Any properties correlating with glass transition temperature

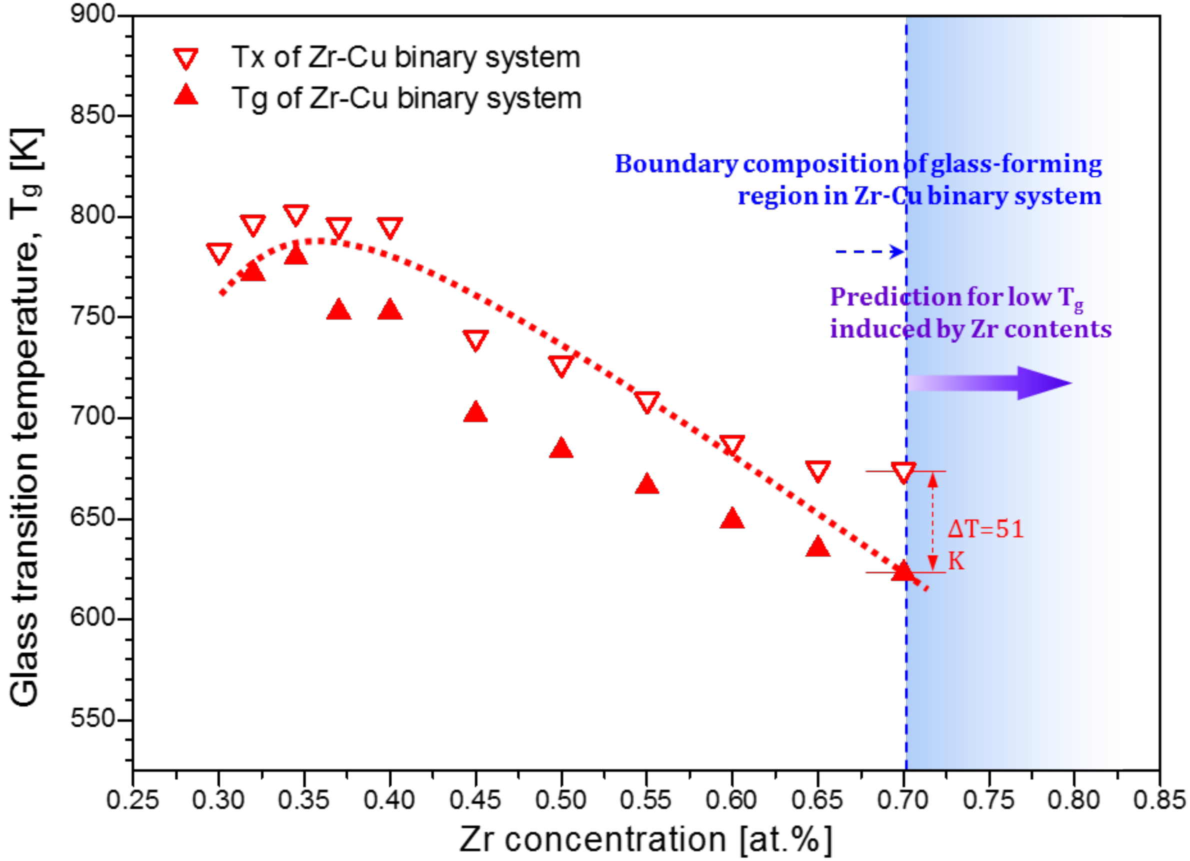
구조재료 심화연구 (Current Status of Structural Materials)

