1. Introduction

Soft magnetic materials are essential for increasing the efficiency of electrical and electronic equipment, such as transformers, memories, magnetic shields, and sensors [1,2]. Thereinto, Fe-based amorphous alloys have drawn much attention as a result of their outstanding soft magnetic performances, such as excellent saturation magnetization ($B_s$), high effective permeability, extremely low coercivity ($H_c$), and low core loss [3,4]. Fe-Si-B amorphous alloys are typically representative, with broad practical applications in transformers and inductors [5]. The newly developed Fe-P-C-B amorphous alloys have drawn more attention because of their superior comprehensive properties, including excellent soft magnetic properties, large electric resistivity, good processibility, and low cost [6–9]. For the green development of the next-generation devices, soft magnetic amorphous materials with lower $H_c$ will play a significant role.

The chemical composition design has been widely applied in Fe-based amorphous alloys to improve the performance of glass-forming ability (GFA) and various properties. For this reason, multiple elements have been adopted to enhance $B_s$ and decrease $H_c$ values [10–12]. Typically, the addition of high-melting-point metals with large atoms, such as Mo, Nb, and W, can significantly affect the microstructure of the melt-spun alloys, which is helpful for obtaining good soft magnetic properties [13–15]. Tungsten, which shows the highest melting point among all metals, can strengthen thermal stability, extend the supercooled liquid region, and enhance the GFA of Fe-based amorphous alloys [16–19]. Moreover, W alloying can enhance the soft magnetic performances of Fe-based metallic glass and amorphous alloys. For example, the addition of the W element in Fe-Y-B amorphous alloys leads to low $H_c$ values below 2 A/m [20]. With the addition of W, Fe$_{86}$Co$_{10}$Zr$_3$W$_4$B$_{20}$

Abstract: In this work, the thermal behavior, soft magnetic properties, and structure of Fe$_{66-x}$P$_{11}$C$_2$B$_7$W$_x$ ($x = 0, 0.1, 0.2, 0.4, 0.6, 0.8, 1, 2,$ and $4$) amorphous alloys were researched by several experimental methods and ab initio molecular dynamics. The addition of W improved the thermal stability of the alloy system when the first onset crystallization temperature ($T_{x1}$) increased from 655 K to 711 K, significantly reduced the coercivity $H_c$ and decreased the saturation magnetization $B_s$. The Fe$_{66.6}$P$_{11}$C$_2$B$_7$W$_{0.4}$ alloy showed optimal soft magnetic performance, with low $H_c$ of 1.4 A/m and relatively good $B_s$ of 1.52 T. The simulation results suggested that W atoms increased the distance of the neighboring Fe-Fe pair, reduced the coordination number, narrowed the gap between the spin-up and spin-down electrons of each atom, and decreased the average magnetic moment of the Fe atoms. This work demonstrates a micro-alloying strategy to greatly reduce $H_c$ while maintaining high $B_s$.

Keywords: amorphous alloys; Tungsten addition; soft magnetic property; ab initio molecular dynamics simulation
showed a very low $H_c$ of 1.4 A/m [21]. However, the influences of the W element on the Fe-P-based amorphous alloys, especially in newly developed Fe-P-C-B alloy systems, is unclear and has not been systematically studied.

In this work, the authors have attempted to investigate the soft magnetic performances and structure of the newly developed Fe-P-C-B amorphous alloys concerning W addition. The results suggest that the $H_c$ of the Fe-P-C-B amorphous alloy decrease obviously with the minor addition of W. Moreover, the Vienna ab initio simulation package (VASP) was used to investigate the evolution of atomic and electronic structures caused by the composition adjustment.

2. Experimental

Alloys with nominal atomic compositions of $Fe_{86-x}P_{11}C_2B_1W_x$ ($x = 0, 0.1, 0.2, 0.4, 0.6, 0.8, 1, 2, \text{ and } 4$) were prepared by the induction-melting method in an Ar atmosphere. The specific crude materials were as follows: Fe (99.9 wt.%), C (99.9 wt.%), W (99.95 wt.%), Fe-B prealloy (B: 20.0 wt.%), and Fe-P prealloy (P: 22.1 wt.%). The ingots were remelted many times to guarantee the uniformity of composition. Amorphous ribbons with a width of approximately 1.5 mm and a thickness of approximately 20 $\mu$m were produced by single roller melt-spinning method in an Ar atmosphere. The corresponding samples were annealed at different temperatures in evacuated and sealed quartz tubes in a muffle furnace (TKD-1400, Beijing, China) to obtain inner-stress relief samples. The annealing processes of ribbons were performed in the presence of Earth’s field, and no extra external field was applied during the annealing process.

