Composition interpretation of binary bulk metallic glasses via principal cluster definition

Dandan Dong, Shuang Zhang, Zijian Wang, C. Dong, Peter Häussler

PII: S0264-1275(16)30166-6
DOI: doi: 10.1016/j.matdes.2016.02.020
Reference: JMADE 1370

To appear in:

Received date: 27 December 2015
Revised date: 2 February 2016
Accepted date: 5 February 2016

Please cite this article as: Dandan Dong, Shuang Zhang, Zijian Wang, C. Dong, Peter Häussler, Composition interpretation of binary bulk metallic glasses via principal cluster definition, (2016), doi: 10.1016/j.matdes.2016.02.020

Composition Interpretation of Binary Bulk Metallic Glasses via Principal Cluster Definition

Dandan Dong, Shuang Zhang, Zijian Wang, C. Dong* and Peter Häussler[1]
Key Laboratory for Materials Modification by Laser, Ion and Electron Beam (Dalian University of Technology), Ministry of Education, Dalian 116024, China
*dong@dlut.edu.cn

Abstract

It has been pointed out that a bulk metallic glass composition could be formulated as [cluster](glue atoms)$_x$, where the cluster is derived from a devitrification phase. However, the selection rule of the so-called principal cluster should be specified because an alloy phase usually contains multiple clusters. In this paper, two important properties of the principal clusters are emphasized, i.e., spherical periodicity and cluster isolation, both being structural features of metallic glasses. According to these two criteria, the principal clusters are rigorously identified in devitrification phases and are used to construct cluster formulas to explain binary bulk-metallic glasses of Cu-(Zr,Hf), Ni-(Nb,Ta), Al-Ca, and Pd-Si.

Key Words: Principal cluster; Spherical periodicity; Cluster-plus-glue-atom model; Bulk-metallic glasses

Ⅰ. INTRODUCTION

A coordination polyhedral cluster is an ordered range at nearest-neighbor scale caused by chemical interaction between neighboring atoms and atomic-size effects. It is widely accepted that metallic glass structures are characterized by the presence of special clusters [1-8]. Some of us proposed in previous publications a 'cluster-plus-glue-atom' model which regards any structure as being composed of a cluster part and a glue-atom part [9]. Subsequently, a glassy structure is always expressed with a cluster formula [cluster](glue atom)$_x$, where x=1, 3 denotes the number of glue atoms. This model actually identifies a local short-range unit, representative of the most general structural feature of the overall phase. Good glass formers satisfy special composition formulas. Here the cluster is derived from the most prominent crystalline devitrification phase. For instance, the binary bulk-metallic glass (BMG) $Cu_{64}Zr_{36}$ is interpreted as [Cu-Cu_7Zr_5]Cu [10]. Enclosed by square brackets, the central atom is separated from its nearest neighbors by a hyphen. The type and number of glue atoms are given outside of the square brackets.

In general, there are multiple non-equivalent atomic sites within unit cells. Centered around each of them, a cluster will develop. For instance, there are eight clusters in Cu_8Zr_3 (Cu_8Hf_3-type). Since only one cluster enters into the cluster formula for the glass, the selection rule of the right cluster among the multiples present in a devitrification phase should be specified before one can establish a reliable cluster formula. Such a cluster has been called the 'principal' cluster [11] and should be the most representative local structure in the devitrification phase. A cluster formula as the local structural unit, on which the composition resides, somehow mimics the

[1] On leave from: Chemnitz University of Technology, Physics Institute, 091107 Chemnitz, Germany