analysis (FEA) of the impact stage. Although dislocation generation during ultrasonic vibration is not included in the analysis, ultrasonic vibration has an important role in the oxide layer removal that is crucial for bare-metal contacts and the initiation of diffusion even if it is not a large contributor to dislocation density.

FEA is used to simulate stress-strain distribution in the deformed copper ball and aluminum pad after the contact stage. These results are used for estimating dislocation density, a required variable for the calculation conducted in the next section. Since wire bonding is a highly dynamic process, ANSYS/LS-DYNA software was chosen due to its explicit method solving, which is suitable for simulating short-