April 10th, 2017

Kyung-jun Kim

1. Introduction: Change of T_g depending on composition

T_g and T_x Change Depending on Zr Content in Zr-Cu Binary System

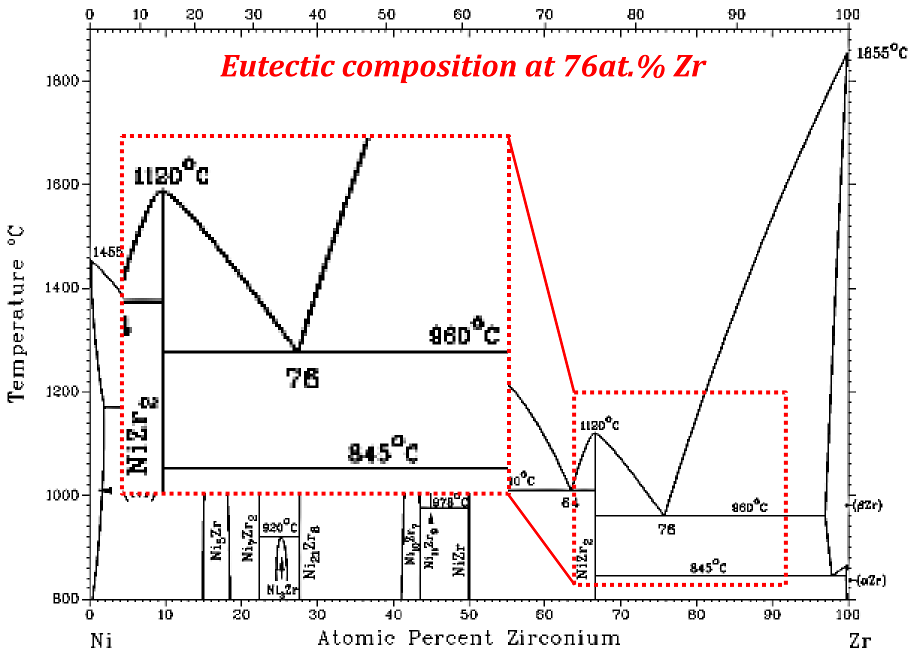


Decrease of T_g depending on Zr content

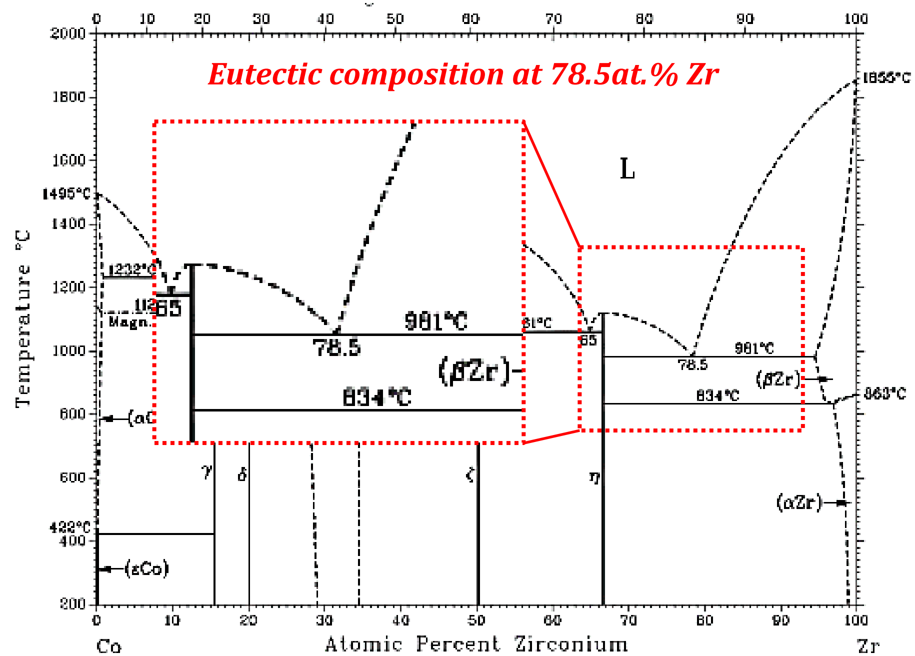
"Develop novel Zr-rich Zr-TM glassy alloy system for low T_g"

