

MOLECULAR DYNAMICS STUDY OF STRUCTURE, CRYSTALLIZATION AND PHASE TRANSITION IN BULK CO-MATERIALS: EFFECT OF TEMPERATURE, NUMBER OF ATOMS AND ANNEALING TIME

Dung Nguyen Trong^{1, 2}, Umut Saraç³, Van Cao Long¹, and Ștefan Țălu^{4, *}

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Abstract

In this work, the structure, crystallization, and phase transition of the bulk Co materials have been characterized via the Molecular Dynamics Simulation (MDS) method combined with the Sutton-Chen (SC) embedded potentials and periodic boundary conditions under various factors such as temperature (T), number of atoms (N), and annealing time (t). The common neighbor analysis revealed the coexistence of Amorphous (Amor) and crystalline Face Centered Cubic (FCC), Body Centered Cubic (BCC), and Hexagonal Close Packed (HCP) phases at an equilibrium state irrespective of the aforementioned factors. Compared with the crystalline FCC and BCC phases, the HCP and Amor phases were found to be dominant in the bulk Co₁₀₉₇₆ material at T = 300 K. Decreasing N from 10976 to 4000 atoms at T = 300 K and increasing T from 300 to 1000 K in the bulk Co₁₀₉₇₆ material didn't change the dominant phases. It was found that the glass transition temperature (T_g) of the bulk Co₁₀₉₇₆ material was 700 K. Increasing t from 0 to 10 ps at T_g = 700 K abruptly changed the dominant phase of the bulk Co₁₀₉₇₆ material into the FCC structure. The radial distribution function (RDF) analysis showed that the distance between Co atoms in the bulk Co₁₀₉₇₆ material was 2.475 Å at T = 300 K. The N and T didn't affect the distance between Co atoms, but t caused an increase. The size (l) increased from 3.8391 to 5.3320 nm, while the energy (E) decreased from -4.195 to -4.218 eV with increasing N. The first peak height of the RDF (g(r)) first increased and then decreased as the N increased. Increasing T from 300 to 1000 K led to an increment in the E value from -4.218 to -4.087 eV and a slight increase in the l from 5.3320 to 5.3323 nm.

Keywords: Annealing time; Atomic number; Co bulk materials; Crystallization; Glass transition temperature; Molecular dynamics simulation; Structure

¹ Institute of Physics, University of Zielona Góra, Poland. E-mail: dungntdt2018@gmail.com; vancaolong2020@gmail.com

² Faculty of Physics, Hanoi National University of Education, Vietnam.

³ Department of Science Education, Bartın University, Turkey. E-mail: usarac@bartin.edu.tr

⁴ The Directorate of Research, Development and Innovation Management (DMCDI), Technical University of Cluj-Napoca, Romania. E-mail: stefan_ta@yahoo.com*

* Corresponding author

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Introduction

Cobalt (Co) and Co-based materials are one of the most interesting materials for industrial and magnetic applications thanks to their unique properties (Puntes *et al.*, 2001; Gubin *et al.*, 2003; de la Peña O' Shea *et al.*, 2009; Purja Pun and Mishin, 2012; Shatrova *et al.*, 2018; Kumar *et al.*, 2019). It is well known that the properties of materials are strongly related to their structural characteristics (Sarac *et al.*, 2015; Khan *et al.*, 2019; Babayevska *et al.*, 2022; Cao Long *et al.*, 2022). The structural characteristics of ultrafine grain films of Co were experimentally investigated as a function of annealing temperature (T) and a transition from HCP phase to FCC one was found at the annealing temperature above 573 K (Kumar and Gupta, 2007). Experimental studies showed that the HCP structure in pure Co changes to FCC one at the temperature range of 680–720 K (Nishizawa and Ishida, 1983; Bidaux *et al.*, 1989; Bedi and Forker, 1993; Adjam *et al.*, 2020; Guillermet, 1989). It was reported that Co exhibits only the HCP phase at $T \leq 604$ K while at $T = 771$ K it exhibits only the FCC phase (Lindgren *et al.*, 1978). In addition to experimental studies, advances in simulation technologies facilitate the study of the structure, crystallization process, and phase transition of materials at an atomic scale. This has been achieved using various theoretical functional approaches such as Density Functional Theory, Effective Field Theory, Monte Carlo Simulation, and Molecular Dynamics Simulation (MDS) (Oukhrib *et al.*, 2021; Tran *et al.*, 2020; Goudeli, 2019; Sewak *et al.*, 2022; Starikova *et al.*, 2018; Lizárraga *et al.*, 2017). Among the theoretical approaches, the MDS method is widely utilized to explore the influence of various factors on the structural and mechanical features of a wide variety of metallic materials (Purja Pun and Mishin, 2012; Deng and Tüysüz, 2014; Nguyen *et al.*, 2017; Ou, 2017; Dung, 2018; Tuan and Dung, 2018; Tuan and Dung, 2019; Dung and Phuong, 2020; Dung *et al.*, 2020a; Dung *et al.*, 2020b; Long *et al.*, 2020; Dung and Van, 2021; Nguyen Trong *et al.*, 2021; Zhang *et al.*, 2021; Hoc *et al.*, 2022; Quoc *et al.*, 2022a; Quoc *et al.*, 2022b; Trong *et al.*, 2022; Xue *et al.*, 2022). With simulation methods, the Embedded Atom Method (EAM) interatomic potential and Sutton-Chen (SC) potential are widely applied to identify the interactions between atoms (Dung and Phuong, 2020; Quoc *et al.*, 2022b). In a recent study, the transition from the HCP structure to the FCC one in Co layers of Ni/Co multilayers is found in the temperature range of 500–700 K using the MDS method with the EAM potential (Vu *et al.*, 2022). In another study using the EAM interatomic

