Accepted Manuscript

Insights into the plasticity of Ag_3Sn from density functional theory

Ian N. Bakst, Hang Yu, Mohammadreza Bahadori, Haibo Yu, Seok-Woo Lee, Mark Aindow, Christopher R. Weinberger

PII: S0749-6419(18)30131-1

DOI: 10.1016/j.ijplas.2018.06.008

Reference: INTPLA 2363

To appear in: *International Journal of Plasticity*

Received Date: 7 March 2018

Revised Date: 15 June 2018

Accepted Date: 15 June 2018

Please cite this article as: Bakst, I.N., Yu, H., Bahadori, M., Yu, H., Lee, SW., Aindow, M., Weinberger, C.R., Insights into the plasticity of Ag3Sn from density functional theory, *International Journal of Plasticity* (2018), doi: 10.1016/j.ijplas.2018.06.008.

Insights into the plasticity of Ag_3Sn from density functional theory

Ian N. Bakst[a,*], Hang Yu[c], Mohammadreza Bahadori[c], Haibo Yu[d,e], Seok-Woo Lee[d,e], Mark Aindow[d,e], Christopher R. Weinberger[a,b]

[a] *Department of Mechanical Engineering, Colorado State University, Fort Collins CO, 80523, USA*
[b] *School of Advanced Materials Discovery, Colorado State University, Fort Collins CO 80523, USA*
[c] *Department of Mechanical Engineering and Mechanics, Drexel University, Philadelphia PA 19104, USA*
[d] *Department of Materials Science and Engineering, University of Connecticut, 97 North Eagleville Road, Unit 3136, Storrs CT 06269-3136, USA*
[e] *Institute of Materials Science, University of Connecticut, 97 North Eagleville Road, Unit 3136, Storrs CT 06269-3136, USA*

Abstract

The intermetallic Ag_3Sn is a strengthening phase in both silver amalgams as well as Sn–Ag lead-free solders, but is also a relatively ductile compound. Experimental reports have suggested the compound can both readily slip via dislocations as well as deform via twinning. To better understand the deformation mechanisms in Ag_3Sn, we investigate the energetics of slip via generalized stacking fault (GSF) curves as well as the structure and energetics of the twins using both density functional theory and analytical modeling. Our results suggest that [100](001) slip, which is equivalent to $\langle a \rangle_{\text{hcp}}$ slip on a prism plane in the hcp structure, is favorable due to a very low antiphase boundary energy. Slip on the (010) plane, which is equivalent to the basal plane in hcp metals, can occur in either the [100] or [001] directions via the formation of four superpartials. Our results further suggest that slip in the $\langle 102 \rangle$ direction could occur easily on either the {201} or {211} planes with the former being more likely since it is similar to prism planes in the hcp crystal. The overall values of the GSF curves are quite low, similar to high stacking fault energy metals, resulting in a rather ductile intermetallic. Simulations of the twins in Ag_3Sn demonstrate that they are structurally similar to twins in hcp metals with similar energy magnitudes. However, the experimentally observed activation of the {011} and {211} is likely a result of the small shear required to form the twins, and the suppression of other twin types is a likely a result of chemical ordering. Finally, our results point out that twinning is likely a necessary deformation mode to account for a general state of plastic deformation.

Keywords: Ag_3Sn; twinning; dislocations; nanostructure; plastic deformation; intermetallics; density functional theory;

1. Introduction

Ag_3Sn is an intermetallic that has been of interest for a number of years since it is one of the main constituents of silver amalgams used in dentistry [1–3]. Ag_3Sn appears as a major

*Corresponding author
Email address: Ian.Bakst@colostate.edu (Ian N. Bakst)