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Molecular dynamics simulation of polyhedron analysis of Cu–Ag alloy under rapid quenching conditions

Fatih Ahmet Celik *

Bitlis Eren University, Faculty of Arts & Sciences, Physics Department, 13000 Bitlis, Turkey

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ABSTRACT

In this study, the formation mechanism of polyhedron clusters in $Cu_{50}Ag_{50}$ binary alloy system consisting of 50 000 atoms has been investigated by using molecular dynamics simulations based on embedded atom method (EAM) during the rapid cooling processes. The cluster-type index method (CTIM) has been used to describe the evaluation properties of clusters and the structural development has been investigated by using radial distribution function (RDF). The simulation results show that the amorphous phase is formed by the main bonded pairs of 1551, 1541 and 1431 in the system, and ideal icosahedral (icos) cluster (12 0 12 0) and other basic polyhedron clusters, such as defective icos, Frank–Kasper, Bernal polyhedron, play a critical role under the rapid cooling conditions. The results of our simulations that have been disclosed show that high cooling rate favors the icos and defective icos clusters for model alloy system.

1. Introduction

Cu-based alloys are a great interest for a wide range of materials sciences applications because of the understanding of mechanical, electrical and magnetic properties. Especially, Cu–Ag alloys have been exhibited to have interesting physical properties, such as high strength, high conductivity and heat treatments during the phase transformations processes. Recently, some investigators have devoted themselves to improve the Cu–Ag alloys for the application in mechanical properties. At the present time, it is very important to have a good understanding of the formation mechanism of atomic clusters in Cu–Ag alloy during the quenching processes [1–4].

Nano-atomic clusters are the bridge between the microstructures and the macroscopic properties of materials [5]. It is well known that under the experimental conditions it is difficult to obtain information about the atomic cluster formation mechanism in the quenching processes of model alloy system. However, with the fast development of computer techniques, some microstructure information can be realized by using molecular dynamic simulation. In addition to this, several clusters analysis techniques, such as cluster-type index method (CTIM), Honeycutt–Andersen (HA) method, have been used to investigate the formation of cluster structure during the cooling processes [6–8].

Today's developed technological facilities remain to be insufficient in reaching the desired experimental level in determining the atomic sizes mechanical and thermo dynamical properties of materials. However, when the same condition is theoretically examined, the researchers had the chance to investigate and control several properties of the materials by using methods based on different approaches in strong computer setting. For example, the commonly used methods are the Monte Carlo (MC) and Molecular Dynamic (MD) simulation, which give positive results that shed light on or pioneer the experimental studies in investigating both mechanical and thermo dynamical properties of the materials [9]. One of the important potential energy methods is the embedded atom method (EAM) based on the many-body interactions proposed by Daw and Baskes [10].

In the present work, the rapid solidification processes of Cu–%50Ag alloy consisting of 50 000 atoms have been performed based on embedded atom method (EAM) by using molecular dynamics simulation under different quenching conditions. The formation and evaluation of polyhedron clusters during the rapid cooling processes have been investigated by using HA bond-type index method and cluster-type index method. The structural development, also, has been performed by using radial distribution functions at different temperatures. In the present simulation, we use the EAM to observe various body potential functions, because of metallic bonding. We should, however, note that we shall avoid discussing the potential functions here since it was explained before in an early study and hence, we refer to the study given in Refs. [11,12].

* Tel.: +90 (0434) 228 5270; fax: +90 (0434) 228 5271.
E-mail address: facelik@beu.edu.tr.

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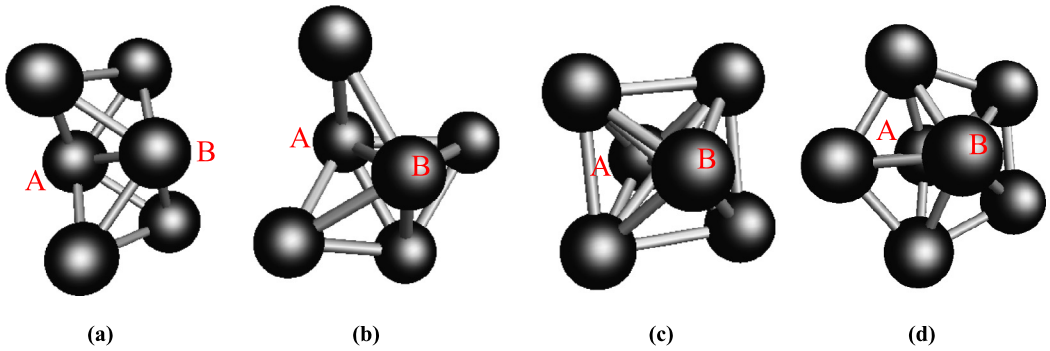

Fig. 1. The diagram for some bonded pairs: (a) 1421, (b) 1422, (c) 1441, (d) 1551. A and B represent pair atoms (root pair).

