Bulk Metallic Glasses: General Note with Effect of Fraction Change in Constituent Elements on Various Temperatures.

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Abstract

Metallic glasses are amorphous metallic solids which have high strength, good magnetic properties and better corrosion resistance and will possess both the properties of metals and glasses. Metals can be made into a glassy state by increasing the rate of cooling to a very high level. At that state the atoms will not be able to arrange orderly because of its rapid cooling rate. Thus, the atoms will not be allowed to go to crystalline state, rather it goes to amorphous state, and it will form a new type of material, such materials are called metallic glasses. Glass formation is a phenomenon commonly associated with non-metallic materials, but it is relatively new for metals. In most material classes, crystallization occurs when a material is melted and then cooled. However, in some cases, crystallization can be avoided if the material is rapidly cooled, resulting in the formation of a glassy, amorphous structure instead of a crystalline one. The temperature-related properties of BMGs can include crystallization temperature (T_x), glass transition temperature (T_g), melting temperature (T_m) or liquidus temperature (T_l), and the coefficient of thermal expansion (α). These temperatures can vary widely depending on various factors of the BMG alloy, such as composition, cooling rate, alloying element and their fraction, atomic structure, processing condition etc.

Keywords: Crystallization temperature (T_x), glass transition temperature (T_g), the coefficient of thermal expansion, thermal conductivity, and covalent radius.

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Introduction

Bulk metallic glasses exhibit exceptional physical and chemical properties. They demonstrate high wear resistance and corrosion resistance, coupled with remarkable characteristics such as high flexibility at elevated temperatures and extraordinary strength in low-temperature conditions. Notably, akin to certain polymer materials, they boast a substantial elastic limit of nearly 2%. In comparison to their crystalline counterparts, bulk metallic glasses display a significantly heightened strength, often ranging from 2 to 3 times greater. These remarkable attributes make bulk metallic glasses an alluring candidate for practical applications as a

novel class of functional and structural materials. These qualities, rarely found in crystalline materials, open new avenues for advanced designs and systems.

The scientific significance of comprehending the intricacies of glass phenomena and the formation of bulk metallic glasses, alongside the technological potential for real-world applications, has garnered widespread research interest in the exploration of these materials. Since their initial discovery by Duwez in 1990, substantial endeavours have been dedicated to developing glassy or amorphous alloys. These pursuits encompass techniques encompassing solid-state amorphization and rapid solidifications.

The first instance of what we now categorize as "bulk" amorphous alloy dates back to 1969 when Chen and Turnbull uncovered it in ternary Pd-Cu-Si alloys. The critical cooling rate for these ternary bulk glass-forming alloys hovers around 102 K/s. Particularly noteworthy is the surge in attention from the scientific community, triggered by the emergence of new multi-component bulk metallic glasses. Examples include $La_{55}Al_{25}Ni_{20}$ (discovered by Inoue et al. in 1989) and $Zr_{41.2}Ti_{13.8}Cu_{12.5}Ni_{10}Be_{22.5}$ (unveiled by Peker and Johnson in 1993). These alloys can be produced at lower cooling rates through direct casting from molten liquid, marking a significant advancement in BMG fabrication techniques. On the basis of metallic composition, bulk metallic glasses can be divided into two types: one is metal-metal (TE-TL) type and another is metal-metalloid (TL-MD). In metal-metal type BMGs, all constituent elements are metallic, while in metal-metalloid type BMGs, 80% are metallic and the remaining 20% are metalloid elements.

Metal-metal(TL-late transition metal (Fe, Co, Ni, Pd, Pt, Cu), TE-early transition metal (Y, Sc, Ti, Zr, Hf, Mo, W)) bulk metallic glasses are more applicable than metal-metalloid (TL-MD (metalloid (B, P, C, Si) type bulk metallic glasses. Metal-metal type bulk metallic glasses generally exhibit lower glass forming abilities than metal-metalloid type bulk metallic glasses.

A proper grid is an atomic percentage according to a grid system because glass-forming compositions exhibit different properties (hence different alloys) on that scale. Applying the grid system to two different alloys in one component gives a total of $\sim 10^{12}$ metallic glass alloys that can be formed from 32 elements. These do not include the rare earth elements and high-cost elements such as Sc, Ta, Ru, and Rh elements; if these are included the total number of metallic glass alloys would be much larger than $\sim 10^{12}$.

Nearly 54 elements are used in the fabrication of bulk metallic glasses. If we apply the fabrication's law of bulk metallic glasses then there are so many bulk metallic glasses that can fabricate.

These three guidelines to enable BMG formation instead of crystallization as given by Inoue are as follows-

1. The atomic size ratios of at least two constituents of the alloy should be $\alpha < 0.89$ for small relative to large.
2. The value of negative heat of mixing should be large.
3. Atomic components should be several.

