AIP | Journal of Applied Physics

Properties inheritance in metallic glasses

Wei Hua Wang

Citation: J. Appl. Phys. **111**, 123519 (2012); doi: 10.1063/1.4730441

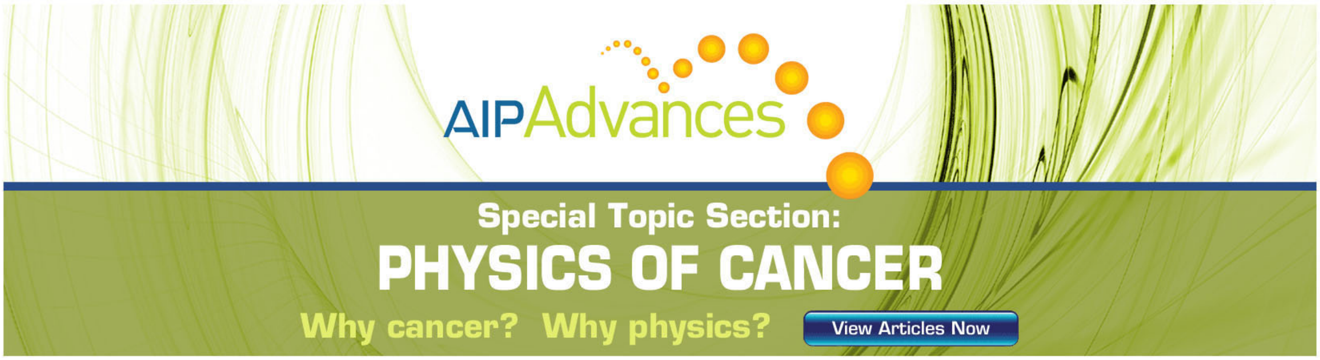
View online: http://dx.doi.org/10.1063/1.4730441

View Table of Contents: http://jap.aip.org/resource/1/JAPIAU/v111/i12

Published by the American Institute of Physics.

Related Articles

Additional information on J. Appl. Phys.



JOURNAL OF APPLIED PHYSICS **111**, 123519 (2012)

Properties inheritance in metallic glasses

Wei Hua Wang (汪卫华)[a)]
Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China

(Received 9 April 2012; accepted 21 May 2012; published online 25 June 2012)

It is widely accepted that the structural features of a metallic glass inherits from its liquid state. The survey of the elastic, plastic, mechanical and physical properties, and glass transition of various metallic glasses indicates that metallic glasses can inherit their properties from their solvent components (or base components). It is found that the elastic properties are mainly determined by the weakest solvent-solvent bonds in metallic glasses, and the plastic events and glass transition prefer to be initiated in the regions with high density of weak solvent-solvent bonds and propagate toward the regions with less density of solvent-solvent bonds in metallic glasses. Some physical properties of the metallic glasses are found to be determined by the electronic structure of the solvent components. The properties inheritance allows new understanding of the glassy structure as well as the properties and structure relationship in metallic glasses, and also indicates the hierarchical atomic bands and inhomogeneous microstructure in metallic glasses which is helpful for understanding the mechanisms of plastic and elastic deformations and glass transition in metallic glasses. © *2012 American Institute of Physics*. [http://dx.doi.org/10.1063/1.4730441]

I. INTRODUCTION

In contrast to conventional alloys, glassy alloys have liquid-like disordered structure which is regarded to inherit from their liquid state.[1–3] To understand and ultimately control the unique mechanical and physical properties of metallic glasses (MGs), it is vital to characterize their structure and their structure and properties relationship. Macroscopically, metallic glass is isotropic and homogeneous, however, it has atomic-scale short-range orders (SRO) and nanoscale medium-range orders (MRO), and the SRO of metallic glasses is a structural heredity of liquids.[1–5] The short-range orders in MGs are modeled by a cluster of solute atoms surrounded by a majority of solvent atoms, and the nanoscale MRO is described by highly structured superclusters consisting of interconnected clusters.[6–10] Both of the two types of orders of SRO and MRO affect the features and properties of MGs, but are extremely hard to distinguish. The way of atoms pack inside metallic glass and the role of the local atomic orders in physical and mechanical properties remain a mystery.[1–10] The current understanding of glassy structure relies to large extent on models and simulations.

The metallic glasses not only inherit disordered structure and SRO from the liquid state. It is recently found that Poisson's ratio of a glass is determined by the viscous character of its liquid, which demonstrates that the properties of a glass could be inherited from their liquid state.[11–13] The subtle structure and proprieties inheritance from liquids in metallic glass could help for understanding the nature and some fundamental issues in metallic glasses.

The elastic moduli as readily measurable parameters are the key physical parameter for controlling the main thermodynamic and kinetic, mechanical, and physical properties of metallic supercooled liquids and metallic glasses. The elastic moduli also offer a realistic and simple picture for understanding the glass transition and deformation, and the natures in MGs and MG-forming liquids.[14–24] It is found that the elastic moduli of a MG show a correlation with a weighted average of the elastic constants for the constituent elements.[17–20,25] That is, the moduli (M) of a MG can be approximated by a type of "rule of mixtures,"[17]

$$\frac{1}{M} = \sum \left(\frac{V_i \cdot f_i}{\sum V_i \cdot f_i} \cdot \frac{1}{M_i} \right). \tag{1}$$

Assuming all elements have the same atomic volume, the equation can be simplified to[17]

$$M^{-1} = \sum \left(f_i \cdot \frac{1}{M_i} \right), \tag{2}$$

where M_i is the modulus of constituent element, f_i is the atomic percent of element i, and V_{mi} is the atomic volume. The theoretically derived elastic moduli data for various MGs show rough consistency with their corresponding experimental ones.[17–20,25] However, very recently, it is found that some metallic glasses can inherit their moduli from their solvent components.[17,26,27] The elastic moduli inheritance suggests a hierarchy of atomic bonding structure in MGs,[26] and helps for revealing the structural secret of MGs, and allows a new understanding of complex metallic glassy structure and its relations with deformation and mechanical properties. The finding would promise fertile ground for deep studies in metallic glass field.

In this paper, we systematically investigate the elastic, mechanical, and physical properties of various MGs available and compare the properties of the MGs and their base elements. We find that not only the elastic properties but also the plasticity, some physical properties, glass transition, and even electronic structure in some metallic glasses can inherit

---

[a)] Author to whom correspondence should be addressed. Electronic mail: whw@iphy.ac.cn.

0021-8979/2012/111(12)/123519/8/$30.00

from their solvent components. The properties inheritance helps judge different structural features of MGs, and allows a new understanding of the relations between the glassy structure and properties, as well as the structural origins of plastic deformation and relaxations.