Retention of Liquid Phase

Phase diagram of Ni-Zr binary system

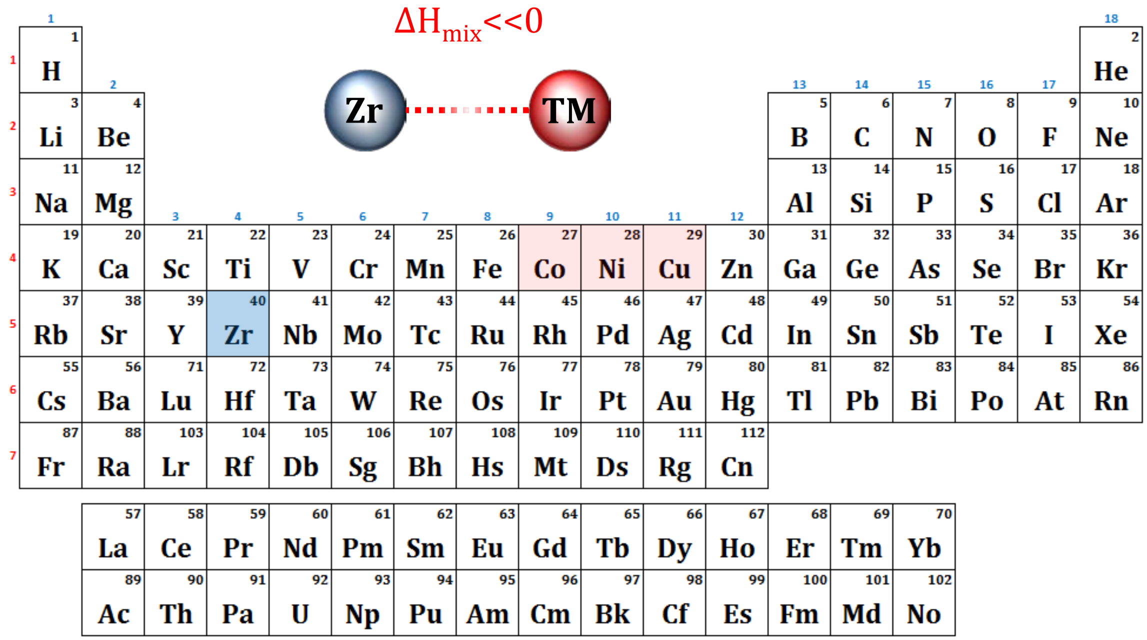


Phase diagram of Co-Zr binary system



Near eutectic composition, liquid phase keeps stable even at low temperature → " Large GFA "

Thermodynamic and Structural Point



A. Takeuchi et al., Materials Transactions, 46, 12, 2005, 2817-2829

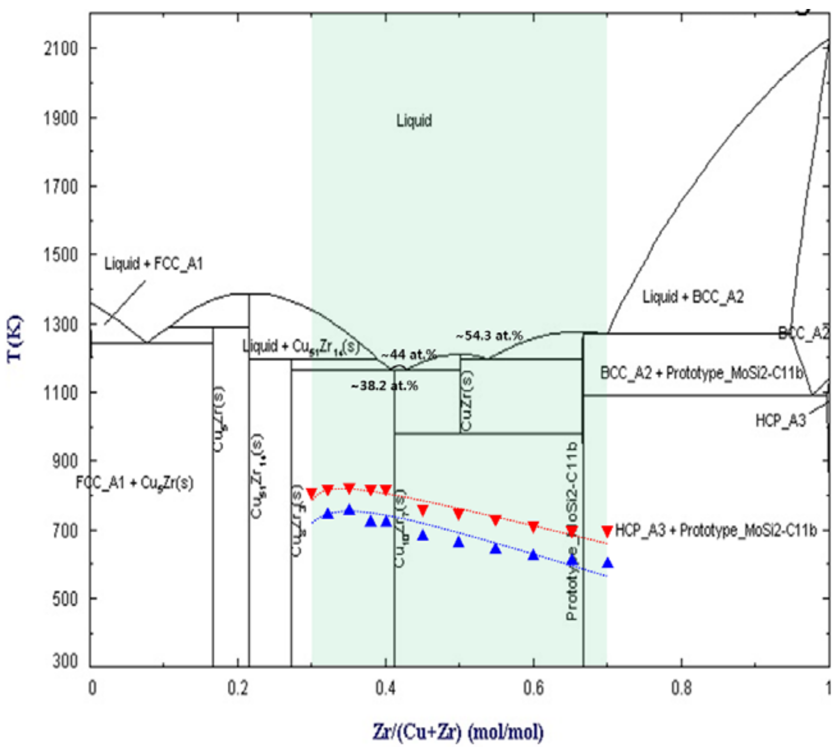
	Atomic radius [Å]	Atomic radius difference [%]	ΔH_{mix} [kJ/mol]
Zr	1.62	–	–
Cu	1.28	21.0	-23
Ni	1.25	22.8	-49
Co	1.25	22.8	-41

