Structure, Plastic Deformation of Polyethylene: A Molecular Dynamics Method

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Abstract

This paper studies the influence factors of atoms number (N) at temperature (T) and after annealing time (t) on the structure shape and the plastic deformation of Polyethylene C₂H₄ (PE) by the Molecular Dynamics (MD) method with Dreading pair interaction, cyclic boundary conditions and plastic deformation of Polyethylene (PE) be done by stretching method according to the z-axis. The results of structure, plastic deformation of PE are analyzed through size (l), the total energy of the system (E_{total}), shape and associated energy (E_{bond}), angular binding energy (E_{angle}), energy E_{dihedral}, interactive energy Vander Walls (E_{non-bonding}). When increasing N, t leads to the number of structural units of Face-Centred Cubic (FCC), Body-Centered Cubic (BCC) and Hexagonal Close-Packed (HCP) increasing, but Amorphous (Amor) decreases while the angle between the atoms is a constant corresponding to 109.5°. Besides, the length of the link (r) increases from r = 1.529 Å to r = 1.558 Å while the plastic deformation energy of PE gets an enormous change and the bonding angle at 109.27°. The length of the link r = 1.529 Å and the size (l) of the PE material increase from l = 3.73 nm to l = 6.63 nm while the total energy of system (E_{total}) decreases from E_{total} = −1586 eV to E_{total} = −7891 eV with the transition temperature is T = 103 K. Increasing the number of atoms leads to increasing the length of the link. The total energy E_{total} of the system decreases, but the number of structural units in FCC, HCP, BCC and Amor increase, which leads to the length of the link increases, the E_{total} decreases, and there is a change in the plastic deformation characteristics of PE. In contrast, increasing T leads to the plastic deformation increases, and PE moves from the amorphous state to the liquid state. The obtained results are very significant for future experimental research.

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Keywords

Molecular Dynamics, Atoms Number, Annealing Time, Polyethylene, Plastic Deformation

1. Introduction

Polyethylene C2H4 (PE) is a flexible plastic existing in an amorphous state and widely used in consumer products. In particular, PE plays an important role in material science, which is considered as a bright candidate for new industrial materials. When PE is combined with wood, it creates an environmentally friendly Wood Plastic Composite material (WPC) [1] [2] such as reducing energy consumption in production, lightweight, and sound insulation [3] [4] [5]; reducing pollution and greenhouse effect; enhancing biodegradability [6] [7] [8]. Also, WPC is widely used in industries such as automotive, construction, et al. [6] [9]. The flexible plastic resins are made of Polyethylene (PE) [8], Polypropylene [10], Polyvinyl Chloride (PVC) [11] and polystyrene (PS) [12]. The Wood components include wood pulp, cotton, wheat straw, bagasse, and rice husk [13] [14] [15] [16] [17]. PE plastic is used in practice including both High-Density Polyethylene (HDPE) and low-density WPC [18]. PE, as a binder and wood pulp as an additive; HDPE includes material hydrophilic wood pulp and PE hydrophobic wood pulp [19] [20]. Therefore, PE is considered as an important additive component in industrial applications. PE is divided into many types, mainly based on density, monomer, flexibility [21], and copolymer [22] [23] [24]. In particular, with Low-Density Polyethylene (LDPE) which is the most commonly used and commercially produced at high pressure (P), P = 2400 Bar, temperature (T) from T = 363 K to T = 383 K [25].