The simple empirical rules in the search of compositions likely to yield new metal/metalloid bulk metallic glasses given by Shen and Schwarza for Bulk ferromagnetic glasses prepared by flux melting and water quenching are:

1. The alloy must have at least three components, two of which are metallic.
2. The alloy must contain two or more metallic elements with different atomic sizes and near-zero heats of mixing.
3. The metallic elements must have large negative heats of mixing with the metalloid(s).
4. The total metalloid content must be in the vicinity of 20 at. %.
5. Heteronucleants, such as crystalline oxide inclusions, must be carefully removed by dissolving the oxides in a flux, or by neutralizing the oxygen dissolving it in (dissolving it in the melt)

BMG: Significance and Interest

When metals are cooled at critical cooling rates (typically 1000 K/s or less), they can form bulk metallic glasses (BMGs). These are alloys that vitrify upon cooling, maintaining an amorphous atomic structure rather than forming crystals. BMGs have garnered significant attention due to their unique combination of properties, processability, and amorphous structure. The properties and characteristics of BMGs make them both technologically and scientifically interesting. They have a range of potential applications due to their unique combination of mechanical, magnetic, thermal, and electrical properties. The ability to process these materials in bulk dimensions is a key advantage.

Over a hundred different compositions of BMGs have been discovered. These compositions involve various combinations of elements that result in the formation of bulk metallic glasses. This diversity allows for tailoring properties to suit specific applications. The critical cooling rate is a crucial factor in quantifying the glass forming ability (GFA) of an alloy. Higher GFA indicates that the alloy is more likely to form a glassy structure upon cooling, rather than crystallizing.

To understand and predict the compositions of BMGs, various theories have been developed. These theories aim to explain the underlying principles of glass formation and

provide insights into which combinations of elements are likely to lead to the formation of BMGs. As researchers continue to study BMGs and their potential applications, knowledge about the range of possible BMG-forming alloys will guide the development of appropriate techniques for producing these materials. This knowledge is valuable for advancing both scientific understanding and technological applications.

Temperatures for amorphous alloys

The temperature-related properties of BMGs can include crystallization temperature (T_x), glass transition temperature (T_g), melting temperature (T_m) or liquidus temperature (T_l), and the coefficient of thermal expansion (α). These temperatures can vary widely depending on various factors of the BMG alloy, such as composition, cooling rate, alloying element and their fraction, atomic structure, processing condition etc.

(i). Composition: The constituent elements and their proportions in the bulk metallic glass amorphous alloy can affect the temperature-related properties. For instance, adding elements that promote atomic mobility can lower the glass transition temperature.

(ii) Cooling Rate: The rate at which the bulk metallic glass amorphous alloy was cooled during its fabrication can influence its temperature-related properties.

(iii) Alloying Elements: Certain alloying elements can disrupt the atomic arrangement and lower the temperature-related properties.

(iv) Atomic Structure: The arrangement of atoms and the degree of disorder in the amorphous structure can impact temperature-related properties.

(v) Processing Conditions: The manufacturing process, including the preparation and cooling methods, can influence temperature-related properties.

Crystallization temperature (T_x)

The crystallization temperature, T_x, is the temperature at which the bulk metallic glass amorphous structure starts to transform into a crystalline structure. This transition embraces the atoms rearranging themselves into sequenced, crystalline arrangements. The particular temperature at which crystallization begins can vary based on the specific composition of the bulk metallic glass. Crystallization can affect the properties of bulk metallic glasses and hence, it may lead to changes in their mechanical, electrical, magnetic, and thermal characteristics.

The crystallization temperature can vary depending on the specific composition of the bulk metallic amorphous alloy. There is a lack of the long-range atomic order of crystalline metals, and exhibit disordered or non-crystalline atomic structures in BMGs. When BMGs are heated, they undergo a transition from a non-crystalline to a crystalline state.

Glass transition temperature (T_g)

The glass transition temperature, T_g, is the temperature at which a bulk metallic glass amorphous material transitions from a rigid or glassy state to a more viscous or rubbery state. The glass transition temperature is undoubtedly the temperature range at which the amorphous structure of a material system starts to experience molecular mobility and relaxation, leading to changes in mechanical, electrical, thermal, etc. properties. This phenomenon is considerable in understanding the behaviour of bulk metallic glasses and other amorphous materials.

Glass transition temperature (T_g) is a critical factor for bulk metallic glasses in determining the temperature limits for their processing and application. Below Tg, the material system is in a glassy, rigid state, while above T_g, it becomes more ductile and shows properties typical of a liquid with a supercooled state. Therefore, the glass transition temperature (T_g) is indeed a key parameter in the behaviour of BMGs. It represents the temperature at which a bulk metallic glass amorphous material, transitions from a glassy, rigid state to a more rubbery and ductile state.

