Postprint: Composition Design of Fe-B-Si-Ta Bulk Metallic Glass Based on Cluster-Plus-Glue-Atom Model

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Abstract

Based on the cluster-plus-glue-atom model, Fe-B-Si-Ta soft magnetic bulk metallic glasses with high glass-forming ability were designed. Starting from the eutectic phase Fe2B corresponding to the eutectic point Fe83B17, the [B-B2Fe8] principal cluster centered by B was obtained according to the principles of maximum radial atomic number density and isolation. Combined with the electron concentration criterion for ideal metallic glass cluster formulas, the ideal cluster formula [B-B2Fe8]Fe for Fe-B binary metallic glasses was constructed. To enhance the glass-forming ability of Fe-B binary alloys, Si, which exhibits a large negative mixing enthalpy with Fe, was selected to substitute the center atom B in the [B-B2Fe8] cluster, yielding the ideal cluster formula [Si-B2Fe8]Fe for Fe-B-Si ternary metallic glasses. Since Ta possesses large negative mixing enthalpies with both B and Si, Fe atoms at shell positions in the [Si-B2Fe8]Fe cluster formula were further substituted by Ta to design a series of quaternary amorphous compositions [Si-B2Fe8-xTax]Fe. The results demonstrate that [Si-B2Fe8-xTax]Fe can form amorphous alloy rods with a diameter of 1.0 mm at compositions of x=0.4~0.7. Among these, the [Si-B2Fe7.4Ta0.6]Fe alloy exhibits the optimal glass-forming ability, with a reduced glass transition temperature Trg of 0.584, a glass transition temperature Tg of 856 K, and a supercooled liquid region width ΔTx reaching 33 K. The Vickers hardness Hv of [Si-B2Fe8-xTax]Fe (x=0.4~0.7) bulk metallic glasses increases from 1117 HV (x=0.4) to 1154 HV (x=0.7) with Ta addition. The [Si-B2Fe7.6Ta0.4]Fe amorphous alloy demonstrates excellent room-temperature soft magnetic properties, with a saturation magnetization Bs of 1.37 T and a coercivity Hc of 3.0 A/m.

Full Text

Composition Design of Fe-B-Si-Ta Bulk Amorphous Alloys Based on the Cluster-Plus-Glue Atom Model

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Abstract

The structural and compositional features of amorphous alloys can be effectively described by the cluster-plus-glue atom model, which provides a powerful method for composition design. In the Fe-B binary system, the Fe_2B phase is an intermetallic compound associated with the $Fe_{83}B_{17}$ eutectic point. Under the framework of the highest radial number density and isolation principle, the local structure of Fe_2B is characterized by a B-centered Archimedean octahedral antiprism [B-B_2Fe_8] atomic cluster. Combined with the electron concentration criterion, [B-B_2Fe_8]Fe (where the center and shell atoms are separated by a hyphen, a cluster is enclosed in square brackets, and glue atoms appear outside the brackets) is determined as the ideal cluster formula for Fe-B binary amorphous alloys. To further enhance the glass-forming ability (GFA), Si and Ta are introduced to replace the center B and shell Fe atoms, respectively, due to their large negative enthalpy of mixing with Fe and B/Si. This yields a series of Fe-B-Si-Ta quaternary compositions, namely [Si-B_2Fe_8 Ta]Fe. Experimental results reveal that bulk amorphous rods with a diameter of 1.0 mm can be achieved for [Si-B_2Fe_8 Ta]Fe compositions with x = 0.4–0.7. Among them, [Si-$B_2Fe_{7\cdot4}Ta_{0\cdot6}$]Fe (i.e., $Fe_{70}B_{16\cdot67}Si_{8\cdot33}Ta_5$, atomic fraction, %) exhibits the best glass-forming ability, with a glass transition temperature Tg of 856 K, a supercooled liquid region ΔTx of 33 K, and a reduced glass transition temperature Trg of 0.584. The Vickers hardness Hv of [Si-B_2Fe_8 Ta]Fe (x = 0.4–0.7) bulk amorphous alloys increases from 1117 HV (x = 0.4) to 1154 HV (x = 0.7) with Ta addition. The [Si-$B_2Fe_{7\cdot6}Ta_{0\cdot4}$]Fe amorphous alloy demonstrates excellent soft magnetic properties at room temperature, with a saturation magnetization Bs of 1.37 T and a coercivity Hc of 3.0 A/m.