2. The method of calculation

2.1. Simulation and application process

In order to obtain phase transformations for model alloy system, radial distribution function (RDF) has been widely used to describe the structure analyses such as characterization of liquid and amorphous phases. This approach has been studied in this work. The RDF have expressed with,

$$g(r) = \frac{V}{N^2}\left\langle \frac{\sum_i n_i(r)}{4\pi r^2 \Delta r} \right\rangle$$

where r is the radial distance, $n_i(r)$ is the coordination number of atom i separated with r within Δr interval, and brackets denote the time average.

The classical molecular dynamics simulation has been studied for model alloy system [13,14]. The simulations were performed with the system consisting of 50 000 atoms in a cubic box with periodic boundary conditions under constant pressure. The Cu–%50Ag model alloy system has been chosen as the starting configuration for the MD computer simulation. The temperature of the system has been controlled and the initial velocities of particles follow the Boltzmann distribution. The equation of motion is integrated by using Gears' 5th order predictor–corrector algorithm. The molecular dynamics time step was set up as 6.64 fs. The lattice parameter for CuAg has been taken as $a = 3.61$ Å and the potential functions were truncated at a cut off distance of $2.5a$. The temperature of the system has been controlled by rescaling the atomic velocities at every two integration steps. In a simulation, because we have computed the number of neighbor atoms bounded a centre atom in the MD cell we have used a cut-off distance taken from the minimum of the RDF between the first and the second maximum.

The model alloy system is run for 50 000 MD step at 1400 K to guarantee an equilibrium liquid phase to obtain the initial configuration for cooling processes. For the quenching conditions, the temperature of system is decreased with two different cooling rates of $Q1 = 1.5 \times 10^{13}$ K/s and $Q2 = 3 \times 10^{13}$ K/s, respectively.

3. Polyhedron formation

3.1. Pair analyses technique

The pair analyses technique is an important method to characterize short-range order and this technique widely is used to define the configurations of the microstructures of different systems, such as amorphous and liquid phases as described by Honeycutt–Andersen (HA) [15]. The various bonded pairs are also described by the HA method, such as 1421, 1441, 1551, 1661, 1431, etc. For example, the 1551 bonded pairs represent the two root pair atoms with five common neighbors that have five bonds forming a pentagon of near-neighbor contact. The 1551 bonded pairs have five-fold symmetry, and the ratio of 1551 bonded pairs gives a measure of the degree of ideal icosahedral (ICOS) order. The 1661 and 1441 bonded pairs are the characteristic bonded pairs for bcc crystal structure [16]. Fig. 1 shows some of the corresponding bonded pairs.

3.2. Polyhedron analyses

When various combinations of bonded pairs formed by each atom in the system with its neighbor atoms are different, the cluster configurations formed by these bonded pairs are also different. In this regard, the HA bond-type index method, which represents bonded pairs, is very difficult to describe clearly for polyhedron cluster configurations of various types. For a more clear description of various types of polyhedron cluster configurations, based on the work of Qi and Wang [17], the CTIM which was proposed by Liu et al. as given in Refs. [6–8].

According to the definition of a basic cluster, four integers are approved to describe the main clusters. In this context, the four integers which are used in CTIM are as follows: the first integer represents the number of surrounding atoms which form a basic cluster with the central atom, i.e. the coordination number Z of the central atom; the second, third and fourth integers represent the numbers of 1441, 1551 and 1661 bond-types, respectively. For example, (12 0 12 0) mean an ideal icosahedral cluster that is composed of 13 atoms: the central atom is connected to the surrounding atoms through twelve 1551 bond-types (i.e., the coordination number of the central atom $Z = 12$); (13 1 10 2) mean the defective polyhedron cluster composed of 14 atoms, the core atom is connected to the surrounding atoms with one 1441, ten 1551 and two 1661 bond-types (the coordination number $Z = 13$). The CTIM has been successfully used to describe various clusters in liquid and amorphous metals, from basic clusters to larger clusters, as those shown in Refs. [18,19].

On the other hand, if the central atom has 14 neighboring atoms, 12 of which are joined to the central atom by 1551 bonded pairs and two of which are joined to the central atom by 1661 bonded pairs, then they define a Frank–Kasper (FK) polyhedron with $Z = 14$. If the central atom has 14 neighboring atoms, 8 of which are joined to the central atom by 1551 bonded pairs and two of which are joined to the central atom by 1441 bonded pairs, then they define a Bernal polyhedron with $Z = 10$.

4. Result and discussion

Fig. 2 shows the radial distribution function (RDF) curves as a function of temperature which drops from 1400 K to 300 K under the quenching conditions Q1 and Q2. It can be clearly said from this figure that the second peak of RDF curve become more