potential, the transition temperature for Co was estimated to be 717 K (Purja Pun and Mishin, 2012). The study reported only the HCP phase (Lindgren *et al.*, 1978), but other studies showed that both HCP (predominant) and FCC phases coexist at room temperature (Bedi and Forker, 1993; Lizárraga *et al.*, 2017; Sewak *et al.*, 2022). Earlier studies reported that the reason for the phase transition can be attributed to the absence and/or reduction of magnetism at higher temperatures (Söderlind *et al.*, 1994; Uhl and Kübler, 1996; Yoo *et al.*, 1998). However, recent theoretical studies have shown that the weakening of magnetism alone is not responsible for the stabilization of the FCC phase at 700 K (Sewak *et al.*, 2022; Lizárraga *et al.*, 2017). The largest energy contribution to the stabilization of FCC arises from ionic lattice vibrations (Lizárraga *et al.*, 2017). To our best knowledge, the effect of temperature (T), number of atoms (N), and annealing time (t) on the structure, crystallization, and phase transition of the bulk Co materials has not been studied until now using MDS method combined with the Sutton-Chen (SC) embedded potentials and periodic boundary conditions. In the present study, the glass transition temperature (T_g) of the bulk Co_{10976} material was found to be 700 K. It was also revealed that increasing t from 0 to 10 ps at $T_g = 700$ K caused an abrupt change in the dominant phase of the bulk Co_{10976} material.

Method of Calculation

In this work, the MDS combined with SC potential and periodic boundary conditions were used to investigate the structural changes of the bulk Co materials under various factors (Spearot *et al.*, 2007; Tschopp *et al.*, 2007; Yanqiu and Shuyong, 2018). With the applied periodic boundary condition, all size effects and surface effects of the material will be eliminated when the Co-material model is included in the study. The interaction between atoms with periodic boundary conditions occurs. If an atom flies out of the periodic boundary region, there will immediately be another atom flying in to replace the symmetry position in the research model.

In our model, the Co atoms in the bulk material are arranged randomly. The size (l) of the Co material is determined by the following formula (1):

$$l = \sqrt[3]{\frac{N}{\rho_0}} \quad (1)$$

Table 1. The parameters of the bulk Co material

Coefficient	E_i^0 (eV)	R_i^0 (Å)	α_i	A_i	$\beta_i^{(0)}$	$\beta_i^{(1)}$	A
Value	4.41	5.0	5.24	0.9	3.5	4.0	2.5
Coefficient	$\beta_i^{(2)}$	$\beta_i^{(4)}$	$t_i^{(0)}$	$t_i^{(1)}$	$t_i^{(2)}$	$t_i^{(4)}$	r_c
Value	0.0	0.0	1.0	3.0	5.0	-1.0	4.5

In that l is the size, N is the number of atoms, ρ_0 is the density, $\rho_0 = 7.75 \text{ g} \cdot \text{cm}^{-3}$, and the lattice constant size of Co is $a = 3.54 \text{ Å}$.