Key words: cluster-plus-glue atom model, cluster formula, Fe-B-Si-Ta bulk amorphous alloy, magnetism

Introduction

Iron-based amorphous alloys are important soft magnetic and structural materials, offering high saturation magnetization (Bs), high permeability (e), low coercivity (Hc), high strength, and excellent corrosion resistance [1-5]. Early Fe-based amorphous alloys were primarily produced as ribbons, which significantly limited their applications. In the 1990s, Inoue et al. [6] prepared Fe-(Al, Ga)-(P, C, B) bulk amorphous alloys using copper mold suction casting, expanding the scope of Fe-based amorphous materials. Since then, several Fe-based bulk amorphous alloy systems have been developed, which can be broadly classified into four categories based on alloying elements: Fe-(Al, Ga, Mo)-(P, C, B, Si), Fe-Cr-Mo-C-B-RE (where RE denotes rare earth elements), Fe-B-Si-(Zr, Nb), and Fe-B-(Zr, Hf, Nb, Ta) [7-10].

Despite nearly two decades of development, the composition design of Fe-based bulk amorphous alloys has relied primarily on semi-empirical rules such as Inoue' s three principles [11], requiring extensive experimental effort. Recently, Dong et al. [12] proposed the cluster-plus-glue atom model for ideal amorphous alloys, which describes compositions with optimal glass-forming ability in a unified cluster formula cluster (where x = 1 or 3). This approach correlates composition, structure, and glass-forming ability, enabling quantitative composition design of amorphous alloys. The cluster formula method has successfully rationalized optimal glass-forming compositions in Zr-based, Cu-based, and rare-earth-based metal-metal alloy systems [13,14], and has been used to design new bulk amorphous alloy systems such as Ni-Ta [15,16]. However, its application to metal-metalloid amorphous alloy systems remains limited. Since metal-metalloid atomic pairs generally exhibit strong interactions, the resulting amorphous alloys possess more pronounced cluster structural features [17], better satisfying the prerequisites of the cluster-plus-glue atom model. Based on this rationale, the present work employs the cluster-plus-glue atom model to establish ideal cluster formulas for Fe-B and Fe-B-Si amorphous alloys from the Fe-B binary equilibrium phase diagram, combined with electron concentration criteria. Building upon this foundation, the element Ta is introduced to design novel Fe-B-Si-Ta quaternary bulk amorphous alloys with excellent soft magnetic properties.

1. Composition Design

Amorphous alloy formation requires high cooling rates to suppress crystallization during melt solidification. Consequently, compositions with high melt stability, such as eutectic points in alloy phase diagrams, typically exhibit stronger glass-forming ability. On the other hand, melts near eutectic compositions tend to form eutectic structures when solidified below the critical cooling rate, suggesting a close structural relationship between amorphous alloys and related eutectic phases. In fact, the basic structural units of amorphous alloys can be equated to certain local structures of relevant eutectic compound phases [18,19].

In the Fe-B binary equilibrium phase diagram [20], the eutectic point on the Fe-rich side is $Fe_{83}B_{17}$, with corresponding eutectic phases of γ-Fe solid solution and Fe_2B phase. Among these, the Al_2Cu-type Fe_2B intermetallic compound phase is closely associated with amorphous formation and structure. This phase has one independent atomic site for each Fe and B component [21]. Using Carine structure analysis software, various cluster structures centered on B and Fe atoms can be obtained along with their radial atomic number densities (r). Figure 1 [Figure 1: see original paper] shows the variation of r with cluster radius r (the distance between outermost shell atoms and the central atom) for different clusters in the Fe_2B phase. According to the principle of maximum radial atomic number density for cluster selection in alloy phases [22], [B-B_2Fe_8] and [Fe-$Fe_{11}B_4$] are selected as representative clusters of the Fe_2B phase (where atoms inside “[ ]” constitute the cluster, the atom before “-” is the center atom, the part after “-” represents shell atoms, and subscripts denote the number of corresponding atoms). Their atomic configurations are shown in Figure 2 [Figure 2: see original paper].

