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Computational Materials Science

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Diffusion kinetics of transient liquid phase bonding of Ni-based superalloy with Ni nanoparticles: A molecular dynamics perspective



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ARTICLE INFO

Keywords:

Transient liquid phase bonding
Ni-based superalloy
Ni nanoparticle
Molecular dynamics
Diffusion kinetics

ABSTRACT

Transient liquid phase (TLP) bonding has been broadly utilized to join and repair Ni-based superalloy components; however, the understanding of its diffusion kinetics is still in infancy due to challenges in *in situ* experimental characterization under high operating temperatures. In this research, we examine detailed diffusion kinetics of Ni-based superalloy bonding with Ni nanoparticles employing molecular dynamics (MD), aiming to advance TLP bonding by achieving a desirable diffusion-induced joint microstructure. Diffusion kinetics of TLP bonding is compared with traditional constant heating method (CHM) bonding, by examining diffusion behaviors and microstructure. Self-diffusivity of each specific element is firstly calculated using MD, demonstrating a good agreement with the reported experimental values. The nanoscale size of Ni fillers and high operating temperature induce a large mobility, thus less porosity, while a slower diffusion in TLP bonding than CHM leads to a more crystallized microstructure with nano-sized grains. In addition, non-uniform diffusivity distribution of the surrounding elements influences diffusion pathway and joint microstructure. Therefore, desirable bonding properties can be achieved through Ni nano-filler, optimal temperature, as well as effective composition of atomic surroundings.

1. Introduction

Transient liquid phase (TLP) bonding is a joining technique employing a filler material with low melting temperature for inducing fast atomic diffusion, and subsequent isothermal solidification process of the liquid phase of the filler material, forming strong bonding with the base material [1]. TLP bonding involves minimal microstructure deformation and thermal distortion to the base material, which make it advantageous over traditional joining techniques such as vacuum brazing [2]. The TLP bonding has been widely utilized in joining and repairing of Ni-based superalloys, such as Inconel® 718 [3–7]. Directionally solidified polycrystalline and single crystal (SC) Ni-based superalloys possess excellent high-temperature mechanical properties and high corrosion-oxidation resistance [8], allowing for use in various applications, such as turbine engine, blades and vanes, cogeneration, and heat treatment facilities, which are operated under extreme conditions [9,10]. However, these Ni-based superalloys are expensive and extremely difficult to join and repair, due to challenges in (1) minimization of modification on preexisting precipitations in base materials, (2) remarkable reduction of the bonding time by enhancing the diffusivity, and (3) avoiding formation of undesirable phase, such as Nb-rich Laves phase in Inconel® 718 alloy [11,12].

In traditional TLP bonding, melting point depressants (MPDs), such as carbon, boron, silicon and chromium [9,13,14], are added for enhancing diffusion performance of the filler or base materials. However, the addition of such MPDs induces formation of brittle intermetallic phases within the joint, which deteriorate the joint strength and ductility [1]. Nanomaterials are expected to resolve this problem because melting point can be decreased by their fine size without adding such MPDs [15,16]. Ni nanoparticles (NPs), as a representative example, have been used to braze stainless steel for achieving a high bonding strength [17,18], which is attributed to their high diffusivity.

Most of experimental studies on joining of Inconel® 718 have addressed the isothermal solidification process [19,20], microstructures, and mechanical properties of the joint structure [4,21–23]; however, the *in situ* diffusion process during joining at atomic scale has rarely been reported by experimental investigations due to challenges in high-resolution structural characterization at high temperatures. Nevertheless, diffusion kinetics affects microstructure formation, and an enhanced understanding of diffusion during joining can suggest possible approaches for achieving excellent mechanical and thermal properties for joints.

Motivated by the advantages of Ni NPs in joining and insufficient understanding of diffusion kinetics, we investigate the atomic-scale TLP

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bonding of Ni-based superalloy (i.e., modeling Inconel® 718) with Ni NPs, employing molecular dynamics (MD) to enhance fundamental understanding of diffusion kinetics and to facilitate effective processing design of TLP bonding. Bonding with continuous heating method (CHM), i.e., traditional vacuum joining at a uniform temperature, is also studied for comparison. Although the mechanical and thermal properties of joints are not the main focus of this study, potential property-control mechanisms are discussed.

