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Diffusivities and Atomic Mobilities of Sn-Bi and Sn-Pb Melts

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The recently developed Arrhenius formula of the modified Sutherland equation was first employed to calculate the self- and impurity diffusivities in liquid Sn, Bi, and Pb. The reliability of the calculated results was validated in comparison with the critically reviewed literature data. Based on the reliable tracer and chemical diffusivities available in the literature, the atomic mobility parameters in both Sn-Bi and Sn-Pb melts were then evaluated by the DICTRA (DIffusion-Controlled TRAnsformations) software package with the aid of thermodynamic parameters. Comprehensive comparisons show that most of the measured and theoretical diffusivities in Sn-Bi and Sn-Pb melts can be reasonably reproduced by the currently obtained atomic mobilities. Moreover, the atomic mobilities were further verified by comparing the model-predicted concentration profiles and the measured ones in various liquid Sn-Bi and Sn-Pb diffusion couples.

Key words: Solder alloys, diffusivity, liquid, atomic mobility, Sn-Bi and Sn-Pb melts

INTRODUCTION

Diffusivity in liquids is of great importance in many engineering fields, such as microstructural evolution during solidification,[1] dissolution kinetics in liquid solder,[2] and so on. In comparison with solid phases, however, reliable experimental information for diffusivities in liquid metals is scarce due to the effects of buoyancy-driven convective flow and chemical reactions in melts.[3,4] As a consequence, theoretical self- and impurity diffusion coefficients in liquid metals are of merit.[5–8] Very recently, a modified Sutherland equation, which takes the size of diffusion species into account, was developed by Chen et al.[9] in order to predict the self- and impurity diffusivities in molten metals. With the Arrhenius formula for self- and impurity diffusivities derived from the modified Sutherland equation, atomic mobility databases for liquid alloys can be effectively established by means of the DICTRA (DIffusion-Controlled TRAnsformations) software package,[10] and then various reliable concentration- and temperature-dependent diffusivities in alloy melts can be computed.

Sn, Bi, and Pb are important elements in solder. Information regarding their diffusion in liquid is extremely useful for prediction of the behavior of solder during service, and also for the design of solder materials.[11] Due to the low melting temperatures of Sn, Bi, and Pb, as well as the existence of radioisotopes, experimental measurements of diffusivities in liquid Sn, Bi, and Pb and their binary melts (i.e., Sn-Bi and Sn-Pb) can be performed by means of various experimental methods, such as the capillary reservoir (CR), long reservoir (LR), and shear cell (SC) techniques. However, the data from different sources are not consistent. Thus, there is an urgent need to validate the reliability of the diffusivities from different sources and then to establish atomic mobility databases for Sn-Bi and Sn-Pb melts.

In this work, all kinds of diffusivities in Sn-Bi and Sn-Pb melts were first critically reviewed. The modified Sutherland equation recently developed by Chen et al.[9] was then utilized to compute the

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