The cluster unit that embodies the structural characteristics of an alloy phase is called the principal cluster, which possesses high isolation [18]. Here, isolation is defined as the inverse ratio of Z_2/Z_1, where Z_1 is the number of atoms in an individual cluster, and Z_2 is the effective number of atoms corresponding to this cluster unit after accounting for sharing factors in the crystal phase. A larger Z_2/Z_1 value indicates higher isolation, meaning less sharing between cluster units in the alloy structure. When $Z_2/Z_1 = 1$, the cluster is completely isolated without sharing. For the two clusters obtained above, [B-B_2Fe_8] and [Fe-$Fe_{11}B_4$], their corresponding Z_2/Z_1 values are 3/11 and 1.5/16, respectively. Clearly, the [B-B_2Fe_8] cluster has a larger Z_2/Z_1 value and higher isolation. Therefore, the [B-B_2Fe_8] cluster is identified as the principal cluster of the Fe_2B alloy phase and used as the cluster unit to construct the cluster formula for Fe-B binary amorphous alloys.

Ideal amorphous alloy compositions can be expressed by the cluster formula cluster (where x = 1 or 3) [12]. For Fe-B binary amorphous alloys, the principal cluster is [B-B_2Fe_8], and glue atoms can only be B and/or Fe components. Accordingly, six Fe-B binary amorphous cluster formulas can be obtained: [B-B_2Fe_8]Fe, [B-B_2Fe_8]Fe_3, [B-B_2Fe_8]B, [B-B_2Fe_8]B_3, [B-B_2Fe_8]FeB_2, and [B-B_2Fe_8]Fe_2B. Amorphous alloys are a special class of electron phases, where electron concentration is a crucial factor determining their formation and stability. Recent studies [21] indicate that for amorphous alloys with specific cluster formula compositions, the average number of valence electrons per unit formula can be calculated using:

$$e/u = 1.25\frac{Z}{M}\rho r_1^3 N_0 \tag{1}$$

where e/u is the number of valence electrons per cluster formula; Z represents the total number of atoms in a single cluster formula; M is the average atomic weight of the cluster formula; r_1 is the cluster radius;   is the mass density; and N_0 is Avogadro' s constant (6.02×10^{23} mol^{-1}). Literature [24] shows that the e/u value for ideal amorphous alloy cluster formulas is close to 24, which serves as the electron concentration criterion for amorphous alloy cluster formulas.

Using Equation (1), the e/u values for the six Fe-B binary amorphous cluster formulas are calculated as 24.1, 28.7, 22.8, 25.4, 26.9, and [B-B_2Fe_8]Fe, respectively. The average radius from cluster shell atoms to the center atom is determined using the Goldschmidt radii of Fe and B (rFe = 0.127 nm, rB = 0.098 nm), yielding r_1 = 0.219 nm. The   values are obtained from measured results and fitting in literature [25,26]. As shown in Table 1 , among the listed cluster formulas, [B-B_2Fe_8]Fe has an e/u value closest to 24. Therefore, [B-B_2Fe_8]Fe is identified as the ideal cluster formula for Fe-B binary amorphous alloys, corresponding to the atomic fraction composition $Fe_{75}B_{25}$.

Literature [25] indicates that Fe-B binary alloys only form ribbon amorphous phases within a B atomic fraction range of 12%-28%. To improve the glass-forming ability of Fe-B binary alloys, multi-component alloying is performed based on the [B-B_2Fe_8]Fe cluster formula. According to literature [27], the mixing enthalpies for Fe-Si, Fe-B, and Si-B atomic pairs are ΔHFe-Si = -35 kJ/mol, ΔHFe-B = -26 kJ/mol, and ΔHSi-B = -14 kJ/mol, respectively, with the most negative value for Fe-Si. Therefore, Si atoms are first introduced to replace the center B atom in the [B-B_2Fe_8]Fe cluster formula, yielding the Fe-B-Si ternary amorphous cluster formula [Si-B_2Fe_8]Fe. The atomic fraction composition corresponding to the [Si-B_2Fe_8]Fe cluster formula is $Fe_{75}B_{16\cdot67}Si_{8\cdot33}$, which is close to the optimal glass-forming composition $Fe_{75}B_{16}Si_9$ reported by Luborsky et al. [28] for the Fe-B-Si ternary system. Similarly, since Ta also exhibits relatively negative mixing enthalpy with Si and B (ΔHTa-Si = -56 kJ/mol, ΔHTa-B = -54 kJ/mol), Ta atoms are further introduced into the [Si-B_2Fe_8]Fe cluster formula to replace Fe atoms in the shell positions. This yields a series of Fe-B-Si-Ta quaternary amorphous compositions with the cluster formula [Si-B_2Fe_8 Ta]Fe (x = 0–0.8).