D/max-2500 PC Rigaku X-ray diffractometer (XRD, D/MAX 2500pc, Tokyo, Japan) with Cu Kα radiation was used to investigate the amorphous nature of the melt-spun ribbons and the microstructure of annealed samples. The scanning range was from 30° to 90°, and the scanning rate was 2 degrees per minute. Thermodynamic parameters of melt-spun ribbons were identified by using a differential scanning calorimetry (DSC, PerkinElmer DSC 8000, Waltham, MA, USA) under an Ar gas flow with a heating rate of 0.33 K/s. The Archimedes principle has been used to measure the density of alloys at normal atmospheric temperatures. The hysteresis loops identified the $B_s$ of the melt-spun and annealed ribbons, which were measured by Lakeshore 7407 vibrating sample magnetometer (VSM, Lake Shore 7407, Westerville, OH, USA) under an applied field of 800 kA/m. A DC B-H loop tracer (MATS-2010SA, Loudi, China) was used to measure the $H_c$ of the ribbons under a field of 800 A/m. Moreover, the bright field and the high-resolution transmission electron microscope (HRTEM) microstructure of the samples were characterized via TEM (JEM-2100 F, Tokyo, Japan). The TEM samples were prepared by ion thinning. The magnetic domain structure was observed by the magneto-optical Kerr effect microscope.

By means of density functional theory, the structure of $Fe_{86-x}P_{11}C_2B_1$, $Fe_{85.5}P_{11}C_2B_1W_{0.5}$, and $Fe_{85}P_{11}C_2B_1W_1$ amorphous alloys was simulated by using the Vienna Ab initio simulation package (VASP) [22]. The projected augmented wave method was used to describe electron-ion interactions [23]. Exchange-correlation potentials were calculated by Perdew–Burke–Ernzerh mode with a generalized gradient approximation [24]. The primitive volume of the cubic periodic supercell containing 200 atoms was decided by the experimental density of $Fe_{86}P_{11}C_2B_1$, $Fe_{85.5}P_{11}C_2B_1W_{0.5}$, and $Fe_{85}P_{11}C_2B_1W_1$ amorphous alloys at a normal atmospheric temperature. The systems were melted and well equilibrated for 6000 steps (2 fs for each step) at 2000 K and subsequently quenched to 300 K at a cooling rate of $5 \times 10^{14}$ K/s. In the end, the systems were equilibrated for 5000 steps at 300 K, and at least 1000 configurations were collected to analyze the structure.

3. Results and Discussion

3.1. Amorphous Nature and Thermal Behavior

In order to identify the optimal content of the W element in the Fe-P based amorphous alloys, $Fe_{86-x}P_{11}C_2B_1W_x$ ($x = 0, 0.1, 0.2, 0.4, 0.6, 0.8, 1, 2, \text{ and } 4$) (also denoted as $W_x$
hereafter) ribbon samples were prepared. Figure 1a exhibits XRD patterns of all melt-spun ribbons with different proportions of W elements. All patterns show broad humps without undetectable crystalline features at the 2θ of about 45°, which indicates the amorphous nature of these samples.

![XRD patterns and DSC curves](image)

**Figure 1.** (a) XRD patterns and (b) DSC curves of the melt-spun Fe$_{86-x}$P$_{11}$C$_2$B$_1$W$_x$ ribbons.

As shown in Figure 1b, the crystallization of the melt-spun Fe$_{86-x}$P$_{11}$C$_2$B$_1$W$_x$ (x = 0, 0.1, 0.2, 0.4, 0.6, 0.8, 1, 2, and 4) amorphous alloys was investigated by DSC with a heating rate of 0.33 K/s. Each DSC curve exhibits two exothermic peaks with similar heat release, indicating a two-step crystallization process for these samples. It was reported that the first exothermic peak relates to the precipitation of the soft magnetic phase (α-Fe), while the second peak relates to the hard magnetic phase [25]. No distinct glass transition phenomenon can be observed for all the samples. The relevant thermal parameters, including the first crystallization onset temperature ($T_{x1}$), the second crystallization onset temperature ($T_{x2}$), and the temperature interval $\Delta T$ ($\Delta T = T_{x2} - T_{x1}$), are listed in Table 1. Moreover, it can be seen that $T_{x1}$ (from 655K to 711 K) and $T_{x2}$ (from 736 K to 773 K) rise with the addition of the W element. This shows that the content of W significantly affects the thermostability of the amorphous phase. Considering the $\Delta H_{mix}$ (enthalpy of mixing) of W-P, W-C, and W-B are $-46.5$ kJ/mol, $-60$ kJ/mol, and $-31$ kJ/mol, respectively [26], it is not surpris-
ing because the W atom can strengthen the cohesive energy through the formation of W-metalloid bonds within Fe-based amorphous alloys, which reduce the diffusion ability of metalloid elements in the amorphous structure and impede the precipitation of α-Fe from the amorphous phase [27].