To study this material, it is good to use the experimental, theoretical, and simulation methods. As for the experimental method, using pressing methods and multi-layer extrusion method with low cost has high durability, ductility [26] and increasing stress [27] [28] as Jatin et al. [29], Kurz et al. [30], Pouriayevali et al. [31] for that plastic deformation of PE is an isotropic function with pressure putting on (the deformation (ε) in the experiment which is always less than ε < 0.12); Epee et al. [32] suggested that the deformation of the polymer with ε < 800 s⁻¹; Argon et al. [33] suggested that plastic deformation is due to the twisted bonding pairs along the polymer chain; Roberson suggested that the shear stress is caused by changing angles and movements of molecules [2]; Eyring et al. [1] suggested that the plastic deformation is caused by the shear stress, structural changing, and binding energy [34]-[40]. With the simulation method, Deng et al. [41] suggested that plastic deformation is caused by the local structure. Besides, Maeda, Takeuchi [42], Srolovitz et al. [43] successfully used the molecular statistical method (MS) to study the deformation of three-dimensional metal glasses; Theodorou and Suter [44] [45] successfully simulated the material in the
glass polymer material and studied the deformation. After that, MS. Mott et al. [46], Hutnick et al. [47] used this method to study the plastic deformation of Polypropylene and Polycarbonate. While Mott et al. suggested that the plastic deformation is the result of changing the displacement in atoms or molecular branches, Hutnick et al. suggested that the movement of atoms does not depend on chemical reactions. Similarly, Brown, Clarke [48], Mckechnie, and Clarke [49] successfully investigated the effect of temperature on the bond in glass polyethylene and mechanics of materials. It is said that increasing the plastic deformation and the length of the initial link is necessary. Although there have been many studies on the plastic deformation of PE in the static state or the dynamic state [48] [50]-[57] such as Balsas et al. [58], Haefele et al. [59], using simulation method with Low-Density Polyethylene (LDPE) at high pressure; Astesuain et al. [60] use Graphical Optimization Tool (gOPT) of general PROcess Modelling System (gPROMS) simulator program to optimize LDPE; Bezzo et al. [61] successfully used Fluent, gPROMS for liquids by calculating molecular dynamics. Recently, Clarke [48] has successfully performed uniaxial deformation of amorphous Polymers with different deformation levels at low temperatures, which is obtained in qualitative form. Capaldi et al. [42] suggested that the compressive deformation of Polymer is the same as the change of angle, the angle shift along the chain; Li et al. [62] successfully performed Single-axis plastic deformation of Polyethylene (PE) amorphous by Monte Carlo method (MC) with FCC structure and bonding length (r), r = 1.53 Å. The result shows that there is a dependence on temperature (T), and the heating rate and Uniaxial Tension of the material [63]; Ospina et al. [64] using the MC simulation result of the initial plastic deformation stage of polyethylene gives the consistent result with the experimental result, and it does not reduce the plastic deformation [63] [64] [65]; factors that alter the structure of PE [66] [67] as concentrations of impurities playing an important role in compounds [67] [68].

The result shows that the phase transition of Polyethylene depends on the temperature [69] [70] [71] as the liquefaction process which is just below the room temperature T = 300 K, limited by the movement of atoms at transition layer between the crystal area and the amorphous region. This shift occurs very weakly in HDPE with temperature from T = 123 K to T = 173 K and it is linked with the movement of CH2 groups attached to C2H4 [72], the change in the molecular shape of the polymer depends on the relationship between temperature and pressure [73]; the phase transition depends on the heating rate, the total energy of the system during the deformation process [74]. The results show that the glass transition temperature (Tg) depends on the movement of atoms with valuable in approx from Tg = 133 K to Tm = 408 K [75], and this is performed on experimental measurements [76].

Besides, many authors have successfully studied the plastic deformation of PE by the z-axis stretching method. The results show the influence of the chain length, the number of chains, the strain rate, and the temperature. This depends
on the stress-strain \[77\] \[78\] \[79\] \[80\] which is ended at the source of plastic deformation. Polyethylene is a problem that has not been explained in detail \[81\]. To solve the problem, we focus on studying the effect of atomic number, temperature, annealing time on the structure, and the plastic deformation of PE.

2. Method of Calculation

Initially, randomly sow atomic number (N), N = 2000 atoms, 4000 atoms, 6000 atoms, 8000 atoms, 10,000 atoms Polyethylene (C\(_2\)H\(_4\) or PE) into the cube by the Molecular Dynamics (MD) method \[42\] \[44\] \[82\] \[83\] Dreading pair interaction (1), cyclic boundary conditions \[42\] \[84\] \[85\] \[86\] \[87\] \[88\] through the total energy of the system (\(E_{\text{tot}}\)): \(E_{\text{tot}} = E_{\text{bond}} + E_{\text{angle}} + E_{\text{dihedral}} + E_{\text{non-bonding}}\) (1).

\[
\begin{align*}
E_{\text{bond}}(r) &= \frac{1}{2} K_b (r - r_0)^2, \\
E_{\text{dihedral}}(\phi) &= \sum_{i=1}^{3} C_i (\cos \phi)^i, \\
E_{\text{angle}}(\theta) &= \frac{1}{2} K_\theta (\theta - \theta_0)^2, \\
E_{\text{non-bonding}}(r) &= 4\varepsilon \left[ \frac{\sigma}{r} \right]^{-12} - \left( \frac{\sigma}{r} \right)^6, \\
\end{align*}
\]