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2. Experimental Methods

Master alloy ingots with compositions of [Si-B_2Fe_8 Ta]Fe (x = 0, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, and 0.8) were prepared from raw materials of Fe (99.999 wt% purity), Si (99.999 wt% purity), B (99.5 wt% purity), and Ta (99.95 wt% purity). The master alloy ingots were melted in a high-purity Ar atmosphere after Ti gettering and remelted four times to ensure compositional homogeneity. Ribbon samples with dimensions of 0.02 mm × 0.8 mm were prepared by single-roller melt spinning using a Cu roller with a surface linear velocity of 40 m/s. Rod samples with diameters of 1.0 mm and 1.5 mm were fabricated by copper mold suction casting. Phase structure identification was performed using a Bruker D8 Focus X-ray diffractometer (XRD). Cross-sections of rod samples were observed using a BX51 optical microscope (OM) after etching with a 1% hydrofluoric acid aqueous solution (mass fraction). Thermal analysis was conducted on a Q100 differential scanning calorimeter (DSC) and a Q600 differential thermal analyzer (DTA) at a heating rate of 0.33 K/s. Vickers hardness of bulk amorphous alloys was measured using an HVS-1000 hardness tester with a load of 9.8 N and loading time of 15 s. Saturation magnetization (Bs) and coercivity (Hc) of amorphous ribbon samples were measured using a LakeShore-7407 vibrating sample magnetometer and a MATS-2010SD hysteresis-graph. Prior to testing, ribbon samples were subjected to low-temperature vacuum annealing to remove residual stress.

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3. Results and Discussion

Figure 3 [Figure 3: see original paper] shows the XRD patterns of [Si-B_2Fe_8 Ta]Fe (x = 0–0.8) samples. All ribbon samples exhibit typical broad diffraction peaks characteristic of the amorphous state, indicating that single-phase amorphous ribbons can be formed across this composition range. With increasing Ta content, the diffraction angle 2 of the main amorphous peak gradually decreases from 45.3° at x = 0 to 44.4° at x = 0.8. According to the Ehrenfest equation:

$$Q = \frac{4\pi \sin\theta}{\lambda} = \frac{1.23(2\pi)}{d} \tag{2}$$

where Q is the scattering factor, is the Bragg diffraction angle, λ is the X-ray wavelength, and d is the average atomic distance. This indicates that the diffraction angle of the main amorphous peak is inversely proportional to the average atomic distance. For [Si-B_2Fe_8 Ta]Fe amorphous alloys, the addition of Ta leads to a decrease in 2 , implying an increase in the average atomic distance in the amorphous structure, which is consistent with the cluster design concept. As described earlier, replacing Fe shell atoms in the [Si-B_2Fe_8] cluster with Ta atoms, which have a larger atomic radius (Goldschmidt radii: rTa = 0.147 nm, rFe = 0.127 nm), increases the average atomic distance within the cluster, causing the main amorphous peak to shift to lower angles.

Figure 3b presents the XRD patterns of [Si-B_2Fe_8 Ta]Fe rod samples with a diameter of 1.0 mm. Samples with x = 0.4–0.7 exhibit a fully amorphous structure, while other compositions show varying degrees of crystalline diffraction peaks. When the rod diameter increases to 1.5 mm, all compositions display obvious crystalline diffraction peaks, identified as α-Fe, Fe_3B, and Fe_2B phases [30,31]. These results demonstrate that among the Fe-B-Si-Ta quaternary alloys designed by the cluster formula method, bulk amorphous rods with a diameter of 1.0 mm can be prepared by copper mold suction casting at compositions of [Si-B_2Fe_8 Ta]Fe (x = 0.4–0.7).