Melting Temperature (Tm)

The melting temperature, Tm, refers to the temperature at which a solid material state transitions from a solid state to a liquid state. For bulk metallic glasses, Tm represents the temperature at which the amorphous structure of the alloy material transforms into a liquid during the melting process. Tm indicates the temperature range within which the bulk metallic material alloy can be effectively melted and cast into desired shapes, hence, in the processing of bulk metallic glasses, Tm is a critical parameter. When bulk metallic glasses are heated, they typically exhibit a gradual softening behavior. This transition is often specified as the glass transition, recorded by the glass transition temperature (Tg).

At temperatures below the Tg, bulk metallic glasses behave as rigid materials, glassy. As the temperature increases above Tg, they become softer and more ductile, but a clear phase change from solid to liquid does not appear. One of the characteristics that distinguish BMGs from conventional crystalline metals and alloys is the absence of a sharp melting point. At elevated temperatures, BMGs may undergo crystallization rather than melting, which involves the transformation of the amorphous structure of BMGs into crystalline phases.

Liquidus temperature (T_l)

The term liquidus temperature is relatively uncommon within the realm of bulk metallic glasses. Nevertheless, when applied to bulk metallic glasses, it could denote the temperature range wherein the bulk metallic glass amorphous alloys exhibit characteristics associated

with those of a supercooled liquid. In this supercooled liquid state, the atomic structure resembles that of a liquid, yet it maintains its solid form due to kinetic restrictions or elevated viscosity.

The term liquidus temperature (T_l) typically refers to the temperature at which a material after heating, usually an alloy, transitions completely into a liquid state from a solid state. In reference to bulk metallic glass amorphous alloys, which have disordered atomic structures. Like conventional crystalline alloys, bulk metallic glasses have a less direct concept of apparent liquidus temperature. Bulk metallic glasses are known for their amorphous structure or unique non-crystalline, which means they don't have a pronounced melting point like their counterparts' crystalline materials. Instead, bulk metallic glasses typically exhibit a supercooled liquid region, in this region if the temperature increases, they gradually become more viscous and softer.

Some researchers, in some cases, might use the term "liquidus" for BMGs, informally referring to the temperature range in which the non-crystalline structure of a bulk metallic alloy starts to transition into a state more liquid-like. However, this behaviour shows a clear melting point in crystalline materials but is not as well-defined as BMGs. It's crucial to emphasize that the behaviour exhibited by bulk metallic glasses in relation to temperature, including any observable "liquidus-like" characteristics, can exhibit significant variability. This variability depends on factors such as the composition of the alloy, fraction of constituent elements, processing parameters, and other influencing elements.

Nose Temperature (T_n)

The nose temperature, T_n, is a term used in reference to the TTT (Time-Temperature-Transformation) diagram. The crystallization behaviour of amorphous materials, such as BMGs is illustrated by the TTT diagram, as a function of time and temperature. The highest temperature on the TTT curve is the nose temperature, where crystallization occurs most rapidly. It's the temperature point for crystallization to BMGs at which the rate of the crystallization process is maximum.

Eutectic Temperature (Te)

The eutectic temperature is not commonly associated with directly bulk metallic glass amorphous alloys, and its meaning can vary depending on the context. The eutectic temperature, in the broader field of science of materials, is the lowest temperature at which a mixture of two or more elements that solidify together (a eutectic alloy) undergoes complete melting or solidification. However, eutectic behaviour is less relevant to bulk metallic glass amorphous alloys,

The concept of a eutectic temperature typically applies to a traditional system of alloys, where a eutectic mixture is formed by two or more components with a particular composition and an analogical eutectic temperature. BMGs are characterized by their amorphous / non-crystalline nature, featuring an arrangement of non-regular of atoms. BMGs lack conventional phase transformations like in crystalline. BMGs often have complex stages of glass transition, crystallization, and other structural changes that lead to the absence of eutectic points.

Supercooled Liquid Region (ΔT_x)

It represents the temperature range within which the maintaining solid-state composition BMG exhibits characteristics associated with those of a supercooled liquid.

Mathematically, it is the temperature difference between T_x and T_g.

i.e., $\Delta T_x = T_x - T_g$

In the supercooled liquid region, the arrangement of atoms the BMG becomes increasingly disordered, analogically the atomic arrangement in a liquid. The atoms in the supercooled region are unable to move freely like in a true liquid, this is because of the high viscosity ingrained in the non-crystalline structure / amorphous structure of BMGs. Even in the presence of disorder, the BMG retains its solid-state characteristics, this happens due to they are constrained by their positions.

The supercooled liquid region in BMGs is a unique phenomenon, emphasizing their ability to exhibit liquid-like behaviours and amorphous nature of these materials even at temperatures well below their conventional crystalline melting points. This special behaviour of BMG is important for its various applications, especially in areas where the unique combination of mechanical strength, low corrosion, thermal stability, and strength in electrical and magnetic properties offered by BMG is valuable.

