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Cooling times' dependence on the glassy NiTi at extremely low temperatures: a result from rapid solidification using molecular dynamics simulations

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Abstract. In this paper, we evaluate the structure of glassy NiTi at 10 K obtained from molecular dynamics simulations using various cooling times. The final configurations of glassy NiTi were produced by decreasing the temperature of liquid NiTi rapidly from 2500 K to10 K during 0.1 nanoseconds (ns) to 1.0 ns of cooling times. The results show that the count of BCC-like and Icosahedral-like local structure increases at the longer cooling times, while the count of HCP-like local structure decreases when the cooling times become longer. We also observe that the count of FCC-like local structure almost remains constant for all cooling time variations.

1. Introduction

NiTi alloy is one of the metal alloys formed from nickel and titanium atoms. NiTi alloys are widely used as biomaterials in the medical field because they have bio-functional and biocompatible properties [1,2]. NiTi alloys have been applied in areas such as aerospace, military, building construction, and medical equipment. This material has several unique properties such as biocompatibility, high electrical resistivity, and corrosion resistance [1,2].

As more products from NiTi materials are developed and produced, controlling the manufacturing process becomes an important role to get the results that are in accordance with expectations and to provide consistent material quality [3, 4]. Among the problems that arise are about how cooling rate variations during the solidification process influence the structure of NiTi solids. This study aims to analyze the crystal structure produced due to of the rapid cooling rate from a temperature of 2500 K to 10 K on the NiTi alloy solidification process. This study is the continuation of our previous researches which have discussed the structural change of liquids NiTi at the different pressures [5] and the local structure of glassy NiTi produced with different cooling times from 2500 K to 300 K [6].

2. Methods

2.1 Atomic Configuration

We use the Avogadro package [7] to generate the atomic configurations of NiTi alloy. Figure 1 shows the initial configuration of NiTi alloys with 16000 atoms, of which 8000 atoms are for Ni and Ti, respectively. The supercell size of the system is 61 x 61 x 61 Å^3 in the x-, y- and z- axis direction. Periodic boundary conditions are applied in the system for all directions.
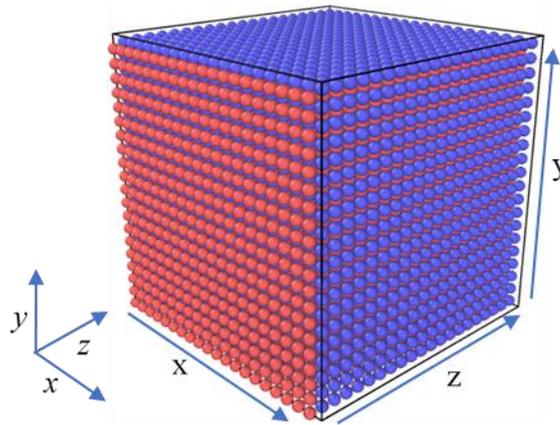
Figure 1. Initial configuration of a NiTi metal alloy with crystal structure B2. The blue and red balls in a row represent the Nickel and Titanium atoms, respectively.

2.2 Numerical procedure

We used the molecular dynamics (MD) calculation with the Large-Scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) package [8]. The potential value of the embedded-atom method (EAM) type potential introduced by Zhou, et al. [9] is used to describe the value of interactions between atoms. This value is used because it has good accuracy in melting temperature and for the types of NiTi metal alloys [10]. To solve the motion equation, we used the Verlet algorithm with time $\Delta t = 1$ fs. Before heating, the system was quantified at a temperature of 300 K for 0.05 ns. The system is then melted by raising the temperature beyond the melting temperature of the alloy from 300 K to 2500 K for 0.05 ns. System equilibration is again carried out at a temperature of 2500 K for 0.1 ns.

Afterwards, the system temperature is reduced from 2500 K to 10 K during cooling, for $t_{cooling} = 0.1$ ns to 1.00 ns (at 0.1 ns intervals) using the NPT Nosé-Hoover nsemble [11, 12]. The system is equilibrated for 0.1 ns using the same ensemble. The NVT ensemble is carried out or 0.03 ns (30,000 MD steps) after solidification as data to be analyzed. For image rendering, we used the Ovito [13] as well as the RINGS package or structural analysis [14].

