Research progress of molecular dynamics simulation for nanoparticles

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Abstract With the continuous development of high-power electronic devices, the traditional tin-lead brazing materials no longer meet the conditions of use, and sintered nanometal solder paste is promising for a new generation of packaging materials. The mechanism of microstructural changes of nanoparticle sintering during the sintering process has not been well studied at present. Molecular dynamics (MD) simulations can effectively track the diffusion process of metal atoms during the sintering process and help to reveal the dynamic evolution of nanoparticles. This review presents many MD simulations of nanoparticle sintering, including the growth mechanism of nanoparticles, the effect of different sintering parameters on the performance of sintered joints, the connection mechanism between the reinforced phase and nanoparticles and the performance of composite sintered joints. The low temperature and low pressure sintering of nanopaste are still in face of some problems, and MD simulations are very helpful for improving the sintering process and verifying the mechanism of the reinforcing phase.

Key words Molecular dynamics, nanoparticles, sintering

0 Introduction

The operating temperature of wide-bandgap semiconductors (gallium nitride, silicon carbide) may reach as high as 250 ℃[1], causing solder joints in service in the risk of melting due to the low melting point of conventional tin-based brazing materials thus bring about irreversible damage to the electronics[2]. Electronic devices are subjected to greater current density as well as greater heat, and the service environment of solder joints is becoming increasingly harsh, requiring more advanced encapsulation materials.

In recent years, silver nano-solder paste has gradually become a research hotspot in the field of chip interconnects, which has good thermal and electrical conductivity[3 − 4]. With low radius of curvature and high specific surface area, silver nanoparticles can be solid-phase connected at low temperatures and serve at high temperature conditions. Sintered silver has excellent material properties and is an ideal material for achieving power device packaging.

The properties of nanometallic particles are closely related to their crystal structure, so it is essential to study the dynamic evolution of metal particles during the sintering process. In the past two decades, molecular-based simulations have been widely used to reveal the changes in the microstructure of metal particles during the sintering process. At high temperatures, sintering can occur rapidly within a few hundred picoseconds[5], and researchers using molecular dynamics simulations (MD) can study the properties of materials at the atomic level, offering better understanding of the phenomena in macroscopic experiments.

In MD simulations, the diffusion process of atoms on the surface or inside the nanoparticles, the formation of defects, and changes in the lattice structure can be directly

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traced, which can visually help researchers understand the dynamic evolution of nanoparticles during sintering. The mechanical properties of sintered joints are related to the sintering temperature[6], time[7 – 8], pressure [9 – 11], and composition[12],etc. For example, increasing the sintering pressure reduces the porosity of the sintered layer, increases the dense density, and has high bond strength, which in turn improves the reliability of the joint. The use of metal particles of different sizes for sintering, with smaller particles filling the gaps between larger particles, not only reduces porosity and increases the density, but also improves the thermal and electrical conductivity of the joint [3 – 4,13 – 14].

In this review, firstly, the principle of MD calculation is introduced in Section 1. The embedded atom (EAM) potential and the modified embedded atom potential (MEAM) are the commonly used potential functions for the sintering of nanometallic particles. The changes in the microstructure of nanoparticles with different sintering parameters during the sintering process, and the changes in the mechanical properties of the sintered joints are presented in Section 2. In Section 3, the effects of different reinforcements on the sintered joints and the mechanism of action are presented. Finally, the current difficulties in the sintering process and the idea of MD simulation for sintering studies are reviewed.

1 Calculation principle

Molecular dynamics simulations use the classical Newtonian laws of kinematics to describe the interactions and motions between atoms or molecules. Through the interaction potential between atoms, the force on each atom is found, and at selected time steps, boundary conditions, initial positions and initial velocities, a finite number of atoms or molecules are subjected to a set of Newtonian kinetic equations, which are solved numerically to obtain the classical trajectories and velocities of these atoms. The results are then statistically averaged over a long enough period of time to obtain the required macroscopic physical and mechanical quantities, such as temperature, pressure, energy, and other physical properties, as well as mean square displacement, radial distribution functions, etc.