Reduced Glass-Transition Temperature ($T_{rg} = T_g/T_l$)

The glass-transition temperature (T_g) is a critical temperature for non-crystalline / amorphous materials like BMGs. It is the temperature at which an amorphous material transitions from a brittle and hard state to a more ductile and rubbery state. The reduced glass-transition temperature (T_{rg}) is mathematically equal to the ratio of the glass-transition temperature (T_g) to the liquidus temperature (T_l).

i.e., $T_{rg} = \frac{T_g}{T_l}$

T_{rg} is a dimensionless parameter that gives an idea of how far above the temperature of the liquid state the glass transition is. A higher T_{rg} value signifies a more pronounced disparity between the temperatures of glass transition and the liquid state.

Analysis of Glass-Transition and Crystallization Temperature

The changes in crystallization temperature and glass transition temperature of different BMGs have been studied based on the following points.

(i) For the base element of the BMG or for elements that have the same crystal structure as the base element, the quantitively fraction of such elements increases. Meanwhile, the quantitively fraction of other elements with a crystal structure other than that of the base element decreases. In this case, the change in glass transition or crystallization temperature corresponds to any two identical changes in the coefficient of thermal expansion, thermal conductivity, and covalent radius. This situation gives the same result in the case when only one element in both the BMGs is partially replaced by another element of the same group and crystal structure.

(ii) For the base element of the BMG or for elements that have the same crystal structure as the base element, the quantitively fraction of such elements decreases. Meanwhile, the quantitively fraction of other elements with a crystal structure other than that of the base element increases. In this case, the change in glass transition or crystallization temperature is inversely related to any two identical changes in the coefficient of thermal expansion, thermal conductivity, and covalent radius.

(iii) For the base element of the BMG or for elements that have the same crystal structure as the base element, the quantitively fraction of such elements increases. Meanwhile, the quantitively fraction of other elements with a crystal structure other than that of the base element decreases or remains unchanged. In this case, changes in the glass transition or crystallization temperature are inversely related to corresponding similar changes in all three thermal expansion coefficient, thermal conductivity, and covalent radius.

(iv) For the base element of the BMG or for elements that have the same crystal structure as the base element, the quantitively fraction of such elements decreases. Meanwhile, the quantitively fraction of other elements with a crystal structure other than that of the base element increases or remains unchanged. In this case, changes in the glass transition or crystallization temperature correspond to similar changes in all three coefficients of thermal expansion, thermal conductivity and covalent radius.

(v) If there is no change in the quantitative fraction of the base element, then the quantitative fraction of elements with the same crystal structure as the base element increases in the BMG. Meanwhile, the quantitative fraction of elements with other structures decreases. In this case, the change in glass transition or crystallization temperature is reversed to any two or all identical changes in the coefficient of thermal expansion, thermal conductivity, and covalent radius.

(vi) If there is no change in the quantitative fraction of the base element, then the quantitative fraction of elements with the same crystal structure as the base element decreases in the BMG. Meanwhile, the quantitative fraction of elements with other structures increases. In this case, the change in glass transition or crystallization temperature is correspond to any two identical changes in the coefficient of thermal expansion, thermal conductivity, and covalent radius.

(vii) If there is no change in the quantitative fraction of the base element and of elements with the same crystal structure as the base element in the BMG. Meanwhile, the quantitative fraction of elements with other base element is decreases. In this case, the change in glass transition or crystallization temperature is reversed to any two identical changes in the coefficient of thermal expansion, thermal conductivity, and covalent radius.

(viii) If there is no change in the quantitative fraction of the base element and of elements with the same crystal structure as the base element in the BMG. Meanwhile, the quantitative fraction of two elements interchange with each other. In this case, the change in glass transition or crystallization temperature is reversed to any two identical changes in the coefficient of thermal expansion, thermal conductivity, and covalent radius. When a metal element interchanges with a non-metal element, BMG with a metallic element is placed first in the sequence. In the case of a metal element interchanging with another metal element, the element with a lower atomic mass in BMG is placed first in the sequence.

(ix) For the base element of the BMG, the quantitively fraction decreases and the quantitively fraction of the second base becomes zero. Meanwhile, the quantitively fraction of other elements with a crystal structure other than that of the base element increases. In this case, the change in glass transition or crystallization temperature is reversed to any two identical changes in the coefficient of thermal expansion, thermal conductivity, and covalent radius.

Note:

1. In BMG, that element is taken as the base element, whose quantitative fraction in BMG is maximum. But if there is no change in the base element, that element is taken as the base element from the rest of the other elements whose quantitative fraction is maximum in that BMG.

2. The points described above can also be applied to the case when there is a change in the fraction of the elements, but there is no consequential change in the crystal structure.
3. If the quantitative fraction of any two elements in BMG is the same, then that element is taken as the base element whose number of atoms is more, that is, the element whose atomic weight is less.
4. Elements should be replaced partially by others.

The following formula is used to calculate the quantitative value of thermal expansion coefficient, thermal conductivity and covalent radius-

$$x = \sum_i f_i x_i$$

Where: x stands for coefficient of thermal expansion or thermal conductivity or covalent radius. f_i means the quantitative fraction of the quantity x_i in BMG.