With: \(E_{\text{bond}}\) is the bond energy, \(E_{\text{angle}}\) is the bond angle energy, \(E_{\text{dihedral}}\) is dihedral energy, \(E_{\text{non-bonding}}\) is van der Waals energy in the Lennard-Jones interaction, \(E_{\text{tot}}\) is the total energy of the system, \(K_b = 350\) kcal/mol, \(K_\theta = 60\) kcal/mol-rad\(^2\) is the stiffness coefficient, the bond angle coefficient, \(r_0 = 1.53\) Å is the bond length, \(\theta_0 = 1.911\) rad (109.5\(^\circ\)) is the link angle, \(C_0 = 1.736, C_1 = -4.490, C_2 = 0.776, C_3 = 6.99\) (kcal/mol) are the coefficients, \(\sigma = 4.01\) Å is the energy at 0 eV, \(\varepsilon = 0.112\) kcal/mol is the dielectric constant, \(r_c = 10\) Å is the radius interrupt.

After obtaining, all PE samples for running \(10^6\) steps molecular dynamics (MD) simulation recovery statistics at temperature (T), T = 500 K; \(10^6\) steps NPT (atomic number, pressure, and constant temperature) MD simulation at T = 500 K. After obtaining PE samples at T = 500 K, the samples were lowered from T = 500 K to T = 100 K. Particularly with N = 10000 atoms at T = 500 K, the temperature is lowered to T = 120 K, 100 K, 80 K, 60 K, 40 K. When increasing t, from t = 0 ps to t = 50 ps, 100 ps, 150 ps, 200 ps at T = 100 K. The temperature was set intentionally, which is to study PE material in the crystalline state with temperature the below glass transition temperature (\(T_g\)), \(T_g = 250\) K \[89\], size (l) of PE material lying in the range from l = 3.73 nm to l = 6.36 nm, the time for each simulation step is \(\Delta t = 0.1\) fs. The program code used to run the PE sample that is the open-source program code LAMMPS \[90\] \[91\] with the heating rate, which is obeyed following the Nosé-Hoover rule \[92\] \[93\] \[94\], van der Waal link \[95\] \[96\] \[97\] \[98\] \[99\]. To study the plastic deformation of PE under the effect of the force in the direction of the z-axis with the constant heating rate at
pressure (P), P = 0 GPa by defining quantities in the direction of the z-axis single tension from the NPT equations of the PE shift process [91]. The stress components are calculated from energy contributions related to the length of the link, bonding angle, bipolar angle, and non-bonding interaction, which are combined with the Common Neighbor Analysis (CNA) method [100] [101] [102] by Ovito software.

3. Results and Discussion

3.1. Effect of Atomic Number

3.1.1. The Phase Transition of Polyethylene

The result of the phase transition Polyethylene C2H4 (PE) is shown in Figure 1.

The results show that after running the Recovery Statistics (RS), RS = 10^6 steps of moving the Molecular Dynamics (MD) simulation at the temperature (T), T = 500 K, then the pressure of the system (P) decreases, with PE 2000 atoms lead to P decreases from P = 4464 Bar to P = −144 Bar. At a steady state, when N increasing from N = 2000 atoms to N = 10,000 atoms leads to P increases from P = −144 Bar to P = 292 Bar (Figure 1(a)). Similarly, with the process of running 10^6 steps NPT (with atoms number, pressures, and temperatures is constant) leads to P changes on the range from P = −558 Bar to P = 706 Bar, with PE 10,000 atoms the P has the smallest change (Figure 1(b)). The process of temperature reduction from T = 500 K to T = 100 K shows that the P of PE 10,000 atoms has not changed significantly (Figure 1(c)). The energy values of PE at T = 100 K has value corresponding change. The total energy pair (Epair) decreases from E pair = −3014 eV to E pair = −15,161 eV (Figure 1(d)), the total electron bond energy (E bond) increases from E bond = 199 eV to E bond = 994 eV (Figure 1(e)), the total angle bond energy (E angle) increases from E angle = 223 eV to E angle = 1158 eV (Figure 1(f)), the total dihedral energy (E dihed) increases from E dihed = 719 eV to E dihed = 3544 eV (Figure 1(g)) and E int decreases from E int = −1873 eV to E int = −9465 eV (Figure 1(h)). Basing on the given result, after 10^6 steps moving of recovering statistics, then PE reached equilibrium; 10^6 steps moving NPT at temperature (T), T = 500 K lead to PE existed in a liquid state. When the temperature decreases from T = 500 K to T = 100 K leading to PE changes from the liquid state to a new crystalline state, running stably 10^6 steps NPT at T = 100 K obtained PE in the new crystalline state corresponds to the shape of PE (Figure 1(i)). As a result, when increasing atoms number (N) leads to the size (l) increases, but E int decreases.