To confirm the critical size and glass-forming ability of bulk amorphous samples, Figure 4 [Figure 4: see original paper] shows optical micrographs of cross-sections from a 1.0 mm rod at x = 0.4 and 1.5 mm rods at x = 0.5–0.7. All rod samples were sectioned 3 mm from the bottom to ensure accurate results. The 1.0 mm rod at x = 0.4 exhibits uniform contrast after etching, with no observable crystalline phase precipitation, confirming a fully amorphous structure. In contrast, the 1.5 mm rods show distinct contrast variations, indicating multiphase microstructures. The bright edge regions, with contrast similar to the 1.0 mm amorphous sample, correspond to the corrosion-resistant amorphous phase, while the darker interior regions represent less corrosion-resistant crystalline phases. This observation is fully consistent with the XRD results. By comparing the relative amount of the bright amorphous phase in the cross-sections of 1.5 mm rods, the glass-forming ability can be evaluated. The sample at x = 0.6 contains the least amount of crystalline precipitates (Figure 4c), indicating the optimal glass-forming ability in the [Si-B_2Fe_8 Ta]Fe (x = 0–0.8) series.

Figure 5 [Figure 5: see original paper] shows the thermal analysis curves of [Si-B_2Fe_8 Ta]Fe (x = 0–0.8) ribbon samples. As shown in Figure 5a, Ta addition transforms the crystallization behavior from a single exothermic peak (x = 0) to a double-peak characteristic. Meanwhile, the initial crystallization temperature (Tx) gradually increases with Ta content, rising from 839 K at x = 0 to 896 K at x = 0.8. At x = 0.4, a discernible glass transition temperature (Tg) appears in the DSC curve, indicating that Ta addition not only improves the thermodynamic stability of Fe-B-Si amorphous alloys but also promotes metallic glass formation, consistent with the previous experimental results. Similar to Tx, the Tg values also increase progressively with Ta content, from 843 K (x = 0.4) to 859 K (x = 0.8). Figure 5b presents the DTA curves of [Si-B_2Fe_8 Ta]Fe (x = 0–0.8) amorphous samples. With increasing Ta content, the liquidus temperature (Tl) first increases, then decreases, and increases again, reaching a minimum value of 1466 K at x = 0.7.

Figure 6 [Figure 6: see original paper] illustrates the variations of supercooled liquid region width (ΔTx) and reduced glass transition temperature (Trg) with Ta content for [Si-B$_2$Fe$_8$ Ta]Fe (x = 0.4-0.8) amorphous alloys. The ΔTx values remain relatively constant, ranging between 30–35 K. The glass-forming ability parameter Trg [32] reaches its maximum at x = 0.6 and 0.7, which is consistent with the copper mold suction casting results. The thermal analysis results and critical size data for [Si-B$_2$Fe$_8$ Ta]Fe (x = 0–0.8) amorphous alloys are summarized in Table 2 .

Similar to the trend in Tg, the Vickers hardness values of [Si-B$_2$Fe$_8$ Ta]Fe (x = 0.4–0.7) bulk amorphous samples also increase with Ta content, as listed in Table 2. Studies [33–35] have shown a positive correlation between the hardness (Hv) and Tg of amorphous alloys. Linear fitting yields the relationship Hv = -570 + 2Tg for the [Si-B$_2$Fe$_8$ Ta]Fe (x = 0.4–0.7) bulk amorphous alloys. In the [Si-B$_2$Fe$_8$ Ta]Fe cluster formula, the negative mixing enthalpy between B/Si and Ta is significantly higher than that between B/Si and Fe, and Ta also exhibits negative mixing enthalpy with Fe. Due to these strong interactions, Ta atoms preferentially occupy shell positions in the cluster formula. Increasing Ta content thus enhances interactions between the cluster center and shell atoms, between shell atoms, and between shell and glue atoms, thereby stabilizing the amorphous cluster structure and raising Tg [36]. On the microscopic level, hardness can be defined as the resistance of chemical bonds per unit area to indentation [37]. Metal-metalloid amorphous alloys exhibit covalent-like bonding characteristics. In Fe-B-Si-Ta amorphous alloys, increased Ta content strengthens atomic bonds, leading to higher hardness values. Thus, from the cluster formula perspective, it is possible to qualitatively and even quantitatively explain the influence of Ta addition on Tg and Hv.

