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Trans. Nonferrous Met. Soc. China 18(2008) 33−39
Transactions of Nonferrous Metals Society of China
www.csu.edu.cn/ysxb/

Formation and evolution properties of clusters in liquid metal copper during rapid cooling processes

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Received 5 March 2007; accepted 23 July 2007

Abstract: Based on the quantum Sutton-Chen many-body potential, a molecular dynamics simulation was performed to investigate the formation and evolution properties of clusters in liquid Cu with 50 000 atoms. The cluster-type index method(CTIM) was used to describe the complex microstructure transitions. It is demonstrated that the amorphous structures are mainly formed with the three bond-types of 1551, 1541 and 1431 in the system, and the icosahedral cluster (12 0 12 0) and other basic polyhedron clusters of (12 2 8 2), (13 1 10 2), (13 3 6 4), (14 1 10 3), (14 2 8 4) and (14 3 6 5) play a critical and leading role in the transition from liquid to glass. The nano-clusters formed in the system consist of some basic clusters and middle cluster configurations by connecting to each other, and distinguish from those obtained by gaseous deposition and ionic spray. From the results of structural parameter pair distribution function $g(r)$, bond-types and basic cluster-types, it is found that the glass transition temperature T_g for liquid metal Cu is about 673 K at the cooling rate of 1.0×10^{14} K/s.

Key words: liquid metal Cu; microstructure transition; nano-cluster; molecular dynamics simulation; QSC many-body potential

1 Introduction

It is well known that it is difficult to obtain the microstructure evolution information in solidification processes of liquid metals under present experimental conditions. However, with the rapid development of computer technique, some important informations of microstructure evolution during solidification processes of liquid metals have been obtained by using molecular dynamics simulation[1−6]. In recent years, for the liquid metal Cu, the molecular dynamics simulation studies have been performed by using some well known model potentials, such as EAM[2, 5, 7], FS [8] and TB[9] potentials, to study the properties of microstructure transition of liquid metal Cu during rapid solidification processes and some important results have been obtained [5−9]. These results, however, from the view point of comprehensive understanding of the structures and properties of liquid Cu, are complementary each other.

To further investigate the microstructure evolution mechanism during solidification processes of liquid Cu, on the basis of previous works[4,10], a tracking simulation study on the formation process of nano-clusters in a larger system consisting of 50 000 Cu atoms was devoted by adopting the quantum Sutton-Chen many-body potential and molecular dynamics method in this work. Using the cluster-type index method(CTIM) and the centre-atom method[4], the complex microstructure transitions were well described and analyzed.

2 Simulation conditions and methods

The conditions for simulation calculation were as follows: 50 000 Cu atoms were placed in a cubic box and then the system was run under periodic boundary conditions. The interacting interatomic potential adopted here is the quantum Sutton-Chen (Q-SC) many-body potentials[11−12], and the total energy of the system is obtained from the following equation:

$$U_{\text{tot}}=\sum_i U_i=\sum_i\left[\frac{1}{2}\sum_{j\neq i}D_{ij}V(r_{ij})-C_iD_{ii}\rho_i^{1/2}\right] \quad (1)$$

Foundation item: Projects(50271026; 50571037) supported by the National Natural Science Foundation of China
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where r_{ij} is the distance between atoms i and j, $V(r_{ij})$ is a pair of repulsive potential between atoms i and j (arising primarily from Pauli repulsion between the core electrons), i.e.

$$V(r_{ij})=\left(\frac{\alpha_{ij}}{r_{ij}}\right)^n \tag{2}$$

While the metallic bonding is captured in ρ_i, a local energy density is associated with atom i and defined as

$$\rho_i=\sum_{j\neq i}\phi(r_{ij})=\sum_{j\neq i}\left(\frac{\alpha_{ij}}{r_{ij}}\right)^n \tag{3}$$

where D sets the overall energy scale, c_i is a dimensionless parameter scaling the attractive term relative to the repulsive term, and α is an arbitrary length parameter leading to a dimensionless form for V and ρ.