3.1.2. Plastic Deformation Process of Polyethylene

The results of the plastic deformation process of Polyethylene (PE) at temperature (T), T = 100 K are shown in Figure 2. Table 1.

The obtained result shows that after the process of the temperature reduction from T = 500 K down to T = 100 K with 10^6 step MD simulation, the
(a) Statistics recovered at $T = 500K$

(b) The NPT running process at $T = 500K$

(c) The NPT running process from $T = 500K$ to $T = 100K$
Figure 1. The phase transition of polyethylene after $10^6$ steps recovery statistics at the temperature at 500 K (a), $10^6$ steps of NPT at the temperature 500 K (b), $10^6$ steps to the lower temperature from 500 K down to 100 K (c), the energy values (d)-(h), and the shape of the PE (i) with atomic number, the number of different displacement steps.
Table 1. The process of transforming the number of structural units after the number of different MD shift steps.

| Shift step number (step) | 0    | $2 \times 10^5$ | $4 \times 10^5$ | $6 \times 10^5$ | $8 \times 10^5$ | $10 \times 10^5$ |
|-------------------------|------|-----------------|-----------------|-----------------|----------------|-----------------|
| FCC                     | 4    | 15              | 13              | 13              | 5              | 12              |
| HCP                     | 56   | 55              | 54              | 58              | 47             | 60              |
| BCC                     | 2    | 4               | 1               | 7               | 9              | 6               |
| Amor                    | 1938 | 1926            | 1932            | 1922            | 1939           | 1922            |

Figure 2. The structural unit number shapes of Polyethylene as FCC structure (a), HCP structure (b), BCC structure (c), Amor structure (d).

Polyethylene has a cube shape (Figure 2(a)-(d)) with the number of structural units is 4 FCC, 56 HCP, 2 BCC, 1938 Amor (Table 1). When increasing moving the number of steps from 0 to $10^6$ of the MD simulation leading to PE changing from the cube shape to the rectangular box shape (Figures 3(a)-(f)), and the of number structural units of FCC, HCP, BCC, Amor changes corresponding (Table 1). When increasing moving the number of steps of the MD leading to the number of structural units unchanged. Particularly, the shape has a huge change raising the question after compressing the PE time of the z-axis, the PE’s shape has changed leading to changing the plastic deformation characteristics of the PE. To confirm that studying the plastic deformation characteristics with different moving the number of steps, the results shown in Figure 4, Table 2.

The results show that the number of structural units with the atomic number (N), N = 2000 atoms is 12 FCC, 60 HCP, 6 BCC, and the characteristics of the plastic deformation include the bonding energy between atoms, $E_{\text{bond}}$ which is
shown by the red color line, $E_{\text{angle}}$ is angular bond energy shown by the blue color line, the $E_{\text{dihed}}$ is energy dihedral shown by the blue color line, $E_{\text{total}}$ shown by the purple color line, (Figure 4(a), Table 2). When increasing $N$ from $N = 2000$ atoms to $N = 4000$ atoms, $6000$ atoms, $8000$ atoms and $10,000$ atoms leads to the total energy pair ($E_{\text{pair}}$) decreases from $E_{\text{pair}} = -2756$ eV to $E_{\text{pair}} = -13,866$ eV (Figure 4(b)), energy bond ($E_{\text{bond}}$) increases from $E_{\text{bond}} = 163$ eV to $E_{\text{bond}} = 812$ eV (Figure 4(c)), angular bond energy $E_{\text{angle}}$ increases from $E_{\text{angle}} = 256$ eV to $E_{\text{angle}} = 1264$ eV (Figure 4(d)), the energy dihedral increases from $E_{\text{dihed}} = 751$ eV to $E_{\text{dihed}} = 3899$ eV (Figure 4(e)), and $E_{\text{total}}$ decreases from $E_{\text{total}} = -1586$ eV to $E_{\text{total}} = -7891$ eV (Figure 4(f)), free volume change the number of atoms (Figure 4(g)), the plastic deformation process of PE (Figure 4(h)), the PE shape (Figure 4(i)) after deformation at $T = 100$ K, and the number of structural units of FCC.