Element	Z	Crystal Structure	Thermal expansion μm/(m·K)	Thermal Conductivity W/(m·K)	Covalent Radius pm
Al	13	fcc	23.1	237	118
B	5	rhombohedral	β form: 5–7	27.4	82
Be	4	hcp	11.3	200	90
C	6	Graphite: simple hexagonal diamond: face-centered diamond-cubic	Diamond: 0.8	graphite: 119–165 diamond: 900–2300	77
Ce	58	B-dhcp, γ-fcc	6.3	11.3	165
Co	27	hcp	13	100	126
Cr	24	bcc	4.9	93.9	127
Cu	29	fcc	16.5	401	138
Er	68	hcp	12.2	14.5	189
Fe	26	fcc	11.8	80.4	125
Ga	31	orthorhombic	18	40.6	122
Hf	72	hcp	5.9	23	150
Ir	77	fcc	6.4	147	141
La	57	dhcp	12.1	13.4	169
Li	3	bcc	46	84.8	128
Lu	71	hcp	9.9	16.4	160

Mg	12	hcp	24.8	156	130
Mo	42	bcc	4.8	138	145
Nb	41	bcc	7.3	53.7	137
Ni	28	fcc	13.4	90.9	121
Os	76	hcp	5.1	87.6	144
P	15	bcc		white-0.236, black-12.1	106
Pd	46	fcc	11.8	71.8	131
Re	75	hcp	6.2	48	151
Rh	45	fcc	8.2	150	142
Ru	44	hcp	6.4	117	146
Si	14	Fc-diamond cubic	2.6	149	111
Ta	73	bcc	6.3	57.5	170
Ti	22	hcp	8.6	21.9	136
V	23	bcc	8.4	30.7	153
W	74	bcc	4.5	173	162
Y	39	hcp	10.6	17.2	162
Zn	30	hcp	30.2	116	131
Zr	40	hcp	5.7	22.6	148

Reference: website -https://en.wikipedia.org/wiki, and https://material-properties.org/.

Table 1: Chemical elements with crystal structure, the coefficient of thermal expansion (α), the value of thermal conductivity (W) and the covalent radius (R).

The coefficient of thermal expansion (α) for Zr, Al, Ni, Cu, and Y is 5.7, 23.1, 13.4,16.5, and 10.6 μm/(m·K) respectively. The quantitative fraction of the constituent elements Zr, Al, Ni, and Cu in BMG $Zr_{54}Al_{15}Ni_{10}Cu_{19}Y_2$ is 0.54, 0.15, 0.10, 0.19, and 0.02 respectively.

By using the formula- $\alpha = \sum_i f_i \, \alpha_i$

The value of coefficient of thermal expansion (α) in BMG $Zr_{54}Al_{15}Ni_{10}Cu_{19}Y_2$ is-

$\alpha = f_{Zr}\,\alpha_{Zr} + f_{Al}\,\alpha_{Al} + f_{Ni}\,\alpha_{Ni} + f_{Cu}\,\alpha_{Cu} + f_{Y}\,\alpha_{Y}$

$= 0.54 \times 5.7 + 0.15 \times 23.1 + .10 \times 13.4 + 0.19 \times 16.5 + .02 \times 10.6$

$= 11.23$ μm/(m·K)

The value of thermal conductivity (W) and the covalent radius (R) in BMG $Zr_{54}Al_{15}Ni_{10}Cu_{19}Y_2$ is 155.6467 W/(m·K), 140.479 pm respectively.

The value of the glass transition temperature (T_g), crystallization temperature (T_x), α, W, and R for various metallic glasses is shown in table 2.