2. Methodology

2.1. Interaction potential

The embedded-atom method (EAM) potential [24] is employed to model interatomic interactions in this work. EAM potential is the most common and accurate interaction model in describing the metallic bonding [25], and has been widely utilized in simulating atomic-scale processes such as diffusion [26], deformation [27], melting and sintering [2], etc. The total energy (E_{tot}) of the EAM potential is formulated as:

$$E_{tot} = \frac{1}{2} \sum_{\substack{j \neq i \\ i, j = 1}}^N v_{ij}(r_{ij}) + \sum_{i=1}^N F_i(\bar{\rho}_i), \quad (1)$$

where $v_{ij}(r_{ij})$ is a pair interaction energy between atoms i and j with a separating distance of r_{ij} , and a factor of 1/2 is included to avoid duplicated calculation of pair interactions. F_i is the embedding energy of atom i , which is a function of local electron density $\bar{\rho}_i$, given by:

$$\bar{\rho}_i = \sum_{j \neq i} \rho_j(r_{ij}), \quad (2)$$

where $\rho_j(r_{ij})$ is the electron density function of atom i assigned to atom j .

The Fe-Ni-Cr EAM potential, developed by Bonny et al. in 2013 (potential 1, P1) [28], can reproduce the self-diffusivity of each element in Fe-Ni-Cr alloys [28]. Thus, it is suitable to simulate the bonding process via atomic diffusion. However, it is parameterized based on properties of Fe10Ni20Cr alloy, whose composition is similar to that of 316L austenitic stainless steel [28]. Whether this potential can be transferred to our simulation subject (i.e., $\text{Fe}_{27}\text{Ni}_{51}\text{Cr}_{22}$, details of this initial structure will be elaborated in the next subsection) with another composition remains uncertain. In order to verify the robustness of this EAM potential, various thermophysical properties of $\text{Fe}_{27}\text{Ni}_{51}\text{Cr}_{22}$ (i.e., solidus and liquidus temperatures, linear thermal expansion coefficient at 300 K, constant-pressure specific heat capacity at 300 K, and latent heat of fusion) are calculated and compared with available experimental results. For further verification, melting temperature of Ni NP is also determined. Another Fe-Ni-Cr EAM potential (potential 2, P2) [29], developed by the same group in 2011, is also verified with the same scenario for comparison of the accuracy in describing the metallic bonding. Detailed methodology of potential verification is elaborated in the Supporting Information (S.I.) Section S1.

2.2. Construction of initial structures

Ni-based superalloy, Inconel® 718 contains more than 10 elements, while almost 90 wt% of the constituent elements are Fe, Ni, and Cr [2]. For simplification of structure model and accuracy of many-body interactions, only the major elements, i.e., Fe, Ni, and Cr, are included in modeling of the Inconel® 718 alloy [30,31]. In step 1, a $20 \times 40 \times 20$ Ni supercell of face-centered cubic (FCC) lattice is created with periodic boundary conditions, i.e., the dimensions of the supercell in x , y , and z directions are $20a_{\text{Ni}}$, $40a_{\text{Ni}}$, and $20a_{\text{Ni}}$, where the a_{Ni} is the lattice constant of Ni ($a_{\text{Ni}} = 3.52 \text{ \AA}$). This supercell contains total 64,000 atoms, and among them, 17,474 Fe and 13,954 Cr atoms are randomly

distributed by replacing the Ni atoms in FCC lattice sites. This replacement results in the number percentages of Fe, Ni, and Cr atoms of 27%, 51% and 22% (the weight percentages are 27.01 wt%, 52.91 wt%, and 20.08 wt%, which are similar to those of realistic Inconel® 718 alloy), and we denote this atomic structure as $\text{Fe}_{27}\text{Ni}_{51}\text{Cr}_{22}$.