Consider atomic radius difference($\Delta r/r_0$) and heat of mixing(ΔH_{mix}) relation by empirical rules about GFA,

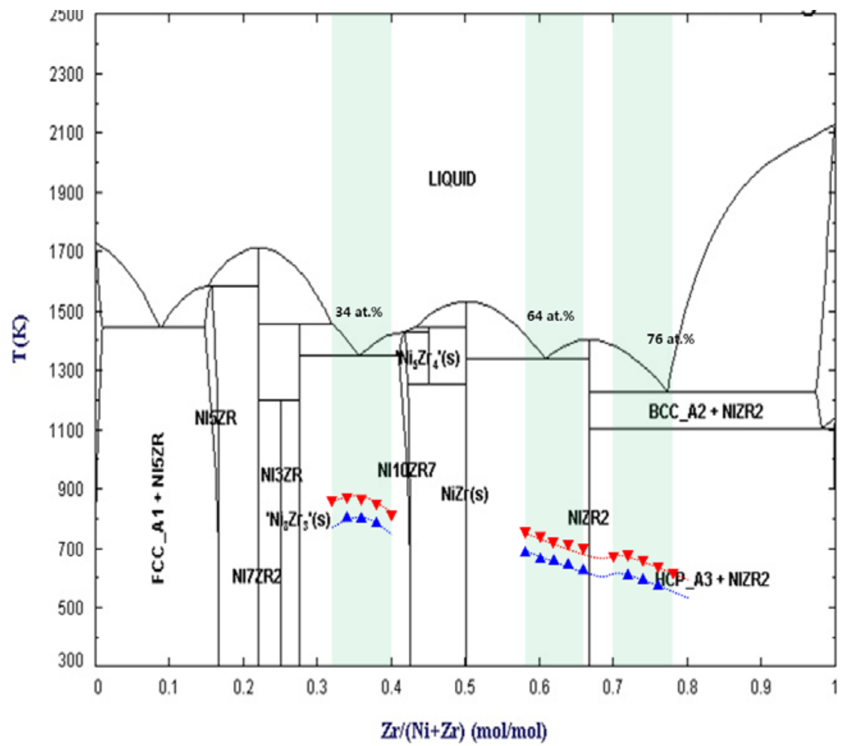
Ni, Co → Large $\Delta r/r_0$ (~22.8%) and negative ΔH_{mix} (over -40kJ/mol)