Figure 7a [Figure 7: see original paper] shows the magnetization curves at an applied field of 1.5 T for [Si-B$_2$Fe$_8$ Ta]Fe samples at x = 0, 0.4, and 0.6. The saturation magnetization (Bs) values are 1.67 T, 1.37 T, and 1.25 T, respectively, demonstrating that Ta addition significantly reduces Bs. This reduction is attributed to the decrease in average atomic spin magnetic moment (mB) caused by the incorporation of non-magnetic Ta atoms [38]. The weak endothermic peaks at low temperatures in the DSC curves (Figure 5a) correspond to the ferromagnetic-paramagnetic transition temperature, i.e., the Curie temperature (Tc). The Tc values for [Si-B$_2$Fe$_8$ Ta]Fe (x = 0–0.8) amorphous samples are also listed in Table 2. With increasing Ta content, Tc decreases rapidly from 723 K to 520 K (x = 0.8). According to the mean field model [39], Tc is determined by both the exchange interaction between atoms and the average spin magnetic moment, where the exchange interaction depends primarily on the average distance between magnetic atoms. XRD results show that increasing Ta content increases the average atomic distance in the amorphous alloys, which would enhance Fe-Fe exchange interactions and increase Tc. However, the decrease in Bs reduces the average spin magnetic moment, leading to a decrease in Tc. Therefore, the variation in Bs dominates the Tc behavior in this alloy series.

Figure 7b presents the magnetic hysteresis loops of [Si-B_2Fe_8 Ta]Fe (x = 0, 0.4, and 0.6) samples. Analysis yields coercivity (Hc) values of 4.3 A/m, 3.0 A/m, and 2.8 A/m, respectively. Compared with known Fe-B-Si-Nb and $Fe_{74}Al_4Ga_2P_{12}B_4Si_4$ bulk amorphous alloys, the newly designed [Si-$B_2Fe_{7\cdot6}Ta_{0\cdot4}$]Fe alloy exhibits significantly higher Bs and lower Hc [40,41].

Conclusions

1. By applying the cluster-plus-glue atom model and starting from the Fe_2B eutectic phase, combined with the electron concentration criterion, the ideal cluster formula for Fe-B binary amorphous alloys was established as [B-B_2Fe_8]Fe. To develop soft magnetic Fe-based bulk amorphous alloys with broader applications, Si atoms with large negative mixing enthalpy with Fe were selected to replace the central B atom, and Ta atoms with large negative mixing enthalpy with B/Si were used to replace shell Fe atoms in the [B-B_2Fe_8]Fe cluster formula. This approach successfully designed and prepared a series of [Si-B_2Fe_8 Ta]Fe (x = 0.4–0.7) quaternary bulk amorphous alloys. Among them, the [Si-$B_2Fe_{7\cdot4}Ta_{0\cdot6}$]Fe (i.e., $Fe_{70}B_{16\cdot67}Si_{8\cdot33}Ta_5$) composition exhibits the best glass-forming ability. The cluster-plus-glue atom model effectively enables composition design of metal-metalloid type Fe-B-Si-Ta bulk soft magnetic amorphous alloys.
2. The [Si-$B_2Fe_{7\cdot6}Ta_{0\cdot4}$]Fe (i.e., $Fe_{71\cdot67}B_{16\cdot67}Si_{8\cdot33}Ta_{3\cdot33}$) amorphous alloy possesses excellent soft magnetic properties, with a saturation magnetization of 1.37 T and a coercivity of 3.0 A/m. The Vickers hardness of [Si-B_2Fe_8 Ta]Fe (x = 0.4–0.7) bulk amorphous alloys increases from 1117 HV (x = 0.4) to 1154 HV (x = 0.7) with increasing Ta content, following a similar trend to that of Tg.

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Note: Figure translations are in progress. See original paper for figures.