1.1 Intermolecular interaction potential

Molecular dynamics is the study of various physical properties of materials by solving the equations of motion of all particles in the system. Molecules interact with other molecules in the system, and various intermolecular interaction potentials affect the total energy of the whole system and control the macroscopic physical properties of the material. The intermolecular interaction potential is a mathematical function used to represent the contribution of a group of atoms to the total energy change. The total potential energy of the system is divided into terms depending on the contributions of atoms, pairs of atoms, triatoms, etc[15]:

$$E = \sum_i \varphi_1\left(\vec{r_i}\right) + \sum_i \sum_{i<j} \varphi_2\left(\vec{r_i}, \vec{r_j}\right) + \sum_i \sum_{i<j} \sum_{j<k} \varphi_3\left(\vec{r_i}, \vec{r_j}, \vec{r_k}\right) + \cdots \tag{1}$$

Where φ_1 indicates the potential energy of the particle in the external field (such as gravitational field, electric field, etc.), and the subsequent terms φ_2, φ_3, etc. indicate the interaction potential of each particle,for example, φ_2 is the two-body potential, which contains all the particles in the system interacting with each other two by two, and its magnitude is only related to the absolute distance between two particles.

Eq. (1) for the three-body potential and higher terms will greatly increase the difficulty of calculation and calculation time, where the four-body potential and higher terms are very small compared with the two-body potential and three-body potential. In order to reduce the difficulty of calculation, generally the impact of these terms on the total energy will not be considered . Alternatively, the average three-body effect can be partially included by defining "effective" pair potentials. For this reason, the rewritten Eq. (1) takes the form:

$$E = \sum_i \varphi_1\left(\vec{r_i}\right) + \sum_i \sum_{i<j} \varphi_2^{\text{eff}}\left(r_{ij}\right) \tag{2}$$

In computer simulations it is usually considered that the effective pair potential, representing all the many-body effects, is represented by $\varphi(r_{ij})$ or $\varphi(r)$, and the effective pair potential may be related to density and temperature, etc.

The two-body potential is generally dominated by the Lennard-Jones (LJ) potential, which is the earliest proposed two-body potential model that considers the intermolecular forces, i.e., the van der Waals forces, and has a relatively simple functional form as follows[16]:

$$\Phi(r) = 4\varepsilon\left(\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right) \tag{3}$$

where ε is the depth of the potential well and σ is the equilibrium distance when the potential energy is zero, i.e., the range of the potential well.

The LJ potential is mainly used to study the properties of gases, and for solids, the accuracy of the calculation can-not be guaranteed if only the interaction between two particles is considered. A more accurate potential function is needed for nanometallic particles in order to describe their various physical properties. The multi-body potential considers not only the two-by-two interaction between the particles inside the whole system, but also the influence of other particles within a certain range on that particle, which makes the calculation results more accurate. In this paper, we introduce two intermolecular potentials commonly used in metal simulations, the embedded atom (EAM) potential and the modified embedded atom potential (MEAM) .

1.1.1 Embedded atom (EAM) potential

The EAM potential was established by Daw and Baskes based on the DFT theory, by introducing the atom-electron density interaction, where the electron density in the vicinity of an atom is constituted by the superposition of its own electron density and the electron density of other particles around it at that place, and the EAM potential function is shown as follows[17]:

$$\Phi = \frac{1}{2}\sum_{i \neq J} \varphi\left(r_{ij}\right) + \sum_{i} F\left(\rho_i\right) \tag{4}$$

where $\varphi(r_{ij})$ is the two-body potential, which represents the interaction between two atoms, and $F(\rho_i)$ is the embedding potential, which represents the potential energy generated by the sum of the electron densities contributed by other atoms at atom i interacting with atom i. The EAM potential is currently the most widely used functional potential for calculating the interaction between metal particles.

1.1.2 Modified embedded atom potential (MEAM) potential

The EAM potential is very accurate for the forces between metal atoms, but it is only applicable to cubic system metals and is not so accurate for non-central force field potentials. The MEAM potential is a non-central force field potential that takes into account the angle factor and can be applied to non-cubic system materials. The potential function is the same for EAM, i.e., Eq. (4), and the embedding potential F is a function of the electron density at atom i[18]:

$$\bar{\rho}_i = \sum_{j \neq i} \rho_j\left(r_{ij}\right) \tag{5}$$

where $\rho_j(r_{ij})$ is the electron density contributed by atom j at atom i.