II. EXPERIMENTS

The bulk MGs samples were prepared by a copper mold suction casting method and the amorphous ribbons were obtained by melt spinning technique.[13,17] The glassy nature was identified by x-ray diffraction, and differential scanning calorimetry and transmission electron microscope. The MGs listed in Table I had a wide range of glass transition temperature, T_g, and significantly different in physical and mechanical properties. Uniaxial compression tests at room temperature were performed on an Instron 5500R1186 machine. Tests were carried out in a constant-crosshead-displacement-rate controlled manner. The samples with gauge aspect ratio (height/diameter) of 2:1 were cut out of the as-cast rods, and the two ends were polished to make them parallel to each other prior to the compression test. For each sample, sets of five measurements are repeated in compression tests.

Elastic moduli of these MGs were monitored using ultrasonic method. The glassy alloy rod ($\phi = 3$–8 mm) was cut to a length of about 8 mm and its ends were carefully polished flat and parallel. The acoustic longitudinal and transverse velocities (v_l and v_s) were measured using a pulse echo overlap method by a MATEC 6600 model ultrasonic system with a measuring sensitivity of 0.5 ns.[17] The excitation and detection of the ultrasonic pulses were provided by X- or Y-cut (for longitudinal and transverse waves, respectively) quartz transducers. The frequency of the ultrasonic is 10 MHz. The density was determined by the Archimedean technique with the accuracy of about 0.1%. The velocity measurements were repeated for each sample for several times to guarantee the minimize error. The elastic constants (the Yong's modulus E, the shear modulus G, and the bulk modulus K and Poisson's ratio ν) were derived from the density and acoustic velocities as follow: $G = \rho v_s^2$; $K = \rho (v_l^2 - 4/3\, v_s^2)$; $v = \rho(v_l^2 - 2v_s^2)/2(v_l^2 - v_s^2)$; $E = 2\,G(1+\nu)$.[17]

III. RESULTS AND DISCUSSIONS

The elastic properties including the elastic moduli of more than 200 various MGs have been systematically studied.[13,17,19,20,27–45] The data are collected in Table I of Ref. 17. We plot the comparison between the calculated Young's modulus (E_{cal}) by Eqs. (1) and (2) and the experimental data, and the results are presented in Fig. 1. Even though the experimental E_{MGs} data are from different groups measured by different methods which bring errors and some composition-dependent discrepancies may exist, it is clear form Fig. 1 that the results calculated by Eq. (1) or (2) are accord with the line $E_{MGs} = E_{cal}$ well, indicating the suitability of the "rule of mixture" for calculation of the elastic moduli of the metallic glasses. The derived elastic moduli data using the rule of mixtures for almost all MGs available show rough consistency with their corresponding experimental ones. However, there remains significant scatter with the data in Fig. 1, and the elastic moduli of some MG systems are obviously deviate from the rule of mixture.

By comparison of both Young's modulus E and shear modulus G of some MGs with their base components as shown in Fig. 2, it is found that both of the G and E of these MGs are almost equal to those of their base elements.[17,26] Figure 3 shows the comparison of Poisson's ratio ν between some MGs and their base metals. The ν also shows nearly a one-to-one correspondence between MGs and their base metals that extend over a broad range.[17] This indicates that the elastic properties of MGs are primarily determined by their base components or solvent components and only base components are responsible for the overall stiffness and rigidity of these MGs. In other words, metallic glasses essentially inherit the elastic moduli from their base components or solvents even though the base element normally makes up only half of such metallic glasses.

It is experimentally demonstrated that one can decompose a metallic glass into the strain-sensitive part of medium-range order (the superclusters), and the strain-insensitive part of short-range order (the solute-centered clusters).[26,46] The subtle elastic moduli inheritance implies that the MGs have a rubber-like structure which can be viewed as stiff solute-centered clusters like molecular units in rubber and much weaker solvent-solvent bonds linking the clusters.[26] The rubber-like structure of MGs can be simply modeled as stiff springs (represents the solute-solvent bonded cluster) connect in series with a much less stiff springs (represents the solvent-solvent bonding)[27] as shown in Fig. 4. The solvent-solvent bonds are simply modeled as the less stiff spring. The elastic and plastic deformation in MGs mainly occurs at the solvent-solvent junctions among the solute-centered clusters and/or superclusters, and the elastic moduli and mechanical properties are essentially determined by the weakest solvent-solvent bonding in MGs (Refs. 26, 27, and 46) as simply modeled in Fig. 5. Only less stiff spring accommodates strain in both metallic glasses and solvent metals, which shows the similar elastic moduli (moduli inheritance). The moduli inheritance confirms the hierarchical atomic banding structure and inhomogeneous atomic microstructure of MGs.

The elastic moduli inheritance has many interesting consequences. One immediate consequence is that the elastic moduli inheritance indicates possible other physical and mechanical properties inheritance in MGs. The elastic moduli have striking correlations with the mechanical properties of MGs.[13,14,17] It is therefore anticipated that MGs have physical and mechanical properties inheritances. It has long been known that in polycrystalline metals the ratio of G to K, alternatively the Poisson's ratio ν, correlates with their mechanical behaviors. That is, low K/G favours brittleness and vice versa.[47,48] The data of some polycrystalline pure metals provide a qualitative ranking from ductile (e.g., Ag, Au, Cd, Cu) to brittle behavior as K/G decreases.[47] On the other hand, the Poisson's ratio ν and plasticity correlation found in MGs suggest that plasticity and/or toughness is favored by high ν,[13,14,17] and the ν of MGs is also primarily determined by the solvent metals. The Zr-, Cu-, Au-, Pt-, Pd-based MGs as shown in Fig. 3 indeed have very similar high ν values and large plasticity to that of their base elements. The results

TABLE I. Data of E, G, σ_f, θ_D, and T_g collected on representative metallic glasses (all compositions in at. %) and the E, and G of the base metals of these metallic glasses. (Refs. 17 and 28–45.)