Figure 3. The PE structure shape of PE with the different number of MD shift steps: In the initial state (a), after $2 \times 10^5$ steps MD (b), $4 \times 10^5$ steps MD (c), $6 \times 10^5$ steps MD (d), $8 \times 10^5$ steps MD (e), $10^6$ steps MD (f).
Figure 4. The plastic deformation process as the energy $E$ (a), the total energy pair $E_{\text{pair}}$ (b), the total electron bond energy $E_{\text{bond}}$ (c), the total energy angle $E_{\text{angle}}$ (d), the total dihedral energy $E_{\text{dihed}}$ (e), the total energy $E_{\text{tot}}$ (f), free volume change the number of atoms (g), stress (h), the PE shape (i) after deformation at $T = 100$ K with atomic number and different moving the number of steps.
Table 2. The process changes the number of structural units with the different number of MD moving steps.

| Atoms number (atoms) | $2 \times 10^3$ | $4 \times 10^3$ | $6 \times 10^3$ | $8 \times 10^3$ | $10 \times 10^3$ |
|---------------------|---------------|---------------|---------------|---------------|----------------|
| FCC                 | 12            | 19            | 18            | 37            | 43             |
| HCP                 | 60            | 112           | 162           | 219           | 265            |
| BCC                 | 6             | 11            | 16            | 24            | 28             |
| Amor                | 1922          | 3858          | 5804          | 7720          | 9664           |

increases from 12 FCC to 43 FCC, HCP increases from 60 HCP to 265 HCP, BCC increases from 6 BCC to 28 BCC, finishes increasing the number of structural units of FCC, BCC, which is not significant, only HCP increases rapidly (Table 2). Consequently, when increasing the number of atoms number and the number of shift steps of MD leads to a rapid increase in shape and the number of structural units of FCC, and the plastic deformation energy of PE also varies greatly. The result of the PE modeling process is consistent with the result [77] [78] [79] [80] and coincide with the previous authors who used the Monte Carlo (MC) method [62] [63] [64] with a PE transition temperature is 103 K [75] [76]. Additionally, when increasing the number of the atoms leads to the angle among the atoms is a constant corresponding to 109.5˚, the length of the link $r$ increases from $r = 1.529 \text{ Å}$ to $r = 1.558 \text{ Å}$, the obtained result is correctly consistent with the result of bonding angle of 109.27˚, and the link length $r = 1.529 \text{ Å}$ [62] [77], the size of the PE material increase from $l = 3.73 \text{ nm}$ to $l = 6.63 \text{ nm}$, the total energy $E_{total}$ decreases from $E_{total} = -1586 \text{ eV}$ to $E_{total} = -7891 \text{ eV}$. This means that when increasing the number the atoms leads to increase the link length, $E_{total}$ decreases and changes the plastic deformation characteristics of PE.

3.1.3. The Effect of Annealing Time

Similarly, the effect of annealing time of PE material with $N = 10,000$ atoms at $T = 100 \text{ K}$, the results are shown in Figures 5-7.

The results show that with $t = 50 \text{ ps}$, the shape (Figure 6(a)), the number of structural units is 54 FCC, 280 HCP, 35 BCC (Figure 7(a)), the plastic deformation characteristics of PE (Figure 5(a)). When increasing the annealing time from $t = 50 \text{ ps}$ to $t = 100 \text{ ps}$, 150 ps, 200 ps lead to FCC, HCP, BCC decreases and Amor increases accordingly: with $t = 50 \text{ ps}$, there are 54 FCC, 280 HCP, 35 BCC, 9581 Amor; $t = 100 \text{ ps}$ has 43 FCC, 265 HCP, 28 BCC, 9564 Amor; $t = 150 \text{ ps}$ has 51 FCC, 268 HCP, 23 BCC, 9508 Amor; $t = 200 \text{ ps}$ has 42 FCC, 278 HCP, 19 BCC, 9461 Amor (Figures 7(b)-(d)), shape (Figures 6(b)-(d)), and the plastic deformation characteristics (Figures 5(b)-(d)). Also, $E_{tot}$ increased (Figure 5(e)), free volume change the number of atoms (Figure 5(f)). This showed that after the annealing time, then FCC, HCP, BCC decreased, Amor, increased after finishing which did not make a significant change in the structure.
Figure 5. The plastic deformation process of PE at temperature $T = 100$ K with $t = 50$ ps (a), 100 ps (b), 150 ps (c), 200 ps (d), total energy of system (e), free volume change number atoms (f).
Figure 6. The shape of PE material after different annealing time as t = 50 ps (a), 100 ps (b), 150 ps (c), 200 ps (d).