3. Results and Analysis

### 3.1 Structure Factor S(q)

We evaluated the results of the glassy NiTi structure's cooling rate, which has been achieved for convergence by analyzing the structure using the radial distribution function $g(r)$ and the structure factor $S(q)$. Figure 2 (a) shows that as the length of the cooling rate increased; the intensity of the first and second peak of the structure factors increased, even though the difference was small by 0.11 and 0.03. Figure 2 (b) shows the existence of a shoulder in the structure factor after the second peak when $t_{cooling} = 0.1$ ns, indicating the presence of ISRO. This shoulder became a new peak when $t_{cooling}$ was getting longer, indicating the face-sharing regular tetrahedra.
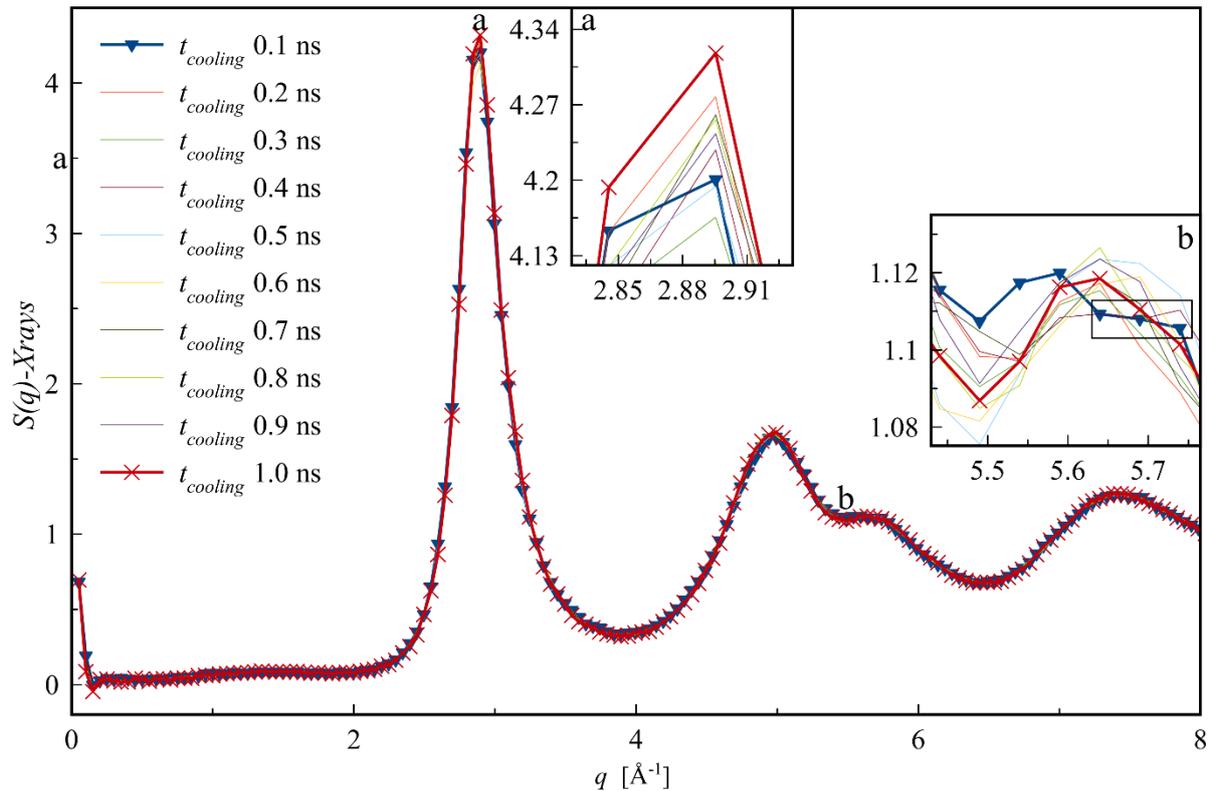
Figure 2. The structure factor $S(q)$ of the NiTi alloy after the solidification process over a number of different variations of the cooling rate. (a) The first peak of the glassy NiTi structure factor; (b) the shoulder of the second peaks of structure factor of glassy NiTi.