This initial structure of Ni-superalloy, $\text{Fe}_{27}\text{Ni}_{51}\text{Cr}_{22}$, for bonding simulations is prepared through three steps: the structure created by random replacement is relaxed at 300 K for 1000 ps in the step 1. In step 2, the relaxed structure at 300 K is heated to 2500 K with a heating rate of 11 K/ps for complete melting, and then relaxed at 2500 K for 1000 ps as well. In step 3, the relaxed structure at 2500 K is quenched to 300 K with a quenching rate of 0.44 K/ps, followed by another 1000 ps relaxation at 300 K. In the above three steps, the temperature (T) and pressure ($P = 1 \text{ atm}$ is employed in all steps) are controlled by Nosé-Hoover thermo- and barostat, using the NPT ensemble (constant atomic number, pressure, and temperature).

A Ni NP with a radius of $9a_{\text{Ni}}$ ($= 31.68 \text{ \AA}$) is constructed using non-periodic boundary conditions. Then, an energy minimization is performed using the conjugate gradient (CG) algorithm [32] with a force or energy precision of 1.0×10^{-15} (eV/Å for force tolerance, unitless for energy tolerance [33]), followed by relaxation at 300 K for 1000 ps with the NVT ensemble (constant atomic number, volume, and temperature).

Two $\text{Fe}_{27}\text{Ni}_{51}\text{Cr}_{22}$ alloy blocks for base materials and Ni NP fillers are then assembled together for bonding simulations as shown in Fig. 1. The adaptive common neighbor analysis (ACNA) [34] is used to characterize crystalline structures of base and filler materials. To avoid overlapping of atoms while maintaining interaction, two Ni NPs are separated with a distance of $2a_{\text{Ni}}$ in y direction, and the NPs are apart

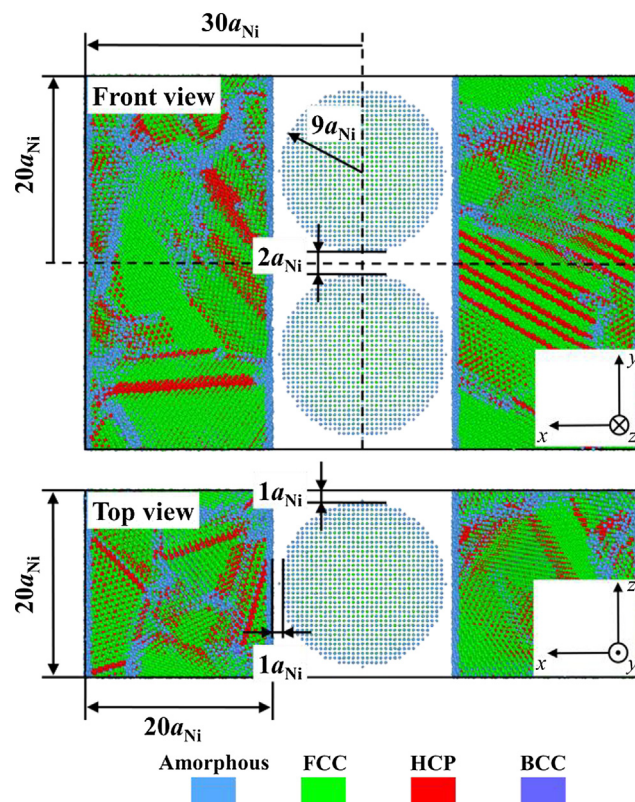


Fig. 1. Front and top views of the simulation configuration for $\text{Fe}_{27}\text{Ni}_{51}\text{Cr}_{22}$ bonding with Ni NPs. Crystalline structure is characterized by the adaptive common neighbor analysis. The base alloy contains a matrix structure of FCC lattice (60.6%, green) with local orders of hexagonal close packed (HCP, red) of 15.4%, body-centered cubic (BCC, purple) of 0.3%, and amorphous (blue) of 23.8%. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

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