Table 1. Thermal parameters of Fe_{86−x}P_{11}C_{2}B_{1}W_{x} amorphous alloys.

| Alloys          | Thermal Parameters |         |         |         |
|-----------------|--------------------|---------|---------|---------|
|                 | T_{x1} (K)         | T_{x2} (K) | ΔT (K)  |
| Fe_{86}P_{11}C_{2}B_{1} | 665                | 736     | 81      |
| Fe_{85.9}P_{11}C_{2}B_{1}W_{0.1} | 661                | 746     | 84      |
| Fe_{85.8}P_{11}C_{2}B_{1}W_{0.2} | 660                | 749     | 89      |
| Fe_{85.6}P_{11}C_{2}B_{1}W_{0.4} | 680                | 758     | 78      |
| Fe_{85.4}P_{11}C_{2}B_{1}W_{0.6} | 682                | 760     | 78      |
| Fe_{85.2}P_{11}C_{2}B_{1}W_{0.8} | 687                | 763     | 76      |
| Fe_{85}P_{11}C_{2}B_{1}W_{1}   | 688                | 766     | 78      |
| Fe_{84}P_{11}C_{2}B_{1}W_{2}   | 692                | 768     | 76      |
| Fe_{82}P_{11}C_{2}B_{1}W_{4}   | 711                | 773     | 62      |

3.2. Magnetic Properties and Microstructure Analysis

For magnetic Fe-based amorphous alloys, the soft magnetic performances can be enhanced after annealing at the proper temperature [28,29]. All samples were annealed at different annealing temperatures (T_{a}) for 10 min. After the annealing process, the magnetic performance and corresponding microstructure of Fe_{86−x}P_{11}C_{2}B_{1}W_{x} alloys were analyzed. All H_{c} curves exhibit V-shaped features, as shown in Figure 2a, which shows low H_{c} for T_{a} ≤ T_{x1} and two H_{c} maxima at low and high temperature ends. The high H_{c} of the melt-spun ribbons is considered to originate from the internal stress caused by rapid solidification during the melt-spinning process, which can be reduced by a proper annealing process [30]. When T_{a} is higher than T_{x1}, H_{c} increases rapidly when T_{a} is higher than T_{x1}, as a result of the rapid growth of α-Fe grains and the precipitation of Fe_{5}(P, C, B) compounds [31]. The appropriate addition of the W element can reduce the H_{c} values of Fe_{86−x}P_{11}C_{2}B_{1}W_{x} alloys. According to previous research, structural defects and surface irregularities have a great influence on H_{c} [32–34]. The addition of W may reduce the structural defects and surface irregularities of FePCB amorphous alloys, which lead to the reduction in H_{c} values. The lowest H_{c} value and corresponding T_{a} and B_{s} values for each alloy are listed in Table 2. Compared to the original Fe_{86}P_{11}C_{2}B_{1} alloy, W_{x} (≤2 at.%) alloys show lower H_{c} values after a proper annealing process. Specifically, the W_{0.4}, W_{0.6}, and W_{0.8} alloys exhibit relatively low H_{c} of 1.4 A/m, 1.9 A/m, and 1.6 A/m, respectively, when T_{a} is around T_{x}. In addition, the B_{s} of all alloys was also investigated at different annealing temperatures, as shown in Figure 2b. The B_{s} values monotonically decrease with the increase in W addition at most temperatures. These characteristics can be explained by the reduction in Fe content and the distance increase between Fe-Fe atoms caused by W addition [35].