			E (GPa)		G (GPa)			
Glasses	Solvent or base metal	T_g (K)	Solvent	*MG*	Solvent	*MG*	σ_f (GPa)	θ_D (K)
$Zr_{41}Ti_{14}Cu_{12.5}Ni_{10}Be_{22.5}$	Zr	620	98	101	35	37.4	1.8	327
$Zr_{46.75}Ti_{8.25}Cu_{7.5}Ni_{10}Be_{27.5}$	Zr	623	98	100	35	37.2	1.83	327
$Zr_{65}Al_{10}Ni_{10}Cu_{15}$	Zr	652	98	83	35	30.3	1.45	267
$Zr_{52.25}Cu_{28.5}Ni_{4.75}Al_{9.5}Ta_5$	Zr	705	98	90	35	…	1.909	…
$Zr_{61}Cu_{17.3}Ni_{12.8}Al_{7.9}Sn_1$	Zr	665	98	77.4	35	28.2	1.77	256.7
$Zr_{57}Ti_5Cu_{20}Ni_8Al_{10}$	Zr	657	98	82	35	30.1	1.77	270.1
$Zr_{57}Nb_5Cu_{15.4}Ni_{12.6}Al_{10}$	Zr	687	98	87.3	35	31.9	1.8	274
$Zr_{35}Ti_{30}Cu_{8.25}Be_{26.75}$	Zr	578	98	86.9	35	31.8		
$Zr_{50}Cu_{25}Be_{25}$	Zr	633	98	96.8	35	35.8		
$Ti_{50}Cu_{23}Ni_{20}Sn_7$	Ti	681	116	85.3	44	…	1.3	…
$Ti_{50}Ni_{24}Cu_{20}B_1Si_2Sn_2$	Ti	726	116	110	44	…	2.1	…
$Ti_{45}Zr_{20}Be_{35}$	Ti	597	116	96.8	44	35.7	1.86	
$Ti_{45}Zr_{20}Be_{30}Cr_5$	Ti	602	116	105.6	44	39.2	1.72	
$Cu_{50}Zr_{50}$	Cu	733	130	85	48	32	1.92	231
$Cu_{50}Zr_{45}Al_5$	Cu	701	130	102	48	33.3	1.89	278
$Cu_{55}Zr_{30}Ti_{10}Co_5$	Cu	714	130	130	48	…	2.31	…
$Cu_{60}Hf_{30}Ti_{10}$	Cu	725	130	124	48	…	2.16	…
$Cu_{60}Hf_{10}\ Zr_{20}Ti_{10}$	Cu	754	130	101	48	36.9	1.95	282
$Pd_{40}Ni_{10}Cu_{30}P_{20}$	Pd	560	121	98	44	35.1	1.52	280
$Pd_{77.5}Si_{16.5}Cu_6$	Pd	630	121	96	44	34.8	1.55	250
$Pd_{40}Ni_{40}P_{20}$	Pd	583	121	108	44	38.6	1.7	292
$Pd_{64}Fe_{16}P_{20}$	Pd	630	121		44	33.1		256
$Pd_{80}Si_{20}$	Pd	607	121	70	44		1.34	
$Pd_{80}P_{20}$	Pd	607	121		44	27.1		224
$(Fe_{0.75}B_{0.2}Si_{0.05})_{96}Nb_4$	Fe	835	211	180	82	…	3.16	…
$[(Fe_{0.8}Co_{0.2})_{0.75}B_{0.2}Si_{0.05}]_{96}Nb_4$	Fe	830	211	205	82	…	4.17	…
$Fe_{61}Zr_8Y_2Co_6Mo_7Al_1B_{15}$	Fe	899	211	222	82			
$Ni_{45}Ti_{20}Zr_{25}Al_{10}$	Ni	733	200	114	76		2.37	
$Ni_{40}Cu_5Ti_{17}Zr_{28}Al_{10}$	Ni	762	200	133.9	76		2.3	
$Co_{43}Fe_{20}Ta_{5.5}B_{31.5}$	Co	910	209	268	…	…	5.185	…
$Co_{56}Ta_9B_{35}$	Co	945	209	240.6	…	91.5	5.80	
$Mo_{52}Cr_{14}Fe_{14}P_{12}B_8$	Mo	1135	329	…	…	…	…	
$Mo_{40}Co_{20}Fe_{20}B_{20}$	Mo	1108	329	…	…	…	…	
$W_{46}Ru_{37}B_{17}$	W	1151	411	309	161	…	…	…
$W_{46}Ru_{37}B_{12}Si_5$	W	1110	411	229	161			
$W_{45}Ru_{36}B_{17}Hf_2$	W	1129	411	262	161			
$Mg_{65}Cu_{25}Tb_{10}$	Mg	417	45	51.3	17	19.6	0.80	272.9
$Mg_{65}Y_{10}Cu_{15}Ag_5Pd_5$	Mg	437	45	59	17		0.77	
$Mg_{65}Cu_{20}Y_{15}$	Mg	420	45	69	17		0.82	
$Sr_{60}Li_5Mg_{15}Zn_{20}$	Sr	331	18	19.7	6.1	7.71	0.30	156
$Al_{88}Ni_9Ce_2Fe_1$	Al	520	70	$\sim$70	26		1.35	
$Ca_{65}Ag_{35}$	Ca	400	20	20	7.4			
$Ca_{57}Mg_{19}Cu_{24}$	Ca	387	20	38	7.4		0.545	
$Ca_{65}Li_{9.96}Mg_{8.54}Zn_{16.5}$	Ca	320	20	23.4	7.4	8.95	0.53	220.7
$Ce_{70}Al_{10}Ni_{10}Cu_{10}$	Ce	359	34	30	14	11.5	0.40	144.1
$Nd_{60}Al_{10}Fe_{20}Co_{10}$	Nd	493	41	51	16	35.1	0.45	189
$Gd_{36}Y_{20}Al_{24}Co_{20}$	Gd	603	55	62.2	22	23.6		221.4
$Ho_{39}Al_{25}Co_{20}Y_{16}$	Ho	649	65	69.1	26	26.2		226.5
$Ho_{55}Al_{25}Co_{20}$	Ho	649	65	66.64	26	25.42	0.87	210
$Tm_{39}Al_{25}Co_{20}Y_{16}$	Tm	664	74	75.0	31	29.4	1.98	236
$Lu_{45}Y_{10}Al_{25}Co_{20}$	Lu	689	69	79.1	27	31.1	1.89	231
$Yb_{62.5}Zn_{15}Mg_{17.5}Cu_5$	Yb	381	24	26.5	9.9	10.4		132
$La_{55}Al_{25}Cu_{10}Ni_5Co_5$	La	466	37	41.9	14	15.6	$\sim$0.5	183
$La_{55}Al_{25}Co_{20}$	La	477	37	40.9	14	15.42	0.99	181
$Pr_{55}Al_{25}Co_{20}$	Pr	509	37	45.90	15	17.35	1.01	190
$Tb_{55}Al_{25}Co_{20}$	Tb	612	56	59.53	22	22.85	0.83	203
$Dy_{55}Al_{25}Co_{20}$	Dy	635	61	61.36	25	23.52	0.72	205
$Er_{55}Al_{25}Co_{20}$	Er	667	70	70.72	28	27.08	1.12	215

TABLE I. (*Continued.*)

Glasses	Solvent or base metal	T_g (K)	*E* (GPa)		*G* (GPa)		σ_f (GPa)	θ_D (K)
			Solvent	*MG*	Solvent	*MG*		
$Au_{76.9}Si_{9.45}Ge_{13.66}$	Au	297	78		27	…		240
$Au_{49}Ag_{5.5}Pd_{2.3}Cu_{26.9}Si_{16.3}$	Au	401	78	74.4	27	26.5		
$Au_{70}Cu_{5.5}Ag_{7.5}Si_{17}$	Au	339	78		27			
$Pt_{60}Ni_{15}P_{25}$	Pt	485	74	96	29	33.8		205
$Pt_{60}Cu_{16}Co_2P_{22}$	Pt	506	74	∼96	29		1.1	206
$Pt_{74.7}Cu_{1.5}Ag_{0.3}P_{18}B_4Si_{1.5}$	Pt	479	74		29	32.4	1.20	
$Pt_{57.5}$Cu14.7$Ni_{5.3}P_{22.5}$	Pt	508	74	94.8	29	33.3	1.4	206

indicate that the MGs have plasticity inheritance, and the properties inheritance can be guidance for designing new glasses with desired properties through the appropriate choice of solvent elements with suitable ν.

