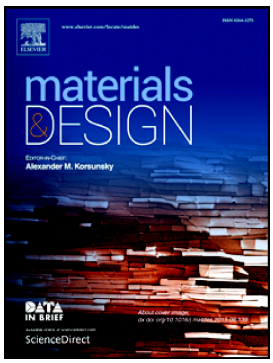
Accepted Manuscript



The effect of pressure and orientation on Cu-Cu3Sn interface reliability under isothermal ageing and monotonic traction via molecular dynamics investigation

Lihua Liang, Jicheng Zhang, Yangjian Xu, Yuanxiang Zhang, Wei Wang, Jian Yang

PII: S0264-1275(18)30266-1
DOI: doi:10.1016/j.matdes.2018.04.004
Reference: JMADE 3817

To appear in: *Materials & Design*

Received date: 19 January 2018
Revised date: 28 March 2018
Accepted date: 3 April 2018

Please cite this article as: Lihua Liang, Jicheng Zhang, Yangjian Xu, Yuanxiang Zhang, Wei Wang, Jian Yang , The effect of pressure and orientation on Cu-Cu3Sn interface reliability under isothermal ageing and monotonic traction via molecular dynamics investigation. The address for the corresponding author was captured as affiliation for all authors. Please check if appropriate. Jmade(2017), doi:10.1016/j.matdes.2018.04.004

The effect of pressure and orientation on Cu-Cu_3Sn interface reliability under isothermal ageing and monotonic traction via molecular dynamics investigation

Lihua Liang [1], Jicheng Zhang [1], Yangjian Xu [1], Yuanxiang Zhang [2], Wei Wang [1], and Jian Yang [3,*]

[1] College of Mechanical Engineering, Zhejiang University of Technology, Hangzhou, 310000, China;
lianglihua@zjut.edu.cn (L.L.); fc_tx@163.com (J.Z.); xuyangjian@163.com (Y.X.); 752843762@qq.com (W.W.)
[2] College of Mechanical Engineering, Quzhou University, Quzhou 324000, China; jarson_zhang@hotmail.com (Y.Z.)
[3] Institute of Process Equipment, College of Energy Engineering, Zhejiang University, Hangzhou, 310000, China

***** Correspondence: zdhjkz@zju.edu.cn; Tel.: +86-571-8795-3098

Abstract: In this paper, the dissipative mechanisms of a Cu pad in a Ball Grid Array (BGA) packaging structure during isothermal ageing and uniaxial tension were investigated. From the result of the isothermal ageing test, a nonuniform consumption of Cu and large amount of Kirkendall voids were observed at the interface of Cu and Cu_3Sn. To study the effect of pressure and orientation on this phenomenon, molecular dynamics (MD) simulations were conducted on four types of Cu-Cu_3Sn interface structures with different orientations of Cu. By comparing the diffusion coefficients of atoms in those cases, it was found that the tensile stress would inhibit the diffusion of atoms, whereas compressive stress would accelerate it, and this would be more significant under a larger magnitude of stress and temperature. Note that, in the model with the (101) surface Cu at the interface, both Cu and Cu_3Sn have a higher diffusion coefficient compared with the model with (001) surface Cu. Thus, the orientation of Cu will also contribute to the uniform consumption of the pad. Uniaxial tension simulation combined with DXA and CSP analyses on those models also shows the model with (001) surface Cu has a greater mechanical reliability in our simulation.

Highlights:

- A nonuniform consumption of Cu in BGA packaging structure is found during isothermal ageing test.
- Tensile and compressive stresses are verified to affect the consumption of Cu via molecular dynamics simulation.
- The Cu_3Sn-(001) Cu structure is verified to have a higher reliability from the perspective of diffusion and interface strength.

Keywords: Solder reliability; Molecular dynamics; Diffusion coefficient; Uniaxial tension; Orientation