S. No.	BMG	T_g (K)	T_x (K)	α {μm/(m·K)}	W {W/(m·K)}	R {pm}	reference
1.	$Zr_{54}Al_{15}Ni_{10}Cu_{19}Y_2$ #	714	787	11.23	133.378	139.18	3
2.	$Zr_{53}Al_{14}Ni_{10}Cu_{19}Y_4$ #	668	766	11.154	131.126	139.76	3
3.	$Zr_{55}Al_{8.9}Ni_{7.3}Cu_{28.8}$	684.6	765.2	10.921	155.647	140.479	3
4.	$Zr_{54.5}Al_{9.6}Ni_{8.4}Cu_{27.5}$	691.3	769.5	10.987	152.980	140.102	3
5.	$Pd_{40}Cu_{25}Ni_{15}P_{20}$	596	668	10.866	145.025	126.250	4
6.	$Pd_{40}Cu_{27.5}Ni_{12.5}P_{20}$	583	665	10.930	152.778	126.675	4
7.	$Ti_{20}Zr_{20}Cu_{30}Ni_{30}$	764*	-	11.83	156.47	134.5	5
8.	$Ti_{20}Zr_{20}Cu_{20}Ni_{40}$	785*	-	11.52	125.46	132.8	5
9.	$Zr_{48}Nb_8Cu_{14}Ni_{12}Be_{18}$	656	-	9.272	118.192	132.04	3
10.	$Zr_{48}Nb_8Cu_{12}Fe_8Be_{24}$	658	-	8.956	117.696	130.16	3
11.	$Zr_{48}Nb_2Cu_{14}Ni_{12}Be_{24}$	668	-	9.512	126.970	129.22	3
12.	$Zr_{48}Nb_8Cu_{14}Ni_{12}Be_{18}$	656	-	9.272	118.192	132.04	3
13.	$W_{46}Ru_{37}B_{15}Si_2$	1167	-	5.390	129.960	143.060	6
14.	$W_{46}Ru_{37}B_{12}Si_5$	1172	-	5.288	133.608	143.930	6
15.	$Zr_{41}Ti_{14}Cu_{12.5}Ni_8Be_{22.5}C_2$	628	-	9.218	117.529	128.44	3
16.	$Zr_{41}Ti_{14}Cu_{12.5}Ni_2Be_{22.5}C_8$	629	-	8.414	120.475	125.8	3
17.	$W_{56}Ir_{23}B_{21}$	1271	-	5.250	136.444	140.370	6
18.	$W_{44}Os_{40}B_{16}$	1298	-	4.980	115.544	142	6

-Thickness of BMGs rod is 5 mm.

* -Heating rate 20 K min^{-1}.

Table 2: Bulk metallic glasses with there glass transition temperature (T_g) and crystallization temperature (T_x).

The proportion of the base element Zr is in a decreasing order in the BMGs with serial numbers 1 and 2, namely $Zr_{54}Al_{15}Ni_{10}Cu_{19}Y_2$ and $Zr_{53}Al_{14}Ni_{10}Cu_{19}Y_4$.The fraction of the hexagonal close-packed (hcp) crystal structure in BMG $Zr_{53}Al_{14}Ni_{10}Cu_{19}Y_4$ increases regarding BMG $Zr_{54}Al_{15}Ni_{10}Cu_{19}Y_2$. This happens because the hcp crystal structure of the base element Zr, due to the similar hcp crystal structure of the other constituent element Y, is partially increased. The value of the coefficient of thermal expansion (α) and value of the thermal conductance (W) in BMGs $Zr_{54}Al_{15}Ni_{10}Cu_{19}Y_2$ and $Zr_{53}Al_{14}Ni_{10}Cu_{19}Y_4$ is 11.23, 133.378 and 11.154, 131.126 are in decreasing sequenced. While, the value of the covalent radius (R) in BMGs $Zr_{54}Al_{15}Ni_{10}Cu_{19}Y_2$ and $Zr_{53}Al_{14}Ni_{10}Cu_{19}Y_4$ is 140.479 and 140.102 pm is in increasing order. As per point (i) the glass transition or crystallization temperature of BMG $Zr_{53}Al_{14}Ni_{10}Cu_{19}Y_4$ must be less than that of the BMG $Zr_{54}Al_{15}Ni_{10}Cu_{19}Y_2$. The experimental value of the glass transition and crystallization temperature both of BMG $Zr_{53}Al_{14}Ni_{10}Cu_{19}Y_4$ and $Zr_{54}Al_{15}Ni_{10}Cu_{19}Y_2$ are 714 K and 787 K, 668 K and 766 K respectively. The experimental value of the glass transition and crystallization temperature both are higher for BMG $Zr_{54}Al_{15}Ni_{10}Cu_{19}Y_2$ than that of $Zr_{53}Al_{14}Ni_{10}Cu_{19}Y_4$.

The proportion of the crystal structure of the base element Zr is in a decreasing order in the BMGs with serial numbers 3 and 4, namely $Zr_{55}Al_{8.9}Ni_{7.3}Cu_{28.8}$ and $Zr_{54.5}Al_{9.6}Ni_{8.4}Cu_{27.5}$. The value of the α and W are increasing sequenced. While the value of R is decreasing in order. As per point (ii) the T_g or T_x of BMG $Zr_{54.5}Al_{9.6}Ni_{8.4}Cu_{27.5}$ must be greater than that of the BMG $Zr_{55}Al_{8.9}Ni_{7.3}Cu_{28.8}$. The experimental value of the T_g and T_x of both of BMGs $Zr_{55}Al_{8.9}Ni_{7.3}Cu_{28.8}$ and $Zr_{54.5}Al_{9.6}Ni_{8.4}Cu_{27.5}$ are 684.6 K and 765.2 K, 691.3 K and 769.5 K respectively, justify the point (ii).