The properties inheritance is helpful for understanding some found experimental phenomena and can be used to distinguish the metallic glasses with different bonding characteristics. For some systems such as Pd-, Cu- and Co-based glasses, their moduli are markedly different from those of their base components. For example, the moduli of $Cu_{60}Zr_{20}Hf_{10}Ti_{10}$ glass are not close to that of its base component of Cu.[19,27] Nevertheless, such deviations can help to understand different microstructural features of MGs. For example, the elastic moduli of $Cu_{50}Zr_{50}$ glass are not close to those of its component Cu

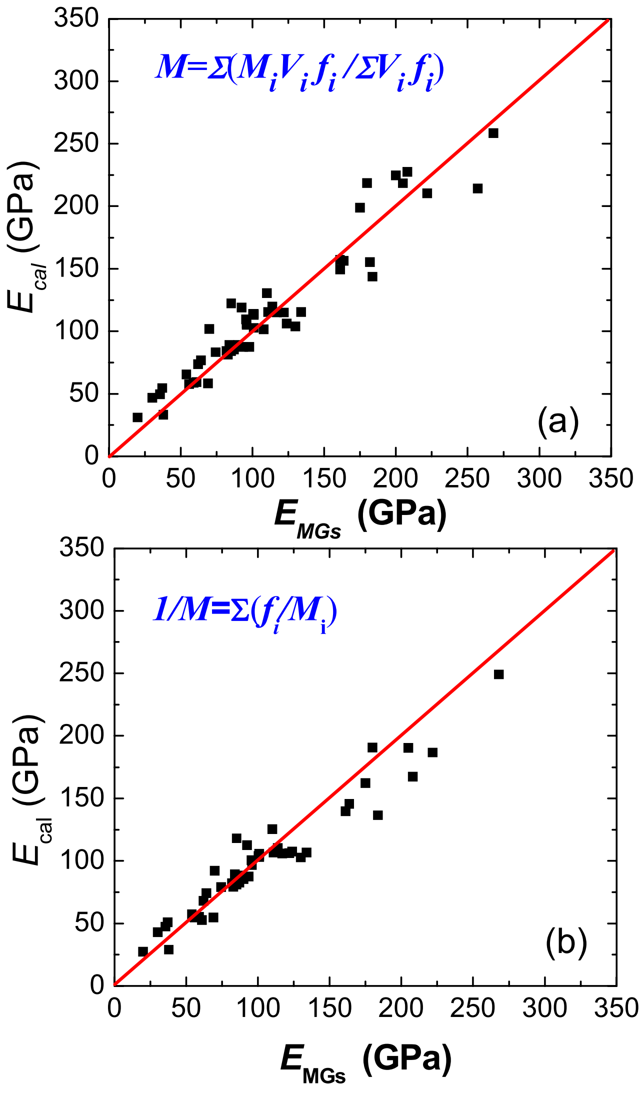


FIG. 1. The comparison the calculated Young's modulus (E_{cal}) by Eq. (1) (a) and Eq. (2) (b) with the experimental moduli data of various MGs.

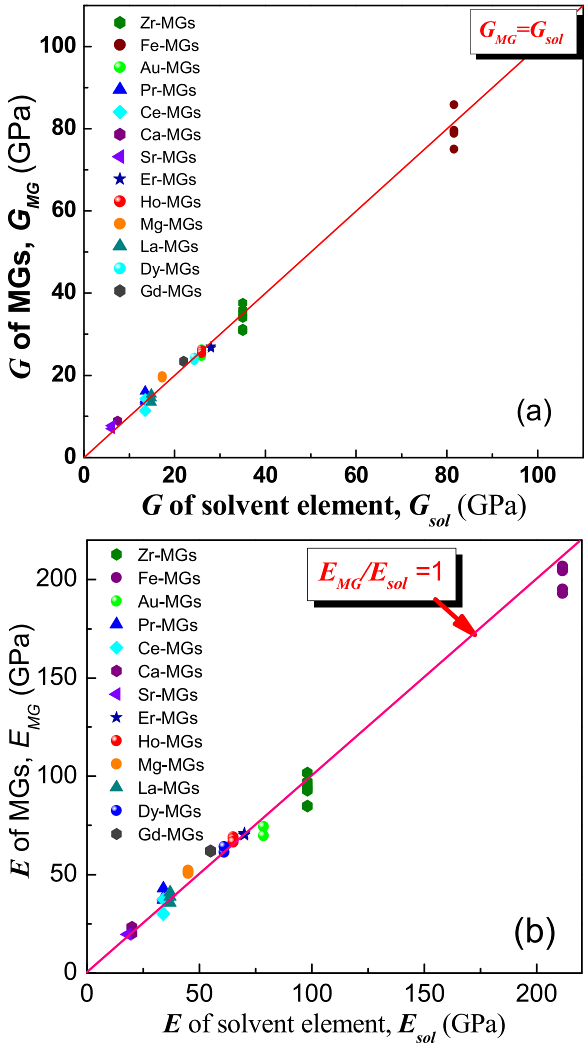


FIG. 2. (a) The average ratio of shear modulus for various metallic glasses (G_{MG}) and their solvents (G_{sol}) and (b) the average ratio of Young's modulus for various metallic glasses (E_{MG}) and their solvents (E_{sol}) are both close to 1, indicating moduli of glasses are primarily determined by base metals.

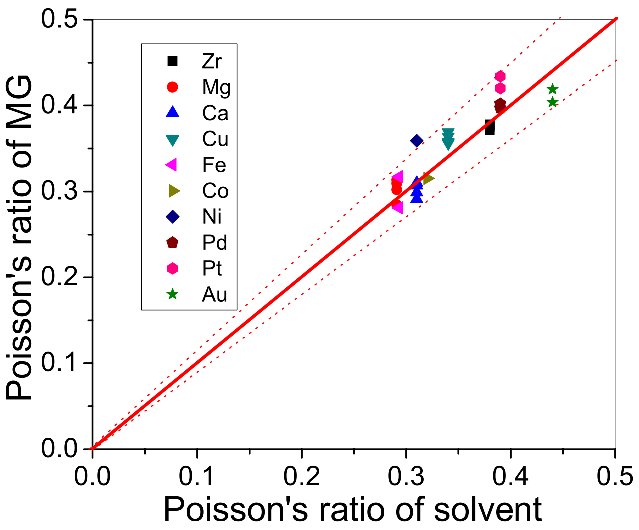


FIG. 3. The comparison of the Poisson's ratios for various metallic glasses and their solvents. Their ratio is also close to 1, indicating the Poisson's ratio of MGs is primarily determined by solvent metals.

but close to those of Zr, indicating that Zr and not Cu is its solvents which has been confirmed by structure study.[49–51] The moduli inheritance can help for understanding the structural change induced by such as minor addition. The alloying of metalloid elements can induce obvious deviation from the elastic moduli correlations.[45] The deviation suggests that the metalloid elements form covalent-like bonding in metallic glasses which changes the atomic structure by strengthening and shortening the atomic bonds according to the moduli inheritance.