The SC potential is one of the most suitable potentials to describe the atomic interactions between Co atoms, which is shown in formula (2): (Yanqiu and Shuyong, 2018).

$$E_{\text{tot}} = \frac{1}{2} \sum_{ij} V_{ij}(r_{ij}) + \sum_i F_i(\bar{\rho}_i), \quad V(r_{ij}) = E_i \left(\frac{a}{r_{ij}} \right)^n,$$

$$F_i(\rho) = A_i E_i^0 \rho \ln \rho, \quad \rho_i^{a(i)}(R) = e^{-b^*}, \quad b^* = \beta_i^{(0)} \left(\frac{R}{R_i^0 - 1} \right),$$

$$(\bar{\rho}_i)^2 = \sum_{l=0}^3 t_i^{(l)} (\rho_i^{(l)})^2 \quad (2)$$

In that, the values of the coefficient of the bulk Co materials are shown in Table 1 (Spearot *et al.*, 2007; Tschopp *et al.*, 2007; Yanqiu and Shuyong, 2018).

All simulations were done using the code LAMMPS (Spearot *et al.*, 2007; Tschopp *et al.*, 2007) with EAM interatomic potential (Murphy *et al.*, 2010). All models of the bulk Co material run NVT (with N is the number of atoms, V is the volume, T being the temperature has constant values) with temperature reduced from 4000 K to 1000, 900, 800, 700, 600, 500, 400, and 300 K with the same heating rate of $4 \times 10^{12} \text{ K/s}$, run to 4×10^5 molecular dynamics steps with 1 fs step. Three models were chosen for the bulk Co material according to the N such as 4000, 8788, and 10976 atoms. After that, the phase transition, structural characteristics, and crystallization process of the bulk Co₁₀₉₇₆ materials under various T and t values were determined. With the bulk Co material, the heating process of follows the Nosé-Hoover formula (Nosé, 1984; Hoover, 1985). It is one of the most accurate and efficient methods for simulating molecular dynamics at a constant temperature. To analyze the structural features of the Co material, the radial distribution function (RDF) (Reed, 2003) and the Common Neighbor Analysis (CNA) (Tsuzuki *et al.*, 2007; Stukowski, 2012) were used. The first peak height of the RDF ($g(r)$) is determined by the following formula (3):

$$g(r) = \frac{n(r)}{4\pi r^2 \rho_0 dr} \quad (3)$$

where r , $g(r)$, n , and ρ_0 represent the link length, the height of the RDF, the number of atoms, and the

atomic density, respectively. In addition, mean squared distance was also used to explore the diffusion mechanism of Co atoms during the simulation process. The mean squared distance between Co atoms is expressed as (Hoover, 1985):

$$r(t) = \sqrt{\frac{1}{N} \left\{ \sum_{i=1}^N |\vec{r}_i(t) - \vec{r}_i(0)|^2 \right\}} \quad (4)$$

where $r_i(0) \rightarrow r_i(t)$ shows the position of atom i at time t . The phase transition was obtained by means of the correlation between the T and the energy (E). OVITO software was applied to visualize the atomic structure and analyze the data obtained from the MDS (Song *et al.*, 2014; Lu *et al.*, 2016).

Results and Discussion

Structural Characteristics

To reveal the structural features of the bulk Co materials, the structural characteristics of the bulk Co₁₀₉₇₆ material were investigated at $T = 300 \text{ K}$. The results obtained are demonstrated in Figure 1.

The CNA was performed to identify the phase structure of the bulk Co₁₀₉₇₆ material (Figure 1(a)) at $T = 300 \text{ K}$. The results of the CNA indicated the coexistence of amorphous (Amor) and crystalline Face-Centered Cubic (FCC), Body-Centered Cubic

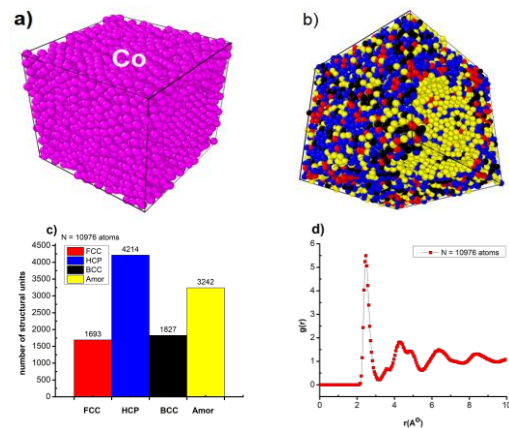


Figure 1. Structural characteristics of the bulk Co₁₀₉₇₆ material at $T = 300 \text{ K}$. The bulk Co (a), the structural shape (b), the structural unit number (c), and the RDF (d)