1.2 **Macroscopic physical parameter statistics**

1.2.1 Surface energy

Surface energy is a parametric quantity that characterizes the surface of a material, and its magnitude depends on the interaction between surface atoms. It is difficult to precisely determine the surface energy of nanometallic particles, and for the surface energy change during the sintering of nanometallic particles, it is difficult to determine it experimentally, in which case, computer simulations using molecular dynamics methods can be used to find the theoretical value of the surface energy of the material. The surface energy γ is expressed by the energy per unit area of the surface, and from Gibbs interface thermodynamics it is known that for an atomic system with a conserved atomic number, the surface energy is[19]:

$$\gamma = \frac{E^s - E^b}{A} \tag{6}$$

where γ is the surface energy, the energy per unit area of the surface; E^s is the total energy of the atomic system with the surface; E^b is the total energy of the atomic system with the surface removed, and A is the surface area of the atomic system.

1.2.2 Radial distribution function (RDF)

The radial distribution function (RDF) is shown below[20]:

$$G(r) = \frac{dN}{\rho 4\pi r^2 dr} \tag{7}$$

where N is the total number of particles and ρ is the ratio of the local density of particles to the average density.

RDF is used to represent the state of particle distribution in the system. In the alloy system, the distribution of molecules is not perfectly uniform throughout the system. The radial distribution function of a particle is defined as the ratio of the probability of the appearance of another particle at position r from the particle to the random distribution. When the distance is large, G(r) tends to 1, indicating that the particle distribution tends to be irregularly distributed.

1.2.3 Mean square displacement (MSD) and diffusion coefficient

The mean square displacement represents the average value of the squared displacement of the particle with respect to the initial state[21]. During the sintering process, all particles undergo microscopic thermal motion and are not fixed in the same position, and the sintering process is dominated by surface diffusion, so the motion of the surface atoms is also more intense. The mean square displacement (MSD) of the particles is given by:

$$\mathrm{MSD} = \frac{1}{N}\sum_{i=1}^{N}\left\langle |r_i(t) - r_i(0)|^2 \right\rangle \tag{8}$$

where r_i(t) is the bit vector of atom i at moment t; $r_i(0)$ is the initial bit vector of atom i at the initial moment.

The diffusion coefficient is a physical quantity characterizing the diffusion ability of a substance molecule and is influenced by the temperature and pressure of the system as well as the concentration of each component. During diffusion, atoms hop irregularly between gaps and vacancies, and the direction of motion of the atoms is not fixed, so that an atom makes almost no contribution to diffusion when it moves in an oscillatory motion somewhere. Therefore, the mean square displacement can be introduced to characterize the diffusion of particles. According to Einstein's equation[22], the diffusion coefficient can be expressed as 1/6 of the slope of the mean square displacement to time curve.

$$D = \frac{1}{6}\lim_{t\to\infty}\frac{\mathrm{d}}{\mathrm{d}t}\left\langle |r_i(t) - r_i(0)|^2 \right\rangle \tag{9}$$

2 Nanoparticle sintering process

The joining of metal materials is a very important technology in material processing and assembly, and the quality of the connection directly affects the reliability of the product. Solid-phase joining of nanoparticles can make nanometallic particles form good solid-phase connections at low temperatures. The joining process of nanoparticles is mainly divided into two stages, the first stage is the formation of the initial sintering neck of nanoparticles; the second stage is the stable growth stage of the sintering neck. The sintering neck is formed by the mutual diffusion of atoms on the surfaces of nanoparticles in contact with each other in the first stage, and the driving force at the nanoparticle interface is given by the Laplace equation[23]:

$$P = P_0 + \gamma\left(\frac{1}{R_1} + \frac{1}{R_2}\right) \tag{10}$$

where R_1 and R_2 are the radii of curvature of the surface contact points. P_0 is the external pressure on the surface and γ is the surface energy. The surface energy is the energy per unit area of the surface and is related to the radius of curvature, stress and composition.