Simulation parameters c_i, D, m, n and α are listed in Table 1. This potential was cut off at 22.0 a.u (atomic units), and the time step chosen was 1.0×10^{-14} s. The simulation calculation was started at 1 773 K (the melting point of Cu is 1 356 K). Firstly, let the system run at the same temperature (1 773 K) to get an equilibrium state (the criterion is the energy of the system being in an equilibrium state). Secondly, the temperature was decreased to some given temperatures from 1 673 to 173 K, the interval of two temperature points was 100 K, and let the system run 20 time steps at each given temperature to measure the structural configurations of this system, i. e., the space coordinates of each atom were recorded. Finally, the bond-types and their indexes between related atoms were detected by means of the index method of Honeycutt-Andersen (HA)[13], and the structural configurations of various clusters formed were described by the cluster-type index method(CTIM)[4]. Analyzing and comparing these results, we can get a clear physical picture on the microstructure transitions in the system from liquid state to amorphous state during rapid solidification processes.

Table 1 Parameters for Quantum Sutton-Chen(Q-SC) many-body potential used in this work[11−12]

D/meV	c	m	n	α/Å
5.792 1	84.843	5	10	3.603 0

3 Simulation results and analyses

3.1 Pair distribution function(PDF)

First of all, we inspect the pair distribution function $g(r)$ of the system obtained from the simulation, and find that it is consistent very well with the experimental results given by WASEDA[14], as shown in Fig.1. From Fig.1, it can be seen that the Q-SC many-body potential function adopted here is successful in reflecting the objective physical nature of the system. In addition, from Fig.2, it can be seen that the first-peak gradually becomes higher and sharper with the temperature decreasing. When temperature drops to the range of 773−673 K, the second-peak of $g(r)$ begins to split. Finally, it entirely splits into two small peaks with a higher front sub-peak and a lower behind one, which is just one of the important characteristics of amorphous structures. This illuminates that the amorphous transition temperature of liquid metal Cu is about 673 K at the cooling rate of 1.0×10^{14} K/s.

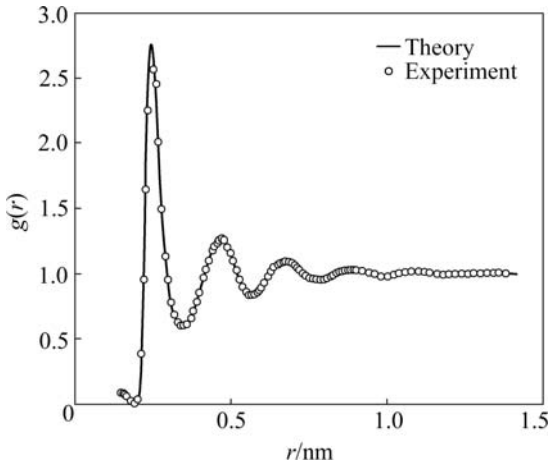

Fig.1 Pair distribution function $g(r)$ of liquid metal Cu at 1 573 K

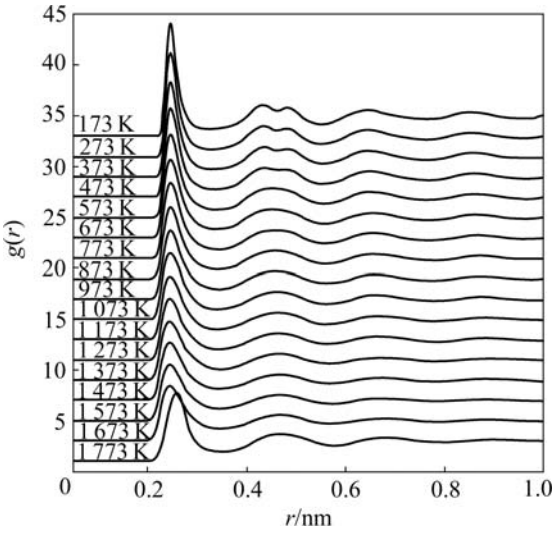

Fig.2 Relationships of pair distribution function $g(r)$ of liquid metal Cu with different temperatures

In order to further confirm the glass transition temperature T_g, we give the relationship between the Wendt-Abraham ratio (g_{min}/g_{max}) and temperature, as shown in Fig.3. The glass transition temperature T_g for the system is located at the intersection of liquid and