Considering the relationships between magnetic domain structure and magnetic property, the MOKE microscopy characterization of different Fe_{86−x}P_{11}C_{2}B_{1}W_{x} ribbons was carried out. Table 2 lists the specific composition and related annealing temperature. The annealing time is 10 min. As can be seen from Figure 3a–i, the wide straight strip domains with smooth edges can be observed, which indicates a homogeneous magnetic structure, a low pinning effect, and small anisotropy of the annealed ribbons. Some defects in domains can be attributed to the edge effect, which is mainly induced by the surface quality and change of inner-stress direction [36]. In contrast, mazing fingerprint-like domains can be seen in Figure 3j,k. The formation of maze domains is mainly due to the
non-uniformity internal stress induced by rapid solidification during the preparation of amorphous alloys [37]. The near-field image also shows the sensitive direction representing the vibration direction of incident polarized light and the strip axis. Accordingly, the results provide solid evidence for the low $H_c$ of all annealed ribbons, especially for $W_{0.4}$, $W_{0.6}$, and $W_{0.8}$ ribbons. The lower domain wall energy $\gamma_B$ causes the widening of the domain, which is correlated to the weak pinning effects induced by the anisotropy fluctuations of the materials and internal stress [38].

Figure 2. Annealing temperatures dependence of (a) $H_c$ and (b) $B_s$ for $Fe_{86-x}P_{11}C_2B_1W_x$ alloy ribbons.

Table 2. The $H_c$ and $B_s$ values of $Fe_{86-x}P_{11}C_2B_1W_x$ alloys annealed at optimal temperature for 10 min.

| Alloys          | $T_a$ (K) | $H_c$ (A/m) | $B_s$ (T) |
|-----------------|-----------|-------------|-----------|
| $Fe_{86}P_{11}C_2B_1$ | 643       | 3.6         | 1.62      |
| $Fe_{85.5}P_{11}C_2B_1W_{0.1}$ | 643       | 3.5         | 1.61      |
| $Fe_{85.5}P_{11}C_2B_1W_{0.2}$ | 663       | 3.7         | 1.55      |
| $Fe_{85.4}P_{11}C_2B_1W_{0.4}$ | 683       | 1.4         | 1.52      |
| $Fe_{85.4}P_{11}C_2B_1W_{0.6}$ | 683       | 1.9         | 1.48      |
| $Fe_{85.2}P_{11}C_2B_1W_{0.8}$ | 683       | 1.6         | 1.45      |
| $Fe_{85}P_{11}C_2B_1W_1$ | 683       | 2.0         | 1.41      |
| $Fe_{84}P_{11}C_2B_1W_2$ | 671       | 2.3         | 1.38      |
| $Fe_{82}P_{11}C_2B_1W_4$ | 691       | 6.3         | 1.17      |

Figure 4 presents the XRD images of annealed samples listed in Table 2. Crystalline peaks can be clearly seen from the $W_{0.2}$ and $W_{0.4}$ ribbons, and minor peaks can be observed from $W_{0.6}$ and $W_{0.8}$ XRD patterns. According to G. Herzer's effective magnetic random anisotropy model, the precipitation of fine and regular nanocrystalline can reduce the $H_c$ of amorphous alloys [39]. This helps explain why $W_x$ ($x = 0.2, 0.4, 0.6, 0.8$, and $1$) ribbons show the lowest $H_c$ when $T_a$ is around $T_x$. Furthermore, TEM is adopted to investigate the phase structure of the annealed $Fe_{85.5}P_{11}C_2B_1W_{0.4}$ and $Fe_{85.2}P_{11}C_2B_1W_{0.8}$ alloy ribbons (683 K for 10 min). As exhibited in Figure 5a,c, the bright field TEM image shows the primary amorphous phase for the annealed ribbons, as also confirmed by the inset selected area electron diffraction (SAED) pattern. As shown in Figure 5b,d, crystallographic planes indicating the presence of nanocrystals can be seen in HRTEM images, which is consistent with the XRD results.
Figure 3. Magnetic domains of (a,b) W0 and W0.1 ribbon annealed at 643 K; (c) W0.2 ribbon annealed at 663 K; (d–g) W0.4, W0.6, W0.8 and W1 ribbon annealed at 683 K; (h) W2 ribbon annealed at 671 K; (i) W4 ribbon annealed at 691 K; (j,k) as-spun W0.4 and W0.8 ribbon. The annealing time is 10 min. The magnitude of the field is 20 Oe, and the orientation of this field is perpendicular to the direction of the long axis of the ribbon.