3.2 Radial Distribution Function g(r)

From figure 3, it can be seen that the results of total $g(r)$ fluctuate. The first peak is highest when $t_{cooling}$ was 0.90 ns with a value of 3.91 with r = 2.64 Å, whereas, at the second peak, there was an increase of height along with the length of the cooling rate. There was a difference of 0.06 when $t_{cooling}$ = 0.1 and $t_{cooling}$ = 1.0, which previously had an initial average of 1.06 becomes 1.12 with r = 4.47 and r = 4.46, respectively. As the cooling rate lengthened, the average position of the neighbor atom became closer to the reference atom.
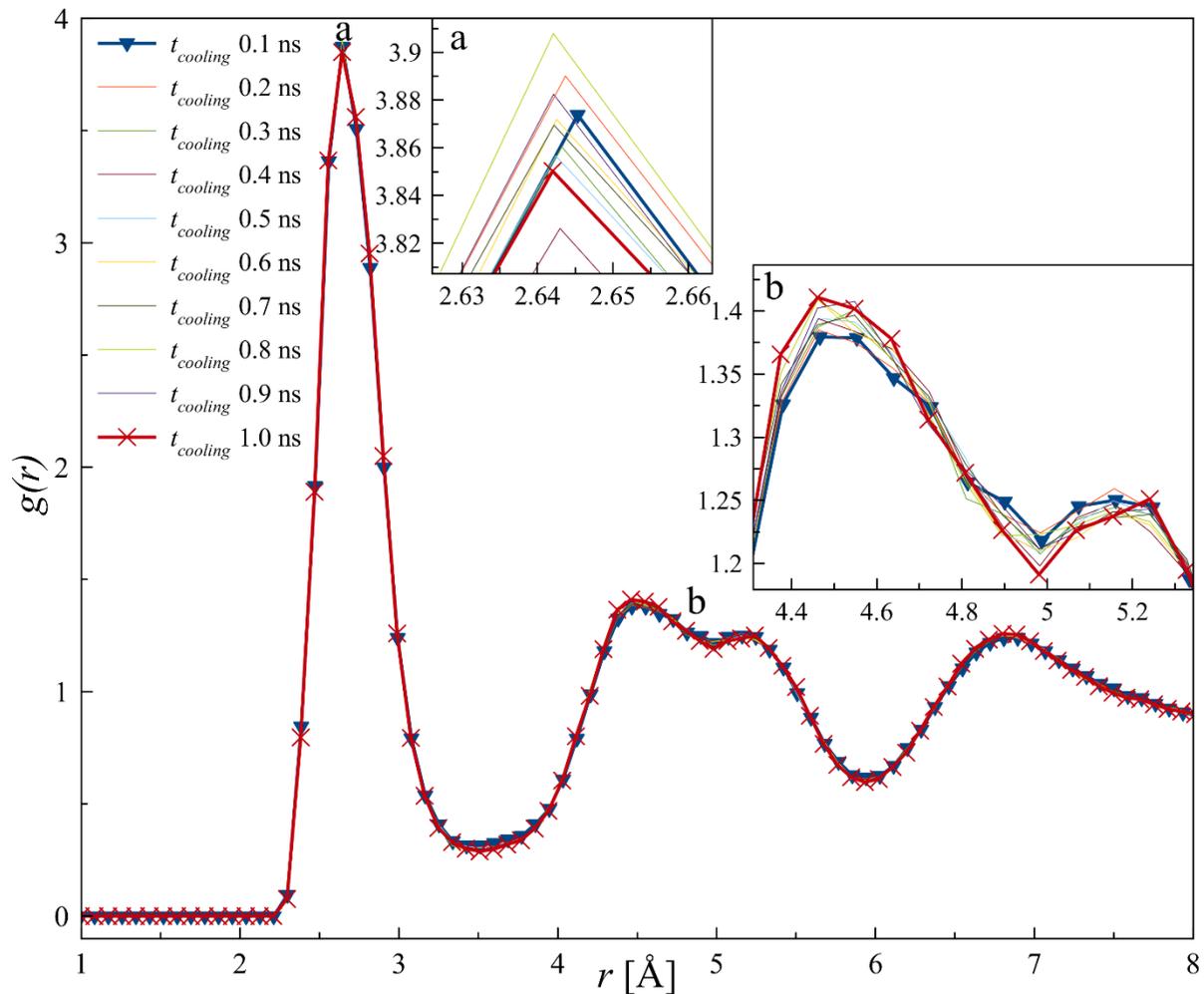
Figure 3. The radial distribution function $g(r)$ of the NiTi alloy after the solidification process over a number of different variations of the cooling rate. (a) The first peak of the radial distribution function $g(r)$; (b) The second and shoulder peaks of the radial distribution function $g(r)$.

3.3 Local Structure

The local structure of glassy NiTi was investigated using the bond-angle method developed by Ackland and Jones [15]. This method evaluates the angle distribution of local neighboring atoms and designates structural types, such as FCC, HCP, BCC, or icosahedral [15]. We conducted this analysis for all atoms without distinguishing Ni and Ti species because the bonding angle method had been designed only for systems containing one type of atom.