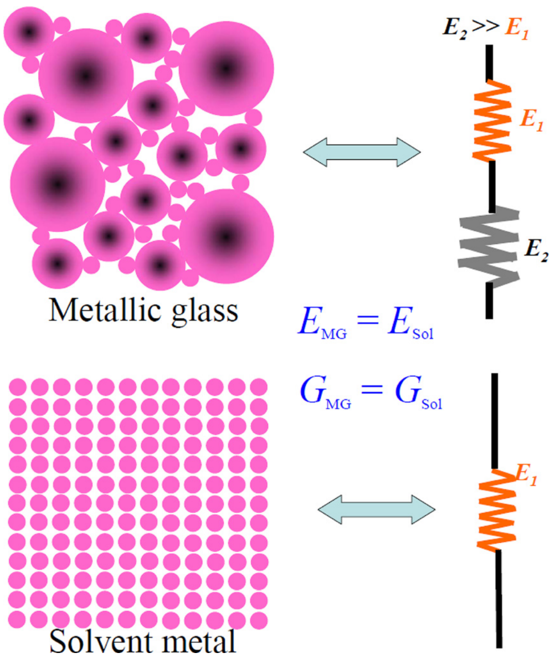


FIG. 4. Metallic glass is simply modeled as a stiff spring (represents the solute-solvent bonded cluster, modulus E_2) connects in series with a much less stiff spring (represents the solvent-solvent bonding, modulus E_1). The solvent metal is simply modeled as the less stiff spring (E_1). The MG is regarded as local packing of solvent atoms (the smallest ball), solute-centered clusters (middle size ball), and superclusters (the largest ball).[26] The darker color in big ball denotes the outmost atomic shell filled with a majority of solvent atoms.

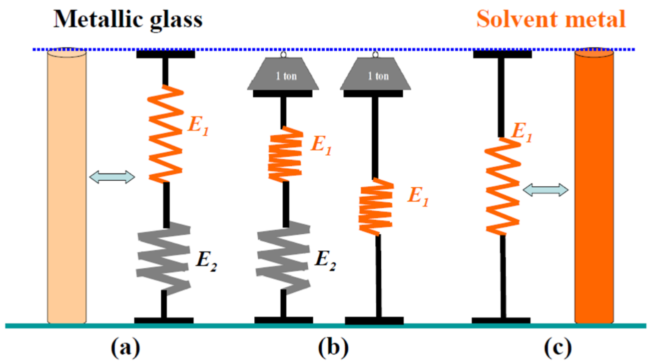


FIG. 5. The simple model shows the elastic deformation in metallic glass. (a) The MG is modeled as a stiff spring connects in series with a much less stiff spring. (b) Under the application of a force such as one ton only the less stiff spring accommodates strain in MG. Therefore, both the MG and the base metal show the similar elastic moduli (or moduli inheritance). (c) The solvent metal is simply modeled as the less stiff spring (E_1).

Due to the elastic moduli of MGs mainly depend on the weak solvent-solvent bonds and correlate with mechanical properties, the minor changes in atom components (e.g., through microalloying) may result in significant bonding changes of a MG and accordingly influence the mechanical properties.[52,53] For example, the moduli of the $Mg_{65}Cu_{25}Y_{10}$ MG are close to its solvent component Mg and the MG has moduli inheritance. It is found that the fracture strength of Mg-based MGs can be dramatically enhanced from 0.68 to 1.1 GPa, and the Poisson's ratio ν of the MG also decreases from 0.329 to 0.261 close to that of brittle oxide glasses when 1 at. % Gd was added (as shown in Table II and Fig. 6). Such significant change in strength, dramatically decrease in the Poisson's ratio, E and G according to the moduli inheritance can be attributed to the bonding changes of the MGs induced by the Gd minor addition. The Gd minor addition changes the weak solvent-solvent bonding structure between clusters in the Mg-based MG which derive in the change of elastic and mechanical properties.[53] Therefore, based on the found property inheritances, the strategy for the design of MGs with desired properties can be obtained. For example, the ductile metallic glasses can be obtained through minor substitution some exceptional "soft" atoms which form weaker bonding comparing with solvent-solvent bonds. The MGs then have some local atomic bonds with less shear resistant, and such a locally modified structure results in topological heterogeneity, which appears to be crucial for achieving enhanced the overall plasticity.[52]

The properties inheritance is helpful for better understanding not only the atomic and bonding structures, the

TABLE II. The Gd addition induced changes in density ρ, G, bulk modulus K, E, and Poisson's ratio ν, and fracture strength σ_f of $Mg_{65}Cu_{25}Y_{10-x}Gd_x$ (x = 0, 1, 2, 5, 10).

MG	ρ (g/cm^3)	G (GPa)	E (GPa)	K (GPa)	ν	σ (GPa)
$Mg_{65}Cu_{25}Y_{10}$	3.284	18.9	50.1	48.8	0.329	0.68
$Mg_{65}Cu_{25}Y_9Gd_1$	3.336	19.5	49.2	34.3	0.261	1.06
$Mg_{65}Cu_{25}Y_8Gd_2$	3.429	20.1	51.7	39.9	0.284	1.03
$Mg_{65}Cu_{25}Y_5Gd_5$	3.650	19.7	50.6	39.1	0.284	1.11
$Mg_{65}Cu_{25}Gd_{10}$	3.79	19.3	50.6	45.1	0.313	0.83

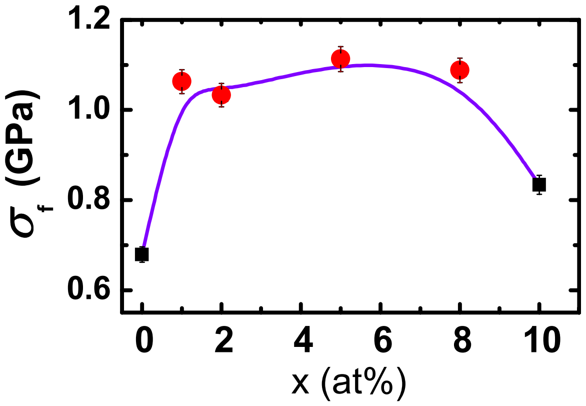


FIG. 6. Fracture stress σ_f of $Mg_{65}Cu_{25}Y_{10-x}Gd_x$ system versus the concentration (x) of Gd. The maximum σ_f is 1.11 GPa for $Mg_{65}Cu_{25}Y_5Gd_5$, which is about 1.7 times of $Mg_{65}Cu_{25}Y_{10}$ and 1.3 times of $Mg_{65}Cu_{25}Gd_{10}$. The blue line is for guiding the eyes.

