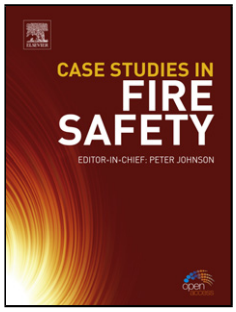

Title: Effects of iron and chromium on the dynamic properties of oxygen in liquid lead-bismuth eutectic alloy

Author: id="aut0005" author-id="S0010938X16307429-3f6a0890e8a19cd50d6d5ef8c1a8090f"> Yichun Xu id="aut0010" author-id="S0010938X16307429-147c102240410c897da3606df4884640"> Yange Zhang id="aut0015" author-id="S0010938X16307429-bda8fbdeead430873e9ee4aa777853df"> Xiangyan Li id="aut0020" author-id="S0010938X16307429-d4446d185bd060084e7417fba512b35c"> Wei Liu id="aut0025" author-id="S0010938X16307429-6902376c9d8f76ef5fe06e1c9259afad"> Dongdong Li id="aut0030" author-id="S0010938X16307429-92d3da97e14e4b452b173530960e12d8"> C.S. Liu id="aut0035" author-id="S0010938X16307429-1449645ce0c5b7c01da36ae4bac22553"> B.C. Pan id="aut0040" author-id="S0010938X16307429-ee6651c1744fb58dfcc171d83309a745"> Zhiguang Wang

PII: S0010-938X(16)30742-9
DOI: http://dx.doi.org/doi:10.1016/j.corsci.2017.01.003
Reference: CS 6968

To appear in:

Received date: 14-9-2016
Accepted date: 6-1-2017

Please cite this article as: Yichun Xu, Yange Zhang, Xiangyan Li, Wei Liu, Dongdong Li, C.S. Liu, B.C. Pan, Zhiguang Wang, Effects of iron and chromium on the dynamic properties of oxygen in liquid lead-bismuth eutectic alloy, *<![CDATA[Corrosion Science]]>* (2017), http://dx.doi.org/10.1016/j.corsci.2017.01.003

Effects of iron and chromium on the dynamic properties of oxygen in liquid lead-bismuth eutectic alloy

Yichun Xu[a], Yange Zhang[a], Xiangyan Li[a], Wei Liu[a], Dongdong Li[b], C.S. Liu[a,*], B.C. Pan[c] and Zhiguang Wang[d]

[a] *Key Laboratory of Materials Physics, Institute of Solid State Physics, Chinese Academy of Sciences, Hefei 230031, P.R. China.*
[b] *Laboratory of Amorphous Materials, School of Materials Science and Engineering, Hefei University of Technology, Hefei 230009, P.R. China*
[c] *National Laboratory for Physical Sciences at Microscale and Department of Physics, University of Science and Technology of China, Hefei 230026, P.R. China.*
[d] *Institute of Modern Physics, Chinese Academy of Sciences, Lanzhou 730000, P.R. China.*

Abstract

Ab initio molecular dynamics simulations were performed to investigate the effects of iron (Fe) and chromium (Cr) on the dynamic behaviour of oxygen in liquid lead-bismuth eutectic (LBE). The results indicated that oxygen atoms could be strongly attracted towards Fe and Cr atoms, forming metal oxide complexes dominated by Fe_3O_4 and Cr_2O_3. These oxide complexes could retard oxygen diffusion and reduce the concentration of free oxygen in LBE, thereby leading to an increase in the output of oxygen sensor in experiments. Besides, the diffusivities of Fe and Cr in LBE were obtained at different temperatures.

Keywords: A. Liquid lead-bismuth eutectic, B. *Ab initio* molecular dynamics simulation, C. Oxygen diffusivity, C. Oxygen concentration

1. Introduction

Lead-bismuth eutectic (LBE) alloys serve as the promising candidates for coolant and neutron spallation source in accelerator-driven systems [1–8]; however, they exhibit high corrosiveness towards structural materials of

[0]†csliu@issp.ac.cn