Figure 4. XRD patterns of the annealed Fe86−xP11C2B1Wx ribbons.

Figure 5. (a) Bright-field TEM and (b) HRTEM pictures of Fe85.6P11C2B1W0.4 sample annealed at 683 K for 10 min. (c) Bright-field TEM and (d) HRTEM pictures of Fe85.6P11C2B1W0.8 sample annealed at 683 K for 10 min. The insets in (a,c) are the corresponding SAED patterns.

3.3. Simulation of Amorphous Structure and Magnetic Properties

To characterize the structure and magnetic performances of amorphous alloys, AIMD is an effective approach. According to the experimental results, the minor addition of the W element causes large changes in magnetic properties. Therefore, Fe86P11C2B1, Fe85.5P11C2B1W0.5, and Fe85P11C2B1W1 are selected as representative alloy components for comparison. The pair correlation function (PCF) of Fe86−xP11C2B1Wx (x = 0, 0.5 and 1) amorphous alloys at a normal atmospheric temperature (300 K) is shown in Figure 6a. The prominent first peak indicates the characteristics of short-range order, while the second one with splitting feature indicates mid-range order, which indicates the amorphous...
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Figure 6. (a) Pair correlation functions and (b) bond pairs distribution of Fe$_{86-x}$P$_{11}$C$_2$B$_1$W$_x$ ($x = 0$, 0.5, and 1) amorphous alloys.

To further understand the effects of W addition on soft magnetic performances, atomic magnetic moments were analyzed. The average magnetic moments of the Fe, P, C, B, and W atoms were calculated by AIMD for the Fe$_{86-x}$P$_{11}$C$_2$B$_1$W$_x$ ($x = 0, 0.5$ and $1$) amorphous alloys. As summarized in Table 3, the electronic magnetic moment of the Fe atoms dominates the total magnetic moments of the whole alloy system. The average magnetic moment of the Fe atoms decreases from 2.225 $\mu_B$ to 2.096 $\mu_B$ with the addition of the W element. In addition, W exhibits a more negative magnetic moment ($-0.578 \mu_B$) than other constituent elements. This can explain the previous experimental phenomenon that the $B_s$ values monotonically decrease with the addition of W. Furthermore, the Fe magnetic moment distribution with the corresponding coordination number was concerned. The average magnetic moment of Fe in Table 3 can be calculated from the weighted average of the data in Figure 7. The coordination number is defined as the number of the first nearest neighbor Fe atoms near the central Fe atoms. The proportion of the high coordination number in the first nearest neighbor was reported to correlate positively with the magnetic moment [43]. This is because the increase in the proportion of high coordination numbers in the first nearest neighbor indicates more neighboring Fe atoms taking part in the ferromagnetic coupling, which increases saturated magnetization [44]. It can be seen in Figure 7 that the proportion of high coordination numbers (13, 14) decreases. In contrast, the proportion of
low coordination numbers (10, 11, and 12) increases with the addition of W. This result shows that the addition of W expands the nearest neighbor Fe-Fe spacing and diminishes the percentage of high coordination numbers. Thus, the average magnetic moment of Fe atoms decreases, which leads to a decrease in the $B_g$ of the Fe$_{86-x}$P$_{11}$C$_2$B$_1$W$_x$ (x = 0, 0.5 and 1) amorphous alloys.

Table 3. Average magnetic moments of each atomic orbital for the Fe, P, C, B, and W atoms in the Fe$_{86-x}$P$_{11}$C$_2$B$_1$W$_x$ (x = 0, 0.5 and 1) amorphous alloys.

| Alloys       | Element | s (μB) | p (μB)  | d (μB)  | Total (μB) |
|--------------|---------|--------|---------|---------|------------|
| Fe$_{86}$P$_{11}$C$_2$B$_1$ | Fe      | −0.009 | −0.034  | 2.268   | 2.225      |
|              | P       | −0.005 | −0.082  | 0.000   | −0.087     |
|              | C       | −0.015 | −0.126  | 0.000   | −0.141     |
|              | B       | −0.026 | −0.137  | 0.000   | −0.164     |
| Fe$_{85.5}$P$_{11}$C$_2$B$_1$W$_{0.5}$ | Fe     | −0.008 | −0.035  | 2.250   | 2.207      |
|              | P       | −0.006 | −0.084  | 0.000   | −0.090     |
|              | C       | −0.015 | −0.126  | 0.000   | −0.141     |
|              | B       | −0.027 | −0.134  | 0.000   | −0.161     |
|              | W       | −0.027 | −0.093  | −0.521  | −0.587     |
| Fe$_{85}$P$_{11}$C$_2$B$_1$W$_1$ | Fe     | −0.008 | −0.033  | 2.137   | 2.096      |
|              | P       | −0.005 | −0.077  | 0.000   | −0.082     |
|              | C       | −0.013 | −0.108  | 0.000   | −0.121     |
|              | B       | −0.026 | −0.127  | 0.000   | −0.153     |
|              | W       | −0.027 | −0.039  | −0.513  | −0.578     |