The proportion of the crystal structure of the base element Pd is in a decreasing order in the BMGs with serial numbers 5 and 6, namely $Pd_{40}Cu_{25}Ni_{15}P_{20}$ and $Pd_{40}Cu_{27.5}Ni_{12.5}P_{20}$. The value of the α, W, and R all are increasing sequenced. As per point (iii) the T_g or T_x of BMG $Pd_{40}Cu_{25}Ni_{15}P_{20}$ must be greater than that of the BMG $Pd_{40}Cu_{27.5}Ni_{12.5}P_{20}$. The experimental value of the T_g and T_x of both of BMGs $Pd_{40}Cu_{25}Ni_{15}P_{20}$ and $Pd_{40}Cu_{27.5}Ni_{12.5}P_{20}$ are 596 K and 668 K, 583 K and 665 K respectively, justify the point (iii).

The proportion of the crystal structure of the base element Cu is in a decreasing order in the BMGs with serial numbers 7 and 8, namely $Ti_{20}Zr_{20}Cu_{30}Ni_{30}$ and $Ti_{20}Zr_{20}Cu_{20}Ni_{40}$. The value of the α, W, and R all are decreasing in order. As per point (iv) the T_g of BMG $Ti_{20}Zr_{20}Cu_{30}Ni_{30}$ must be less than that of the BMG $Ti_{20}Zr_{20}Cu_{20}Ni_{40}$. The experimental value of the T_g of both of BMGs $Ti_{20}Zr_{20}Cu_{30}Ni_{30}$ and $Ti_{20}Zr_{20}Cu_{20}Ni_{40}$ are 764 K and 785 K respectively, justify the point (iv).

The proportion of the crystal structure of the base element Zr is remains unchanged in the BMGs with serial numbers 9 and 10, namely $Zr_{48}Nb_8Cu_{14}Ni_{12}Be_{18}$ and $Zr_{48}Nb_8Cu_{12}Fe_8Be_{24}$. But in BMGs with sequence numbers 9 to 10, the order of crystal structure is increasing, similar to the base structure. The value of the α, W, and R all are decreasing in order. As per point (v) the T_g of BMG $Zr_{48}Nb_8Cu_{12}Fe_8Be_{24}$ must be less than that of the BMG $Zr_{48}Nb_8Cu_{14}Ni_{12}Be_{18}$. The experimental value of the T_g of both of BMGs $Zr_{48}Nb_8Cu_{14}Ni_{12}Be_{18}$ and $Zr_{48}Nb_8Cu_{12}Fe_8Be_{24}$ are 656 K and 658 K respectively, justify the point (v).

The proportion of the crystal structure of the base element Zr is remains unchanged in the BMGs with serial numbers 11 and 12, namely $Zr_{48}Nb_2Cu_{14}Ni_{12}Be_{24}$ and $Zr_{48}Nb_8Cu_{14}Ni_{12}Be_{18}$. But in BMGs with sequence numbers 9 to 10, the order of crystal structure is decreasing, similar to the base structure. The value of the α and W and are decreasing in order, while the value of the R is increasing in order. As per point (vi) the T_g of BMG $Zr_{48}Nb_8Cu_{14}Ni_{12}Be_{18}$ must be less than that of the BMG $Zr_{48}Nb_2Cu_{14}Ni_{12}Be_{24}$. The experimental value of the T_g of both of BMGs $Zr_{48}Nb_2Cu_{14}Ni_{12}Be_{24}$ and $Zr_{48}Nb_8Cu_{14}Ni_{12}Be_{18}$ are 668 K and 656 K respectively, justify the point (vi).

The proportion of the crystal structure of the base element W is remains unchanged in the BMGs with serial numbers 13 and 14, namely $W_{46}Ru_{37}B_{15}Si_2$ and $W_{46}Ru_{37}B_{12}Si_5$. But in BMGs with sequence numbers 13 to 14, the order of crystal structure remains unchanged, similar to the base structure. The value of the α is decreasing in order, while the value of the W and R are increasing in order. As per point (vii) the T_g of BMG $W_{46}Ru_{37}B_{12}Si_5$ must be greater than that of the BMG $W_{46}Ru_{37}B_{15}Si_2$. The experimental value of the T_g of both of BMGs $W_{46}Ru_{37}B_{15}Si_2$ and $W_{46}Ru_{37}B_{12}Si_5$ are 1167 K and 1172 K respectively, justify the point (vii).

The proportion of the crystal structure of the base element Zr is remains unchanged in the BMGs with serial numbers 15 and 16, namely $Zr_{41}Ti_{14}Cu_{12.5}Ni_8Be_{22.5}C_2$ and $Zr_{41}Ti_{14}Cu_{12.5}Ni_2Be_{22.5}C_8$. But Ni and C are interchanging only in these BMGs. The value of the α and R are decreasing in order, while the value of the W is increasing in order. As per point (viii) the T_g of BMG $Zr_{41}Ti_{14}Cu_{12.5}Ni_2Be_{22.5}C_8$ must be greater than that of the BMG $Zr_{41}Ti_{14}Cu_{12.5}Ni_8Be_{22.5}C_2$. The experimental value of the T_g of both of BMGs $Zr_{41}Ti_{14}Cu_{12.5}Ni_8Be_{22.5}C_2$ and $Zr_{41}Ti_{14}Cu_{12.5}Ni_2Be_{22.5}C_8$ are 628 K and 629 K respectively, justify the point (viii).