(BCC), and Hexagonal Close-Packed (HCP) phases (Figure 1(b)). During the entire implementation process, we use the random function to let the atoms move randomly in the interaction force field, so the formation of the structural units FCC, HCP, BCC, Amor is completely random. To be able to determine the number of structural units, we use common neighborhood analysis (CNA) to determine the type of structure and count them (Tsuzuki *et al.*, 2007; Stukowski, 2012). Currently, with Co bulk materials using MD simulation methods to study microstructural characteristics, there are no detailed studies on this issue. The author has also used this method to successfully research other metals and alloys in works (Nguyen *et al.*, 2017; Dung, 2018; Tuan and Dung, 2018; Tuan and Dung, 2019; Nguyen Trong *et al.*, 2021; Dung and Phuong, 2020; Dung *et al.*, 2020a; Dung *et al.*, 2020b; Long *et al.*, 2020; Cao Long *et al.*, 2022; Quoc *et al.*, 2022b; Trong *et al.*, 2022). As clearly seen from Figure 1(c), the HCP and Amor phases were dominant compared with the crystalline FCC and BCC phases at $T = 300$ K. The RDF analysis showed that the distance between Co atoms in the bulk Co_{10976} material is $r = 2.475$ Å (Figure 1(d)); this is very consistent with the values reported in simulation and experimental studies (Nishizawa and Ishida, 1983; Shabib *et al.*, 2009; Purja Pun and Mishin, 2012; Zhang *et al.*, 2014; Trong *et al.*,

2022). It was also determined that the l of the bulk Co_{10976} material is 5.3320 nm and the E of the atom is -4.218 eV. Through the structural shape (Figure 1(b)), it can be seen that the structural shape of the material also has holes on the surface of the material because we have set the number of moving steps to 1 fs, making the elements the atoms not having time to form a crystalline structure. This is because the author wants to research a material with holes on the surface to create a porous material for future applications.

Influencing Factors

In this section, the effects of factors such as N , T , and t are discussed and the results of the analysis are presented. The values of the factors investigated vary between 4000 atoms and 10976 atoms for N , between 300 K and 1000 K for T , and between 0 ps and 100 ps for t .

Effect of N : The influence of the N on the structural characteristics of the bulk Co material from 4000 atoms to 10976 atoms is presented in Figure 2.

Figure 2 revealed that the N affects the structural properties of Co material (Figure 2(a1), 2(b1), 2(c1)). The structural unit number FCC, HCP, BCC, and Amor increased gradually from 577 FCC to 1693 FCC, from 1537 HCP to 4214 HCP,