Figure 7. Fe magnetic moment distribution with corresponding coordination number in the Fe$_{86-x}$P$_{11}$C$_2$B$_1$W$_x$ (x = 0, 0.5, and 1) amorphous alloys.

The tunable electronic performances of Fe$_{86-x}$P$_{11}$C$_2$B$_1$W$_x$ (x = 0, 0.5 and 1) alloys were also researched by the density of states (DOS). The total electron DOS of the Fe atom in Fe$_{86-x}$P$_{11}$C$_2$B$_1$W$_x$ (x = 0, 0.5, and 1) amorphous alloy is illustrated in Figure 8a. The Fermi level lay right above the majority spin band and close to the minimum value of the spin-down band, indicating that ferromagnetism exists in the alloy [45]. Figure 8b shows the partial electron DOS (3d orbital) of Fe atoms for Fe$_{86-x}$P$_{11}$C$_2$B$_1$W$_x$ (x = 0, 0.5 and 1) amorphous alloys. Two dominant peaks separated from the 3d band states can be seen, which were reported as the lower-energy $t_{2g}$ orbital and the higher-energy $e_g$
orbital [46]. According to previous research, ferromagnetism is caused by the distinction in the magnetic moments of the upper and lower spin electrons induced by the asymmetry of band splitting [47]. With the addition of the W element, the number of spin-up electrons $N^\uparrow$ decreases slightly, while the number of occupied spin-down electrons $N^\downarrow$ is almost unchanged. Therefore, the gap becomes much closer, which leads to a decreased Fe atomic magnetic moment of the Fe atom in the alloy system.

Figure 8. (a) Total electron DOS and (b) partial electron DOS of Fe atoms (3d orbital) in the Fe$_{86-x}$P$_{11}$C$_2$B$_1$W$_x$ ($x = 0, 0.5$ and $1$) amorphous alloys. The arrows indicate the spin direction of the electron.

4. Conclusions

Fe$_{86-x}$P$_{11}$C$_2$B$_1$W$_x$ ($x = 0, 0.1, 0.2, 0.4, 0.6, 0.8, 1, 2,$ and $4$) amorphous alloys were developed by melt spinning, and the influences of W addition on the amorphous structure, thermal behavior, and soft magnetic performances were researched by several experiments and AIMD simulation. The addition of W enhances the thermal stability, with $T_{x1}$ and $T_{x2}$ increasing up to 711 K and 731 K, respectively, consistent with the BP analysis of the simulation, which suggests that the GFA of the amorphous alloy can be improved with W addition. The amorphous alloy systems exhibit good $B_s$ and low $H_c$ in the range of 1.17–1.62 T and 1.4–6.3 A/m. The low $H_c$ of annealed ribbons was proved by straight wide stripy magnetic domains. Especially, the Fe$_{85.6}$P$_{11}$C$_2$B$_1$W$_{0.4}$ alloy shows optimal soft magnetic performances, with low $H_c$ of 1.4 A/m and relatively good $B_s$ of 1.52 T. The
magnetic moment and electron DOS analysis demonstrates that the decrease in $B_s$ via W addition results from the distance increase in nearest neighboring Fe-Fe, gap narrowing between spin-up $N_{↑}$ and spin-down $N_{↓}$ electrons, diminishment of the coordination number, and a reduction in the average magnetic moment of the Fe atoms.

**Author Contributions:** C.S.: methodology, investigation, data curation, visualization, and writing—original draft. H.X.: methodology, writing—review and editing. Y.M.: methodology, writing—review and editing. X.W.: simulation, software. M.H.: investigation, data curation. B.Q.: investigation, resources. Y.W.: investigation. T.Z.: conceptualization, methodology, supervision, resources, and funding acquisition. All authors have read and agreed to the published version of the manuscript.

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