origin of elasticity and mechanical properties, but also the structural origin of irreversible plastic deformation and glass transitions of metallic glasses. Despite the long research history of plastic mechanism and glass transition of disordered metallic glasses, understanding their structural origins currently remains at the frontier of condensed matter physics and material science. In the past decade, tremendous efforts were devoted to revealing the primary flow units in MGs by theoretic analysis, experiments, and simulation.[54–64] Several types of flow units, such as the free volume and shear transformation zones (STZs), which were generally considered as relatively loosely bonded atomic clusters, were postulated.[54,55] However, the accurate physical picture describing the plastic deformation mechanisms and structural origin of the relaxations of MGs are still absent. Theories proposed that structural heterogeneity like defects acts as flow units which accommodate plastic deformation or initiate glass transition in glasses,[17,21,56,64] and the activation energy of flow units is uniquely related to elastic modulus G.[14,17,44] The potential energy barrier for an unsheared flow unit can be estimated as[14]: $W = (8/\pi^2)G\gamma_c^2\zeta\Omega$, where G the shear modulus, Ω the average volume of a flow unit, $\gamma_c \approx 0.027$ the average elastic limit, and $\zeta \approx 3$ a correction factor arising from the matrix confinement of a "stressed" flow unit.[14] Microscopically, the elastic moduli reflect the inherent stiffness of atomic bonds.[17] Therefore, the subtle shear modulus inheritance implies that the activation of flow units in metallic glasses should closely relate to the softening of the solvent-solvent bonding in the flow units, and the plastic deformation and glass to supercooled liquid transition in MGs mainly initiates at the solvent-solvent junctions among solute-centered clusters and/or superclusters,[26,27,46] and the initiation of flow induced both by stress (deformation) and temperature (glass transition) are essentially determined by the weakest solvent-solvent bonding as simply modeled in Fig. 5. The moduli inheritance promotes further advances in understanding the long-standing issues of plastic deformation and glass transition.

A simple picture on the relation between the formation or evolution of flow units and the atomic bands and inhomogeneous microstructure can be proposed based on the hierarchical atomic bonding structure. The conventional wisdom of the flow units in MGs is that it occurs in soft "defects" which show low elastic moduli and atomic density, and the bonding information and evolution process about the flow units are unclear. According to the moduli inheritance and structural model of MGs (see Fig. 5), the activation or the spatially heterogeneous irreversible rearrangement of the atoms in flow units occurs only in the solvent-solvent junction bonding among the solute-centered clusters. The local flow events only break the weakest solvent-solvent bonds, and the irreversible rearrangement of the atoms in flow units (i.e., the plastic events) prefers to be initiated in the regions containing high density solvent-solvent bonds due to the activation energy of flow events are determine by G which is close to the G of solvent. In other words, the soft regions where the flow units prefer to be initiated consists more weakly bonded solvent atoms. The heterogeneity of the local atomic structure corresponds to the hierarchical atomic bonding structure and leads to the heterogeneity of the mechanical response found in MGs. Due to the heterogeneity of the local atomic structure and the hierarchical atomic bonding structure, the stiff and soft springs in MGs have an inhomogeneous distribution according to the strings model of MGs. The regions with high density of weak solvent-solvent bonds (soft springs) can accommodate larger plastic deformation, and the irreversible rearrangement is more difficult to be induced in the regions with low density of soft springs, and the plastic events prefer to be initiated in the regions with high density of solvent-solvent bonds and propagate toward the region with low density of solvent-solvent bonds in MGs as strain is increasing. The density of solvent-solvent bonds is the indicator to predict the local plastic deformation. The hierarchical atomic bonding structure and the heterogeneity of the local atomic structure lead to the inhomogeneous plastic deformation in MGs. The results provide evolution information on the flow units and clarify the atomic bonding structure and atom composition of flow units in MGs.

It is generally known that the T_g is dominated by the bonding forces among the components, and T_g of various MGs shows a clear linear relationship with G or E or Debye temperature θ_D.[13,28–30] Figure 7 shows T_g versus E and G of solvent element of various MGs available. The MGs as listed in Table I include Zr-, Cu-, Pd-, Fe-, Co-, Mo-, W-, Mg-, Sr-, Al-, Ca-, Nd-, Gd-, Ho-, Dy-, Tm-, La-, Tb-, Ce-, Er-, Au-, and Pt-based MGs. One can see that the T_g and E or G of solvent element or base component roughly have a linear relationship, and is similar to the correlation between T_g and E of MGs. The survey indicates that the T_g is also mainly determined by the solvent-solvent bonds, and the glass transition relates to the inheritance. The glass state to supercooled liquid state transition can be regarded as the broken of the weakest solvent-solvent bonding in the MGs corresponding to the decrease of G to 0. This has been proven by the dynamic mechanical analysis of glass transition of MGs.[31] On the other hand, the liquid to glass state transition can be considered as the bonded process of the solvent atoms.

The metallic glasses can also inherit the electronic structure of the solvent atom. Recently, polyamorphic transitions have been evidenced in Ce-based MGs upon application of

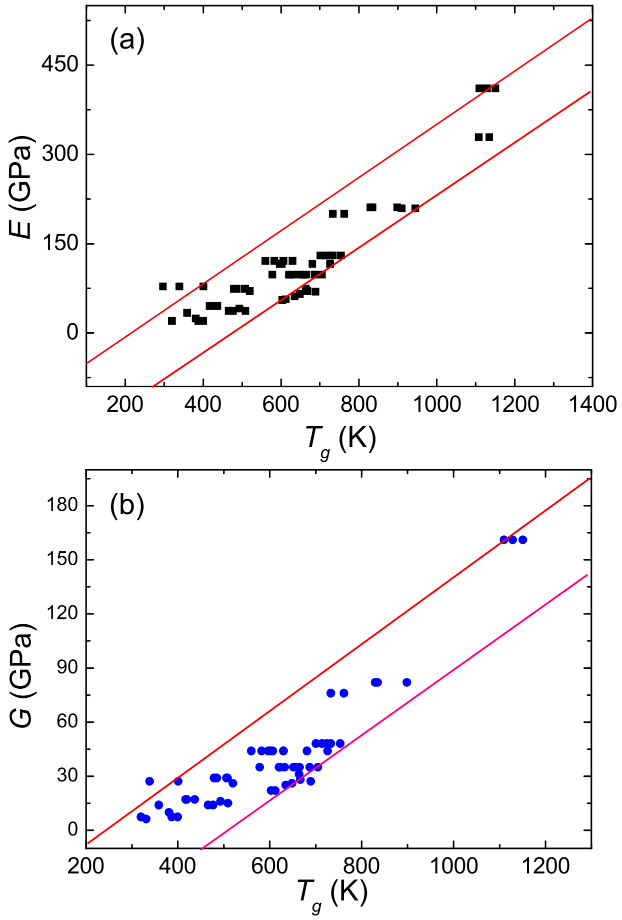


FIG. 7. The T_g versus E (a) and G (b) of various MGs listed in Table I.