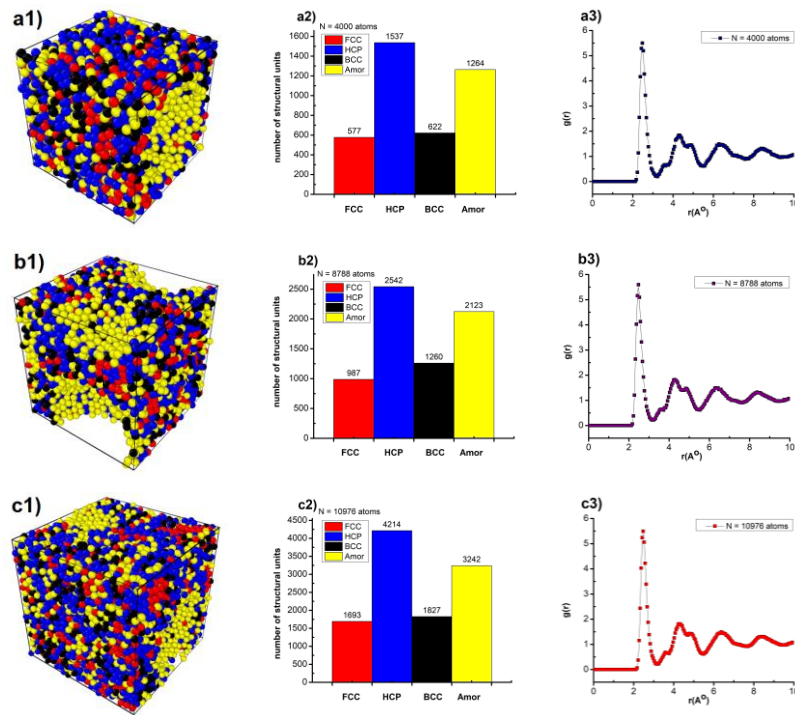


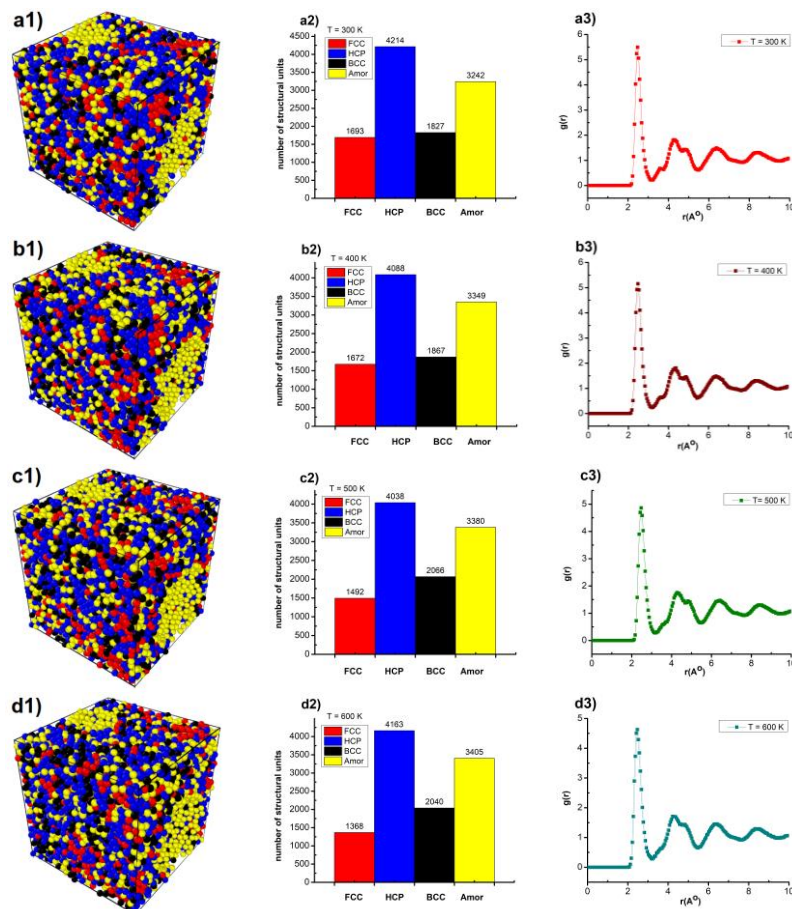
Figure 2. The structural shape (a1, b1, c1), the structural unit number (a2, b2, c2), and the RDF (a3, b3, c3) of the bulk Co material for different N values at a constant T of 300 K.

from 622 BCC to 1827 BCC, and from 1264 Amor to 3242 Amor, respectively, with increasing N from 4000 to 10976 (Fig. 3a2, 3b2, 3c2). However, as clearly seen in Figure 2, the HCP and Amor phases are always predominant compared with the crystalline FCC and BCC phases at $T = 300$ K irrespective of the N. Increasing N from 4000 atoms to 10976 atoms caused no change in the distance between Co atoms ($r = 2.475$ Å) (Figure 2(a3), 2(b3), 2(c3)). However, the $g(r)$ of the RDF first increased from 5.498 to 5.595 with increasing N from 4000 atoms to 8788 atoms and then decreased to 4.494 with a further increase in the N to 10976 atoms. The l increased from 3.8391 nm to 5.3320 nm, while the E of the material decreased from -4.195 eV to -4.218 eV with increasing N from 4000 atoms to 10976 atoms. This may be due to the surface and size effect.

Effect of T: In this section, we showed how the structural characteristics of the bulk Co_{10976} material are affected by the T value ranging from 300 K to 1000 K (Figure 3(a1), 3(b1), 3(c1), 3(d1), 3(e1), 3(f1), 3(g1), 3(h1)). The obtained results are

illustrated in Figure 3. As distinctly noticed from Figure 3, the HCP and Amor phases are always dominant compared with the crystalline FCC and BCC phases regardless of the T value. However, the fraction of the Amor phase gradually increased with increasing T and became more dominant than the HCP phase at higher T values, indicating that the T factor has an effect on the phase structure of the Co materials (Figure 3(a2), 3(b2), 3(c2), 3(d2), 3(e2), 3(f2), 3(g2), 3(h2)). In addition, this increase in the fraction of the Amor phase with increasing T shows that the crystallinity of the Co_{10976} material decreases.

Raising the T from 300 K to 1000 K caused a decrease in the E value from -4.218 eV to -4.087 eV and a slight increase in the l from 5.3320 nm to 5.3323 nm. The RDF analysis indicated a significant reduction in the $g(r)$ value from 5.494 to 3.722 with increasing T from 300 K to 1000 K. However, the T factor had no effect on the distance between Co atoms in the bulk Co_{10976} material ($r = 2.475$ Å) (Figure 3(a3), 3(b3), 3(c3), 3(d3), 3(e3), 3(f3), 3(g3), 3(h3)).