Figure 4 (b) shows that the trend in local ISRO atomic packaging increases when the total cooling time was longer, while the tendency for local FCC atomic packaging remained constant. Figure 4 (a) shows that at very fast cooling rates ($t_{cooling}$ = 0.1 ns to 1.0 ns), the amount of local BCC atomic packing was higher than for HCP structures, with a tendency to increase and decrease, respectively.
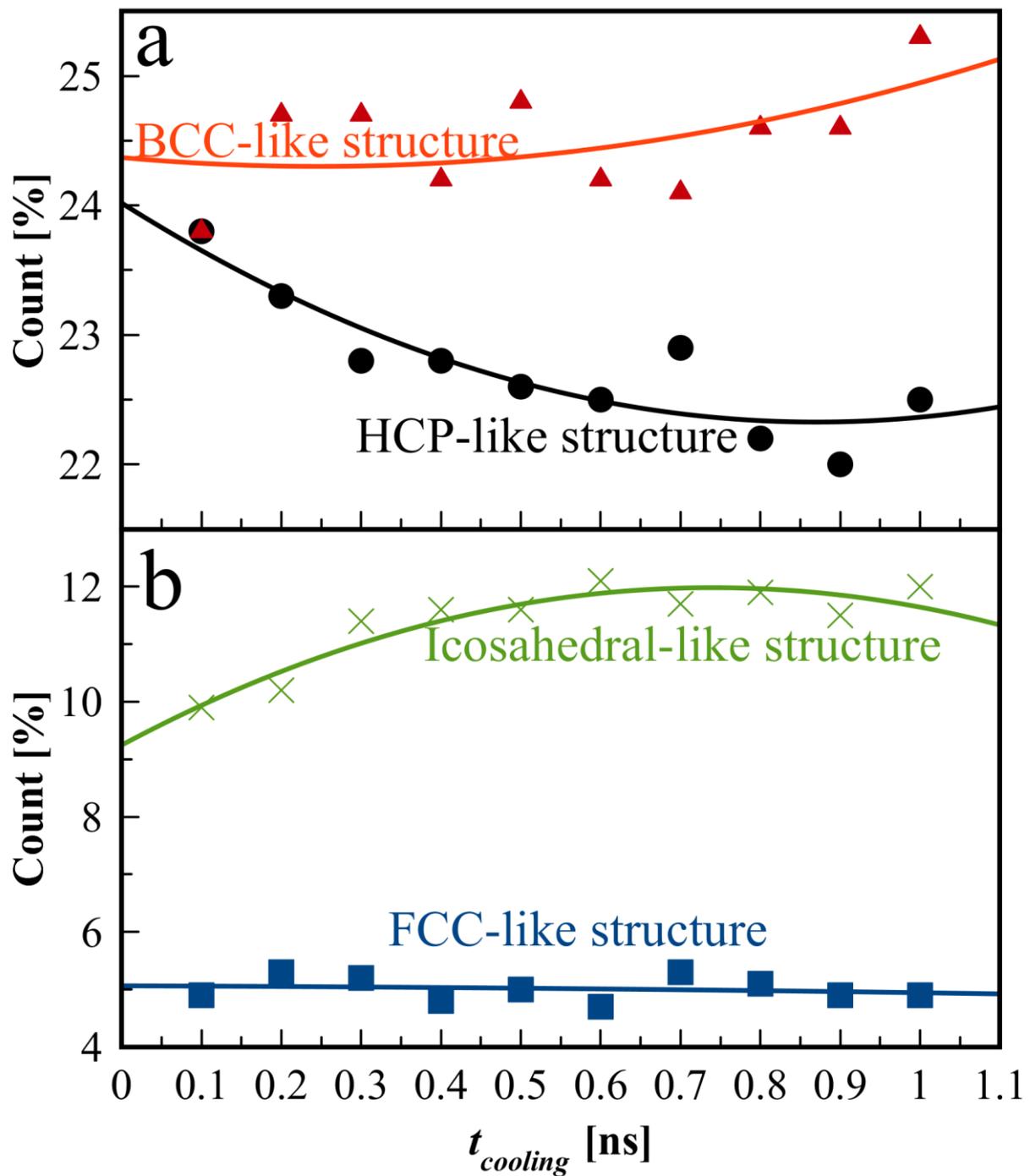
Figure 4. Local structure analysis of glassy NiTi alloy at low temperature of 10 K for (a) BCC- and HCP-like structure, and (b) Icosahedral- and FCC-like structure.

4. Conclusion

It can be concluded from our results that the height of the first peak of the structure factor of glassy NiTi increased slightly with the longer cooling time. The presence of a shoulder after the second peak indicates the presence of ISRO in the system with $t_{cooling}$ = 0.1 ns. Signs of regular face-sharing tetrahedra can be found when cooling time is longer. For the radial distribution function $g(r)$, the first peak fluctuates from the $t_{cooling}$ = 0.1 to 1.0; while for the second peak, there is an increase in the average atom of $g(r)$ during the longer cooling time. From the analysis of local atomic packaging using the bond-angle method, it shows that the number of HCP structures decreases at longer cooling times, which is contrary to the trend for BCC and ISRO structures which have increased percentages. The BCC local atomic packing is found more often than other local structures of glassy NiTi when $t_{cooling}$ at 1.0 ns. It was also observed that the FCC local atomic packing is relatively constant in all cooling times.

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