The proportion of the crystal structure of the base element W is in a decreasing order in the BMGs with serial numbers 17 and 18, namely $W_{56}Ir_{23}B_{21}$ and $W_{44}Os_{40}B_{16}$. The value

of the α and W both are decreasing in order, while the value of the R is increasing in order. As per point (ix) the T_g of BMG $W_{44}Os_{40}B_{16}$ must be greater than that of the BMG $W_{56}Ir_{23}B_{21}$. The experimental value of the T_g of both of BMGs $W_{56}Ir_{23}B_{21}$ and $W_{44}Os_{40}B_{16}$ are 1271 K and 1298 K respectively, justify the point (ix).

There is a list of bulk metallic glasses other than those above in which the glass transition temperature or crystallization temperature can be estimated at these points.

S. No.	**BMG**	**T_g** (K)	**T_x** (K)	**α** {μm/(m·K)}	**W** {W/(m·K)}	**R** {pm}	**reference**
1.	Zr54Al10.2Ni9.4Cu26.4	693.6	771.2	11.0498	150.787	139.762	3
2.	Zr53.5Al10.9Ni10.6Cu25	704.5	775.9	11.1128	147.809	139.368	3
3.	Zr53Al11.6Ni11.7Cu23.7	711.4	778.7	11.1789	145.142	138.991	3
4.	Zr52.5Al12.2Ni12.6Cu22.7	712.8	783.8	11.2446	143.259	138.668	3
5.	Tm55Al25Co20	678	-	15.69	88.545	159.2	4
6.	Tm39Y16Al25Co20	664	-	15.258	88.593	154.72	4
7.	Lu55Al25Co20	701	-	17.395	167.25	142.7	4
8.	Lu45Y10Al25Co20	698	-	16.815	152.97	142.9	4
9.	Lu39Y16Al25Co20	687	-	16.467	144.402	143.02	4
10.	(Ce80La20)68Al10Cu20Co2	355	-	10.0528	121.97	156.464	7
11.	Ce68Al10Cu20Co2	352	-	9.264	121.684	155.92	7
12.	W45 Re23Ru15B17	1273	-	5.431	111.098	143.47	6
13.	W37Ru31Rh18B14	1049	-	5.965	131.116	142.24	6
14.	W38lr17Ru31B14	1119	-	5.622	130.836	142.27	6
15.	Pd45Cu25Ni10P20	595	-	10.775	144.07	126.75	4
16.	Pd45Cu27.5Ni7.5P20	592	-	10.8525	151.823	127.175	4
17.	Pd45Cu30Ni5P20	577	-	10.93	159.575	127.6	4
18.	Fe69Mo7P12C10B2	716*	-	8.598	81.136	118.46	8
19.	Fe66Mo10P12C10B2	721*	-	8.388	82.864	119.06	8
20.	Fe64Cr3Mo10P10C10B3	729*	-	8.359	84.105	119.07	8

21.	Fe45Co3Cr15Mo14C15B6Y2	834#	-	7.679	95.573	119.09	8
22.	Fe43Co5Cr15Mo14C15B6Y2	835#	-	7.703	95.965	119.11	8
23.	Fe41Co7Cr15Mo14C15B6Y2	838#	-	7.727	96.357	119.13	8

* -Thickness of BMGs rod is 2.5 mm.

-Thickness of BMGs rod is 3 mm.

Table 3: BMGs with their T_g, T_x, α, W and R

There are some BMGs that partially follow these points like-

S. No.	**BMG**	**T_g** (K)	**T_x** (K)	**α** {μm/(m·K)}	**W** {W/(m·K)}	**R** {pm}	**reference**
1.	Mg65Cu25Y10	419	-	21.305	203.37	135.2	7
2.	Mg65Cu25Y9Gd1	423	-	21.293	203.304	135.19	7
3.	Mg65Cu25Y8Gd2	420	-	21.281	203.238	135.18	7
4.	Mg65Cu25Y5Gd5	422	-	21.245	203.04	135.15	7
5.	Mg65Cu25Gd10	421	-	21.185	202.71	135.1	7

Table 4: BMGs that partially follow with their T_g, T_x, α, W and R

Conclusion

There is a large list of BMGs whose variation in Tg and Tx values with partial changes in fraction of constituent elements can be determined using points 1 through 9. Some BMGs get partially correct results. A mathematical relation can also be found for how much change will happen in Tg and Tx values with partial changes in a fraction of constituent elements, and these points can also be used to estimate the elasticity coefficients and Poisson's ratio. Partially correct results are obtained in some BMGs, the estimation of the theoretical result can be improved by using Lennard-Jones potential, etc.

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