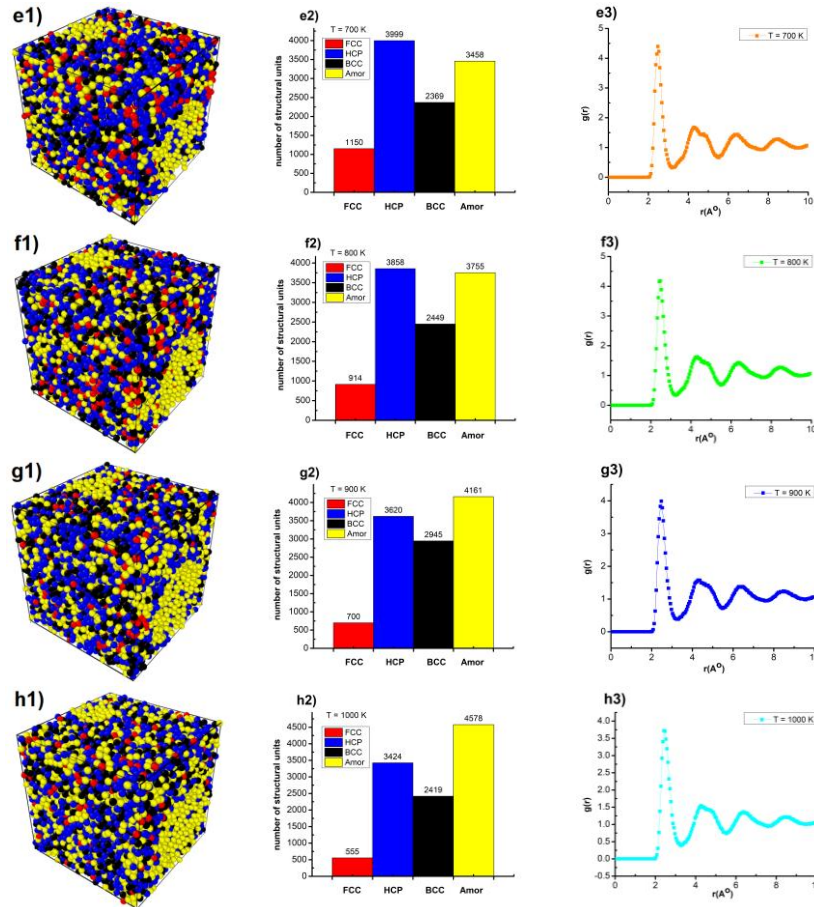


Figure 3. The structural shape (a1, b1, c1, d1, e1, f1, g1, h1), the structural unit number (a2, b2, c2, d2, e2, f2, g2, h2), and the RDF (a3, b3, c3, d3, e3, f3, g3, h3) of the bulk Co_{10976} material for different T values

To estimate the T_g value of the bulk Co_{10976} material, the E-T plot was obtained and the resulting E-T plot is shown in Figure 4. As distinctly noticed from Figure 4, the E-T plot consisted of two different parts. The blue and red lines correspond to the first ($300 \text{ K} < T < 700 \text{ K}$) and second ($700 \text{ K} < T < 1000 \text{ K}$) parts, respectively. In both parts, the E changes linearly with T . However, when T increased, there was a stronger increase in the E in the second part compared to the first part. These two different parts were intersected at $T = 700 \text{ K}$, indicating that the T_g value of the bulk Co_{10976} material is 700 K ; this is in good accordance with the values found in previous experimental and simulation studies (Nishizawa and Ishida, 1983; Guillermet, 1987; Bidaux *et al.*, 1989; Bedi and Forker, 1993; Purja Pun and Mishin, 2012; Adjam *et al.*, 2020).

Effect of t

Figure 5 presents the correlation between the E and the t in the bulk Co_{10976} material at different T

values of 600 K , 700 K , and 800 K . As seen from Figure 5, the E value of the bulk Co_{10976} material is affected by the t value. However, the change in the E value is much stronger at $T = 700 \text{ K}$ compared to the other T values (600 K and 800 K). At $T = 700 \text{ K}$, the E value of the bulk Co_{10976} material decreased rapidly with increasing t from 0 ps to 10 ps (corresponding to the number of simulation steps increased from 0 to 1×10^4 steps). The decline in the E value then gradually slowed down in the t range of 10 ps to 20 ps (2×10^4 steps). The E value reached a constant value at 20 ps and remained almost constant at t values greater than 20 ps . These results reveal that the bulk Co_{10976} material exhibits a strong crystallization at $T_g = 700 \text{ K}$, but a weak crystallization at T values of 600 K and 800 K . To confirm the accuracy of these results, we continue to investigate the influence of the t on the structural features of the bulk Co_{10976} material in more detail as follows.