Due to the high surface energy of nano-sized metal particles, their surface atoms do not require high energy for diffusion and thus can diffuse each other to form sinter necks at temperatures well below the melting point of the material. In the initial stages of sintering, the main mechanisms of sinter neck growth include surface diffusion and grain boundary diffusion. In the early stages of sintering, dislocation generation, mechanical rotation of the particles also contributes to nano-sintering[24].

Nanoparticles undergo crystal structure transformation during the sintering process.Wu et al.[25] found dislocation motion and viscous flow in the particles during sintering in their study of gold nanoparticle sintering. With increasing temperature, the FCC structure in gold nanoparticles keeps decreasing and the amorphous structure on the surface of the particles gradually increases, in addition to the HCP structure was found in the sintering of 4 nm and 6 nm particles.

Wang et al.[26] also found the transition from FCC to HCP structures, and the generation of twin crystal boundaries was observed in MD simulations and eventually formed stable stacking layer dislocations leading to lattice dislocation and particle rotation. Ding et al.[27] performed MD sintering simulations of nanometallic particles with the same and different initial crystal orientations and found that the particles always remained aligned when the initial orientation of the particles was the same, and the particles remained aligned when the initial orientation was different. When the initial orientations are different, they adjust rapidly and maintain the adjusted orientation during the subsequent sintering process. This reorientation behavior is driven by the minimization of grain boundary energy.

Sintered silver is a material with a porous structure, and the porosity of the sintered layer affects not only the mechanical properties of the sintered joints but also the thermal and electrical conductivity[3－4].Yao et al[2] studied the fracture of sintered silver joints with different porosities under tensile conditions, and as the porosity increased, the sintered joints changed from brittle fracture to ductile fracture, and the experimental results are basically consistent with the predicted changes in the simulation predictions.

Increasing the sintering temperature promotes the grain boundary and lattice diffusion of nanomaterials, leading to densification of the sintered joints and contributing to the improvement of the joint strength. In practical applications, a longer sintering time is usually required to decompose the organic matter or solvent in the nano-paste. Increasing the sintering time in a short period of time can substantially improve the mechanical properties of the joints[28], However, overextended sintering time can otherwise lead to coarsening of the sintered layer grains, deteriorating the microstructure of the joints and leading to strength reduction[23].

The porosity of sintered joints has a very significant effect on the joint properties and applying pressure assistance during the sintering process can reduce the porosity. When pressure is applied, it helps to densify the sintered nanomaterials and improve the joint strength[9].

The mechanism of the effect of sintering pressure on the sintering of nanoparticles is still not deep enough, and the mechanism of the effect of external pressure on the dislocation movement and atomic transport inside the joint is not clear. Some researchers have suggested that external pressure applied during sintering creates stress gradients at the sinter neck, which accelerates atomic migration to the neck. Hu et al. investigating through nanocopper sintering found that external pressure leads to defects in nanoparticles, creating fast channels for atomic diffusion[10].

Applying pressure during sintering can reduce the porosity of the sintered layer and increase the dense density. However, the applied pressure can produce defects and cracks on the chip and substrate[29], so it is necessary to reduce the sintering pressure without significantly affecting the quality of the joint. In previous reports[13 – 14], silver nanoparticles were mixed with micron silver particles for pressureless sintering, and the nanoparticles would act as a bridge for bonding between the micron particles. The multi-sized sintered joints had low porosity, high bonding strength and high shear strength.

Researchers have also considered the effect of this multi-size nanoparticle sintering on the thermal and electrical conductivity of the joints[3 – 4]. During the sintering process, the thermal conductivity and electrical conductivity of the joints are improved because the small particles fill between the voids of the large particles, which increase the dense density of the sintered layer. Besides, the cross-sectional area of the contact surface between the large particles is increased, which is also important for the overall electrical conductivity.