Figure 7. The number of structural units of FCC, HCP, BCC, Amor after the different annealing time: t = 50 ps (a), 100 ps (b), 150 ps (c), 200 ps (d).
3.2. Influence of Temperature

The result of the effect of $T$ on the plastic deformation of PE 10,000 atoms, is shown in Figure 8, Figure 9.

The result shows that at the temperature ($T$), $T = 40$ K in which the number of structural units 47 FCC, 307 HCP, 18 BCC (Figure 9(a)) corresponding to the plastic deformation characteristics of PE (Figure 8). When increasing the temperature from $T = 40$ K to $T = 60$ K, 80 K, 100 K, 120 K, then the number of structural units of FCC, HCP, BCC decreases, and Amor increases accordingly with $T = 40$ K, has 47 FCC, 307 HCP, 18 BCC, 9628 Amor; $T = 60$ K, which has 53 FCC, 267 HCP, 33 BCC, 9647 Amor; $T = 80$ K has 56 FCC, 295 HCP, 30 BCC, 9619 Amor; $T = 100$ K has 43 FCC, 265 HCP, 28 BCC, 9664 Amor; $T = 120$ K has 39 FCC, 303 HCP, 18 BCC, 9640 Amor (Figures 9(b)-(e)), the shape and plastic deformation characteristics of PE (Figures 8(a)-(f)). In addition, the $E_{\text{tot}}$ increases (Figure 5(e)), which shows that when increasing temperature leads to the plastic deformation increases, and the structure is unchangeable. The obtained result shows that when increasing N leads to l increasing, $E_{\text{tot}}$ decreases, and the number of structural units increases. When increasing the time of elongation and temperature, l increases, $E_{\text{tot}}$ increases, and the number of structural units of the system decrease. This result is the basis for future empirical research.

4. Conclusion

After studying the effect of the atomic number (N), temperature (T), and annealing time (t) on the structure and the plastic deformation of the polyethylene, the result shows that when increasing N, from N = 2000 atoms to N = 10,000 atoms, the moving number of MD leads to the shape and the number of structural units FCC increase. The angle among the atoms is a constant corresponding to 109.5°. The length of the link $r$ increases from $r = 1.529$ Å to $r = 1.558$ Å. The plastic deformation energy of PE has an enormous change as the bonding angle of 109.27°. The length of the link $r = 1.529$ Å, and the size of the PE material increases from $l = 3.73$ nm to $l = 6.63$ nm. The total energy ($E_{\text{total}}$) decreases from $E_{\text{total}} = -1586$ eV to $E_{\text{total}} = -7891$ eV, and it coincides with the previous authors who used the Monte Carlo (MC) method with a PE transition temperature is 103 K. When N increasing leads to the length of the link increases, $E_{\text{total}}$ decreases, FCC, HCP, BCC, Amor increases, and changes the plastic deformation characteristics of PE with an increase in T and the t. The obtained results are very significant for future experimental research as studying the effect of the number of structural units on the structure, plastic deformation, conductivity, magnetism of PE materials.

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Figure 8. The plastic deformation process of PE 10,000 atoms with the total energy pair $E_{\text{pair}}$ (a), the total electron bond energy $E_{\text{bond}}$ (b), the total energy angle $E_{\text{angle}}$ (c), the total dihedral energy $E_{\text{dihed}}$ (d), the total energy $E_{\text{tot}}$ (e), the free volume change the number of atoms (f) at the temperature $T = 100$ K with different temperatures.
Figure 9. The number of structural units of FCC, HCP, BCC, Amor after different temperature as $T = 40$ K (a), 60 K (b), 80 K (c), 100 K (d), 120 K (e).
Conflicts of Interest
The authors declare no conflicts of interest regarding the publication of this paper.

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