The dependence of the structural properties of the bulk Co_{10976} material on t at $T_g = 700 \text{ K}$ is

presented in Figure 6(a1). The results indicated that the HCP and Amor phases were predominant compared with the crystalline FCC and BCC phases at $t = 0$ ps (Figure 6(b1)). Besides, the RDF analysis revealed that the distance between Co atoms of the Co_{10976} material is $r = 2.475$ Å, $g(r)$ is 4.390, l is 5.3320 nm, and the E is -4.155 eV at $t = 0$ ps (Figure 6(c1)). However, increasing t from 0 ps to 10 ps abruptly changed the dominant phase of the bulk Co_{10976} material into the FCC structure with a small proportion of the Amor, HCP, and BCC phases (Figure 6(a1), 6(a2), 6(a3), and 6(a4)).

The dominant FCC phase remained unchanged even though the t value was increased up to 50 ps. The fraction of the FCC phase continued to increase slightly with increasing t from 10 ps to 50 ps (1×10^5 steps) (Figure 6(b1), 6(b2), 6(b3), and 6(b4)). An increase in the t from 0 ps to 50 ps induced an increase in the $g(r)$ from 4.390 to 4.929, but a decrease in the l and E values from 5.3320 nm to 5.0951 nm and from -4.155 eV to -4.246 eV (Figure 6(c1), 6(c2), 6(c3), and 6(c4)), respectively. The results of the RDF analysis also showed that increasing t from 0 ps to 100 ps caused an increase

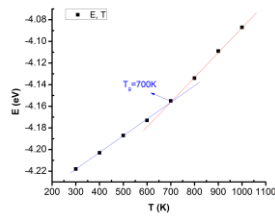


Figure 4. The E-T plot of the Co_{10976} material

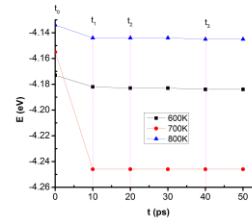


Figure 5. The correlation between the E and the t in the bulk Co_{10976} material at different T values