pressure in the 2–13.5 GPa range.[65–68] Actually, crystalline Ce exhibits a polymorphic transition originated by the 4*f* electrons strong correlation.[69,70] Experimentally, the fcc α phase of Ce transforms into a fcc γ phase when temperature is increased and the transformation is linked to a large change in the volume. When pressure is applied at room temperature, the isostructural phase transition is observed accompanied with a decrease in volume of 15%. This structural behavior has been linked to the electronic behavior of the 4*f* electrons of Ce and pressure induced delocalization was observed. This polyamorphic transition of Ce-based MGs is similar to the behavior observed in the phase transformation in crystalline cerium which is a pressure-driven change in the localization of 4*f* Ce electronic states.[69,70] The particular electronic band structure change induced by pressure of Ce would therefore be expected to affect the pressure behavior of Ce-based amorphous alloys in the same manner and drive the polyamorphic transition. In other words, the pressure-driven polyamorphic transition in the Ce-based MGs inherits from the solvent Ce atoms. Therefore, it is anticipated that polyamorphic transitions could be found in other metallic glasses systems if their solvent components have pressure or temperature driven polymorphic transitions.

The idea of the metallic glasses can inherit the electric properties of the base components, a strategy based on the properties inheritance can be used for fabrication of a series of MGs with various functional physical properties.[32] For example, due to the good magnetocaloric effect of Gd, Er, Ho, and Dy, the Gd-, Ho-, Dy- and Er-based bulk metallic glasses with excellent magnetocaloric effect in helium and hydrogen liquefaction temperature range have been fabricated.[71–74] The Nd, Sm, and Pr have hard magnetism, the Nd(Pr, Sm)-based MGs have been found to have hard magnetic properties at room temperature.[75–77] In Ce- and Yb-based MGs, remarkable heavy fermions behaviors are observed which is similar to the heavy fermions behaviors in Ce and Yb alloys.[78,79] The superconductivity can be found in the MGs systems with superconductive solvent elements such as La, Zr, and Cu.[32,80]

IV. CONCLUSIONS

The metallic glasses have various hereditary traits. Their properties such as elastic property, plasticity, and toughness, glass transition, and even electronic properties are primarily determined by or inherit from their solvent components or base metals. The phenomena can be attributed to the hierarchical atomic bands and inhomogeneous microstructure of metallic glasses. And the hierarchical atomic bands structure of MG can be simply modeled as stiff springs representing the solute-solvent bonded cluster connect with a much less stiff springs representing the solvent-solvent bonding. The found properties inheritance allows new understanding the bonding and heterogeneity structure of metallic glasses, the structure and properties relationship, and structural origins of elastic and plastic deformation and glass transition in metallic glasses.

ACKNOWLEDGMENTS

This work was supported by MOST 973 of China (No. 2010CB731603) and the NSF of China (No. 50921091). The useful discussions and experimental help from X. L. Wang, R. J. Wang, D. Q. Zhao, D. W. Ding, H. Y. Bai, and P. Wen are appreciated.

[1] Y. Waseda, *The Structure of the Non-crystalline Materials, Liquid and Amorphous Solids* (McGraw-Hill, New York, 1980).
[2] J. D. Bernal, Nature (London) **185**, 68 (1960).
[3] R. Wang, Nature (London) **278**, 700 (1979).
[4] W. H. Wang, E. Wu, R. J. Wang, S. J. Kennedy, and A. J. Studer, Phys. Rev. B **66**, 104205 (2002).
[5] D. Holland-Moritz, D. M. Herlach, and K. Urban, Phys. Rev. Lett. **71**, 1196 (1993).
[6] D. B. Miracle, Nature Mater. **3**, 697 (2004).
[7] D. Ma, A. D. Stoica, and X. L. Wang, Nature Mater. **8**, 30 (2009).
[8] A. Hirata, P. F. Guan, T. Fujita, Y. Hirotsu, A. Inoue, A. R. Yavari, T. Sakurai, and M. W. Chen, Nature Mater. **10**, 28 (2011).
[9] Y. Q. Cheng and E. Ma, Prog. Mater. Sci. **56**, 379 (2011).
[10] X. D. Hui, X. Liu, H. Hou, and G. L. Chen, Sci. China, Ser. G **51**, 400 (2008).
[11] J. Dyre, Nature Mater. **3**, 749 (2004).
[12] V. N. Novikiv and A. P. Sokolov, Nature **431**, 961 (2004).
[13] W. H. Wang, J. Appl. Phys. **99**, 093506 (2006).
[14] J. S. Harmon, W. L. Johnson, and K. Samwer, Phys. Rev. Lett. **99**, 135502 (2007).
[15] J. C. Dyre, Rev. Mod. Phys. **78**, 953 (2006).
[16] J. J. Lewandowski, W. H. Wang, and A. L. Greer, Philos. Magn. Lett. **85**, 77 (2005).
[17] W. H. Wang, Prog. Mater. Sci. **57**, 487 (2012).
[18] S. V. Nemilov, J. Non-Cryst. Solids **352**, 2715 (2006).
[19] W. H. Wang, J. Appl. Phys. **110**, 053521 (2011).

[20] W. H. Wang, J. Non-Cryst. Solids **351**, 1481 (2005).

[21] H. Wagner, B. Zhang, and K. Samwer, Nature Mater. **10**, 439–442 (2011).

[22] M. Q. Jiang and L. H. Dai, Phys. Rev. B **76**, 054204 (2007).

[23] J. Q. Wang, W. H. Wang, and H. Y. Bai, J. Non-Cryst. Solids **357**, 223 (2011).

[24] S. J. Poon, A. Zhu, and G. J. Shiflet, Appl. Phys. Lett. **92**, 261902 (2008).

[25] Z. Zhang, R. J. Wang, L. Xia, and W. H. Wang, J. Phys.: Condens. Matter **15**, 4503 (2003).

[26] D. Ma, A. D. Stoica, X.-L. Wang, Z. P. Lu, B. Clausen, and D. W. Brown, Phys. Rev. Lett. **108**, 085501 (2012).

[27] W. H. Wang, Nature Mater. **11**, 275 (2012).

[28] W. H. Wang, P. Wen, and R. J. Wang, J. Mater. Res. **18**, 2747 (2003).

[29] B. Yang, C. T. Liu, and T. G. Nieh, Appl. Phys. Lett. **88**, 221911 (2006).

[30] Y. H. Liu, C. T. Liu, W. H. Wang, A. Inoue, and M. W. Chen, Phys. Rev. Lett. **103**, 065504 (2009).

[31] Z. F. Zhao, P. Wen, C. H. Shek, and W. H. Wang, Phys. Rev. B **75**, 174201 (2007).