3 Composite nanoparticle sintering

Currently, nanoparticle sintering of silver is mainly studied in the field of chip packaging. However, the reliability of sintered silver joints in service still needs to be improved due to the coarsening of silver and other problems. In order to improve the mechanical properties of nanoparticle sintered joints as well as the reliability during service, researchers have added reinforcements to silver nanopaste to study the electrical, thermal and mechanical properties of composite sintered joints. There has been a great development of composite silver nanopaste in recent years, mainly including carbon reinforced matrix, metal reinforced matrix and other reinforced matrix[30].

MD, as an atomic-level simulation method, is well suited to study the sintering behavior of composite nanopaste, and provides good theoretical basis for revealing the mechanism of action of the reinforcing phase. While for the unknown reinforcing phase, the sintering process can be more easily determined after the calculation of MD.

Zheng[31] et al. investigated the interaction of gold nanoparticles around the ends of multi-walled carbon nanotubes with CNTs during sintering. As the diameter of the added multi-walled carbon nanotubes increases, the end-bound gold nanoparticles were closer to spherical shape[31]. Capillary effect can be seen to occur at temperatures well below the melting point of metal particles, where multi-walled carbon nanotubes draw metal atoms near the tube ends. The sintered layer of CNT/Cu nanocomposite sintered joints is dense, and the thermal conductivity of the joints has been improved[32]. In addition, carbon nanotubes can also improve the electrical conductivity of nanocomposites. Some researchers have suggested that carbon nanotubes combined with metal particles can act as conductors of electrons and enhance the electrical conductivity of the material[33].

In addition, metals are often used as nanopaste reinforced substrates because of their good thermal, electrical and mechanical properties and potential applications in packaging. For example, Liu[34] et al. made Ag-Al hybrid nano-paste, and during the sintering process, aluminum particles filled into the voids of the sintered silver matrix, and the interface was tightly fitted to form uniform nano-Ag-Al joints, which reduced the joint voids.

Nanoparticle sintering with core-shell structure exhibits good performance, for example, Cu@Ag core-shell nanoparticles sintered at 250 ℃ in the atmospheric can obtain sintered joints with 26.5 MPa and the obtained sintered joints have high densities and high oxidation resistance[35].Wang et al.[36] performed MD sintering simulations of Cu@Ag core-shell nanoparticles and found that Cu cores do not participate in interfacial reaction. However, it increases the mobility of Ag shell atoms and therefore obtains higher densities and bond strengths than pure Ag nanomaterials do.

In addition to the metal particles in the solder paste, the metallization layer on the solder substrate also affects the sintering. Dai et al. simulated the sintering of copper nanoparticles on Ni, Cu, Ag, and Au, respectively, and found that atomic interdiffusion occurred in the Cu/Ag and Cu/Au systems, leading to an increase in interfacial voids. The generation of Kirkendall voids was also observed in the experiments. Thus after subsequent aging, the shear strength of sintered Cu on Ni and Cu layers increased, while the shear strength of sintered Cu on Ag and Au layers decreased with increasing aging time[21]. Therefore, a suitable metallization coating of the sintered substrate is required for practical applications, which can prevent the diffusion of atoms from the sintered layer to the substrate and the creation of voids.

4 Conclusions

(1) Molecular dynamics simulations can explore the microstructure of materials and help us better understand the atomic motion process and the changes of nanoparticles during nanoparticle sintering.It can be used as a theoretical verification of nanoparticle sintering experiments as well as a guide for the designing of nanoparticle sintering experiments.

(2) Surface diffusion and grain boundary diffusion are the main growth mechanisms during the sintering of nanoparticles. If the orientation of nanoparticles is inconsistent, lattice structure transformation will occur and dislocations will be generated. Increasing the sintering temperature or time during the sintering process can promote the diffusion of atoms, but it will lead to the coarsening of the junction grains. Pressure sintering can improve the densities of the joints, but can lead to defects in the chip and substrate. When sintering with multi-scale stored metal particles, small particles fill the voids of large particles and improve the densities of the joints, which was verified in MD simulations.

(3) Carbon nanotube-reinforced composite paste and metal-reinforced composite paste can improve the performance of sintered joints and are validated in MD simulations.

(4) The sintering mechanism of nanoparticles and the effect of sintering parameters can be better investigated by MD method.

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