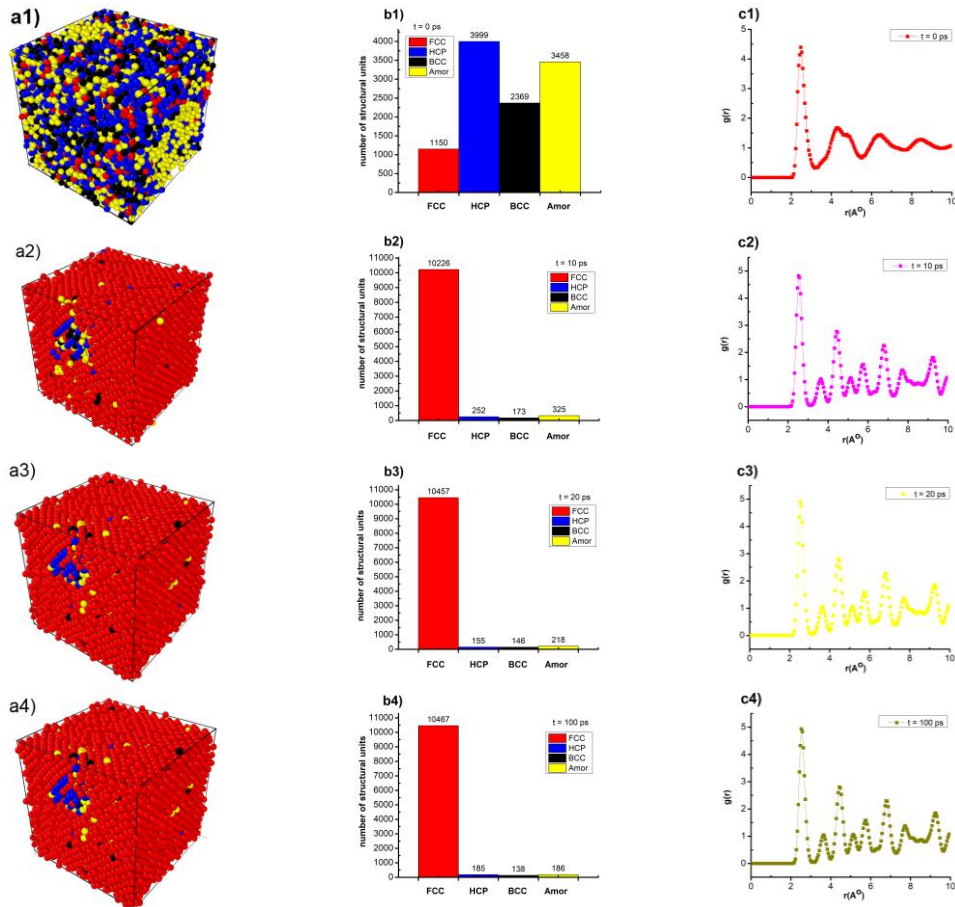


Figure 6. The structural shape (a1, b1, c1, d1), the structural unit number (a2, b2, c2, d2), and the RDF (a3, b3, c3, d3) of the bulk Co_{10976} material for different t values at $T = 700$ K.

in the distance between Co atoms of the Co₁₀₉₇₆ material from 2.475 Å to 2.525 Å. In addition, the obtained results show that when increasing the annealing time t from $t = 0$ ps to $t = 100$ ps, crystallization occurs quickly. With $t = 10$ ps, the crystallization process happened almost completely (Figure 6(a2), 6(b2), and 6(c2)). The cause of the strong crystallization at $T_g = 700$ K is that there appears a low-energy region, and a high-energy region, leading to when an increase in the annealing time t , making the atoms easy to move to the low-energy region increases crystallization (this point is a singularity and is very attractive for theoretical and experimental researchers to focus on exploiting and researching). On the other hand, bulk Co materials are magnetic materials with Curie temperature (T_c), $T_c = 1400$ K (Shabib and Miller, 2009), and FCC structure. When reducing the size from bulk materials to the nanoscale, the crystallization temperature (T_g) of the material is always lower than the phase transition temperature (T_m) of the material, which proves that there is a structural shift from HCP at low temperatures to FCC at high temperature.

Conclusion

In this paper, we have studied the structure, crystallization, and phase transition of the bulk Co materials under various factors such as T , N , and t using the MDS method combined with the SC embedded potentials and periodic boundary conditions. The findings from CNA showed that the Co material has four kinds of atomic structure including Amor and crystalline FCC, BCC, and HCP. Compared with the crystalline FCC and BCC phases, the HCP and Amor phases were found to be predominant in the bulk Co₁₀₉₇₆ material at $T = 300$ K. Decreasing N from 10976 atoms to 4000 atoms at $T = 300$ K and increasing T from 300 to 1000 K did not change the dominant phases in the bulk Co₁₀₉₇₆ material. However, the fraction of the Amor phase gradually increased with increasing T and became more dominant than the HCP phase at higher T values, indicating that the T factor led to a decrease in the crystallinity of the Co₁₀₉₇₆ material. The results of the analysis indicated that the bulk Co₁₀₉₇₆ material exhibits a strong crystallization at $T_g = 700$ K. An increase in the t value from 0 ps to 10 ps at $T_g = 700$ K caused an abrupt change in the dominant phase of the bulk Co₁₀₉₇₆ material into the FCC structure and the FCC dominant phase remained unchanged even though the t value was increased up to 50 ps. The RDF analysis revealed that the distance between Co atoms in the bulk

Co₁₀₉₇₆ material was $r = 2.475$ Å at $T = 300$ K. The N and T had no effect on the distance between Co atoms (2.475 Å), but increasing t from 0 ps to 50 ps caused an increase in the distance between Co atoms from 2.475 to 2.525 Å. The l increased from 3.8391 nm to 5.3320 nm, while the E decreased from -4.195 eV to -4.218 eV with increasing N . The $g(r)$ of the RDF first increased from 5.498 to 5.595 with increasing N from 4000 atoms to 8788 atoms and then decreased to 4.494 with a further increase in the N to 10976. Increasing T from 300 K to 1000 K led to an increment in the E value from -4.218 eV to -4.087 eV and a slight increase in the l from 5.3320 nm to 5.3323 nm. A significant reduction in the $g(r)$ value from 5.494 to 3.722 was detected with increasing T from 300 K to 1000 K. An increase in the t from 0 ps to 50 ps induced an increase in the $g(r)$ from 4.390 to 4.929, but a decrease in the l and E values from 5.3320 nm to 5.0951 nm and from -4.155 eV to -4.246 eV, respectively. The findings revealed in this work are expected to contribute to future studies on not only bulk Co materials but also Co-based alloys and compounds.

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