[32] W. H. Wang, Adv. Mater. **21**, 4524 (2009).

[33] S. Li, R. J. Wang, D. Q. Zhao, and W. H. Wang, J. Non-Cryst. Soilds **354**, 1080 (2008).

[34] Y. H. Liu, G. Wang, R. J. Wang, D. Q. Zhao, and W. H. Wang, Science **315**, 1385 (2007).

[35] W. H. Wang, Q. Wei. M. P. Macht, and H. Wollenberger, Appl. Phys. Lett. **71**, 1053 (1997).

[36] W. H. Wang, M. X. Pan, D. Q. Zhao, and H. Y. Bai, J. Phys.: Condens. Matter **16**, 3719 (2004).

[37] W. H. Wang, Z. X. Bao, and J. Eckert, Phys. Rev. B **61**, 3166 (2000).

[38] V. Ponnambalam, S. J. Poon, and G. J. Shiflet, J. Mater. Res. **19**, 3046 (2004).

[39] J. Schroers and W. L. Johnson, Appl. Phys. Lett. **87**, 061912 (2005).

[40] E. F. Lambson, W. A. Lambson, and D. Turnbull, Phys. Rev. B **33**, 2380 (1986).

[41] M. Ohtsuki, R. Tamura, S. Yoda, and T. Ohmura, Appl. Phys. Lett. **84**, 4911 (2004).

[42] J. S. Harmon, M. D. Demetriou, and W. L. Johnson, Appl. Phys. Lett. **90**, 171923 (2007).

[43] W. H. Wang, J. J. Lewandowski, and A. L. Greer, J. Mater. Res. **20**, 2307 (2005).

[44] J. Q. Wang, W. H. Wang, Y. H. Liu, and H. Y. Bai, Phys. Rev. B **83**, 012201 (2011).

[45] J. Q. Wang, W. H. Wang, and H. Y. Bai, J. Non-Cryst. Solids **357**, 220 (2011).

[46] G. Wang, N. Mattern, J. Bednarčík, R. Li, B. Zhang, and J. Eckert, Acta Mater. **60**, 3074 (2012).

[47] S. S. Hecker, D. L. Rohr, and D. F. Stein, Metall. Trans. A **9**, 481 (1978).

[48] S. F. Pugh, Philos. Mag. **45**, 823 (1950).

[49] H. L. Peng, M. Z. Li, W. H. Wang, and C. Z. Wang, Appl. Phys. Lett. **96**, 021901 (2010).

[50] Y. Q. Cheng, H. W. Sheng, and E. Ma, Phys. Rev. B **78**, 014207 (2008).

[51] W. H. Wang, Q. Wei, and S. Friedrich, Phys. Rev. B **57**, 8211 (1998).

[52] N. Zheng, R. T. Qu, S. Pauly, M. Calin, T. Gemming, Z. F. Zhang, and J. Eckert, Appl. Phys. Lett. **100**, 141901 (2012).

[53] W. H. Wang, Prog. Mater. Sci. **52**, 540 (2007).

[54] A. S. Argon, Acta Metall. **27**, 47 (1979).

[55] F. Spaepen, Acta Metall. **23**, 407 (1977).

[56] J. C. Ye, J. Lu, C. T. Liu, and Y. Yang, Nature Mater. **9**, 619–622 (2010).

[57] M. L. Falk and J. S. Langer, Phys. Rev. E **57**, 7192 (1998).

[58] F. Delogu, Phys. Rev. Lett. **100**, 255901 (2008).

[59] H. B. Yu, Z. Wang, L. Gu, W. H. Wang, and H. Y. Bai, Phys. Rev. Lett. **108**, 015504 (2012).

[60] H. B. Yu, W. H. Wang, H. Y. Bai, Y. Wu, and M. W. Chen, Phys. Rev. B **81**, 220201 (2010).

[61] H. L. Peng, M. Z. Li, and W. H. Wang, Phys. Rev. Lett. **106**, 135503 (2011).

[62] D. Rodney and C. Schuh, Phys. Rev. Lett. **102**, 235503 (2011).

[63] P. Schall, D. A. Weitz, and F. Spaepen, Science **318**, 1895 (2007).

[64] S. T. Liu, Z. Wang, H. B. Yu, Scr. Mater. **67**, 9 (2012); L. S. Huo, J. Ma, H. B. Ke, H. Y. Bai, D. Q. Zhao, and W. H. Wang, J. Appl. Phys. **111**, 113522 (2012).

[65] H. W. Sheng, H. Z. Liu, Y. Q. Cheng, J. Wen, P. L. Lee, W. K. Luo, S. D. Shastri, and E. Ma, Nature Mater. **6**, 192 (2007).

[66] B. Zhang, R. J. Wang, and W. H. Wang, Phys. Rev. B **72**, 104205 (2005).

[67] M. J. Duarte, P. Bruna, E. Pineda, D. Crespo, G. Garbarino, R. Verbeni, K. Zhao, W. H. Wang, A. H. Romero, and J. Serrano, Phys. Rev. B **84**, 224116 (2011).

[68] Q. S. Zeng, W. L. Mao, S. V. Sinogeikin, and H. K. Mao, Phys. Rev. Lett. **104**, 105702 (2010).

[69] P. Soderlind, Adv. Phys. **47**, 959 (1998).

[70] A. B. Shick, W. E. Pickett, and A. I. Liechtenstein, J. Electron Spectrosc. Relat. Phenom. **114–116**, 753 (2001).

[71] Q. Luo, D. Q. Zhao, M. X. Pan, and W. H. Wang, Appl. Phys. Lett. **89**, 081914 (2006).

[72] Q. Luo, D. Q. Zhao, M. X. Pan, and W. H. Wang, Appl. Phys. Lett. **90**, 211903 (2007).

[73] Q. Luo and W. H. Wang, J. Non-Cryst. Solids **355**, 759 (2009).

[74] Y. T. Wang, M. X. Pan, D. Q. Zhao, and W. H. Wang, Sci. China, Ser. G **51**, 337 (2008).

[75] B. C. Wei, L. Xia, S. Roth, W. H. Wang, and J. Eckert, Acta Mater. **50**, 4357 (2002).

[76] B. C. Wei, Y. Zhang, D. Q. Zhao, M. X. Pan, and W. H. Wang, J. Appl. Phys. **89**, 3529 (2001).

[77] Z. F. Zhao, Z. Zhang, P. Wen, D. Q. Zhao, and W. H. Wang, Appl. Phys. Lett. **82**, 4699 (2003).

[78] M. B. Tang, H. Y. Bai, W. H. Wang, K. Samwer, and T. Egami, Phys. Rev. B **75**, 172201 (2007).

[79] B. Huang, H. Y. Bai, and W. H. Wang, J. Appl. Phys. **110**, 123522 (2011).

[80] M. B. Tang, H. Y. Bai, M. X. Pan, and W. H. Wang, J. Non-Cryst. Solids **351**, 2572 (2005).