Characteristic Temperature Plot in Phase Diagram

Phase diagram of Cu-Zr binary system

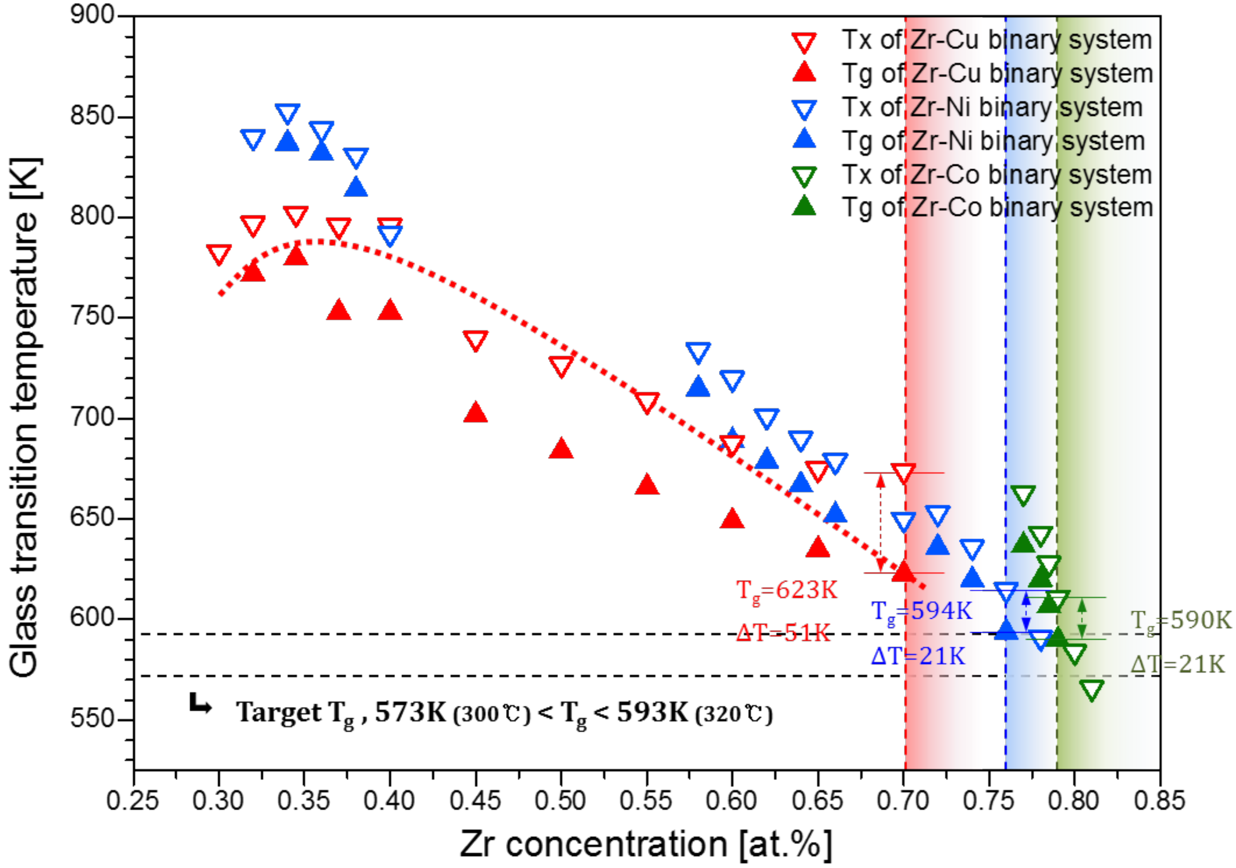


Phase diagram of Ni-Zr binary system



Linear correlation of T_g depending on its composition

Characteristic Temperature of Zr-TM (=Cu, Ni, Co) Binary Metallic Glass



Linear correlation of T_g depending on its composition

2. Other property changes depending on its composition

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Scripta Materialia 57 (2007) 805–808
Scripta MATERIALIA
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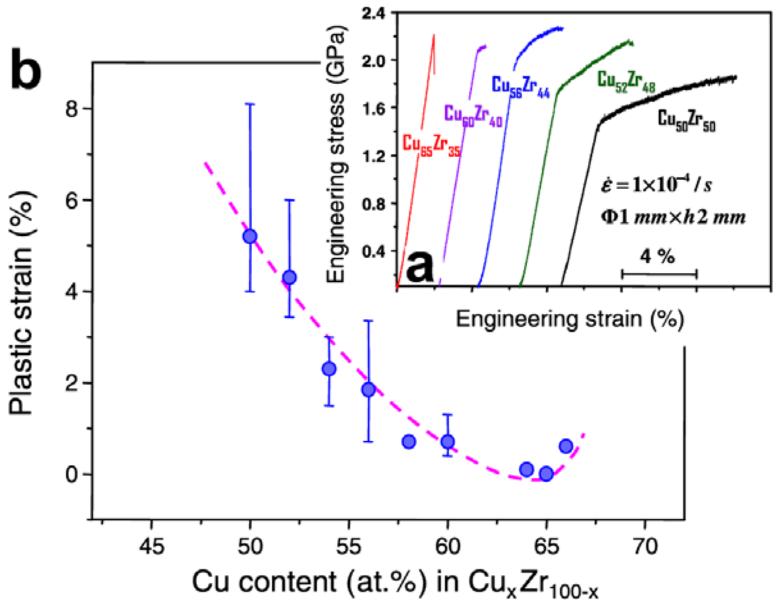
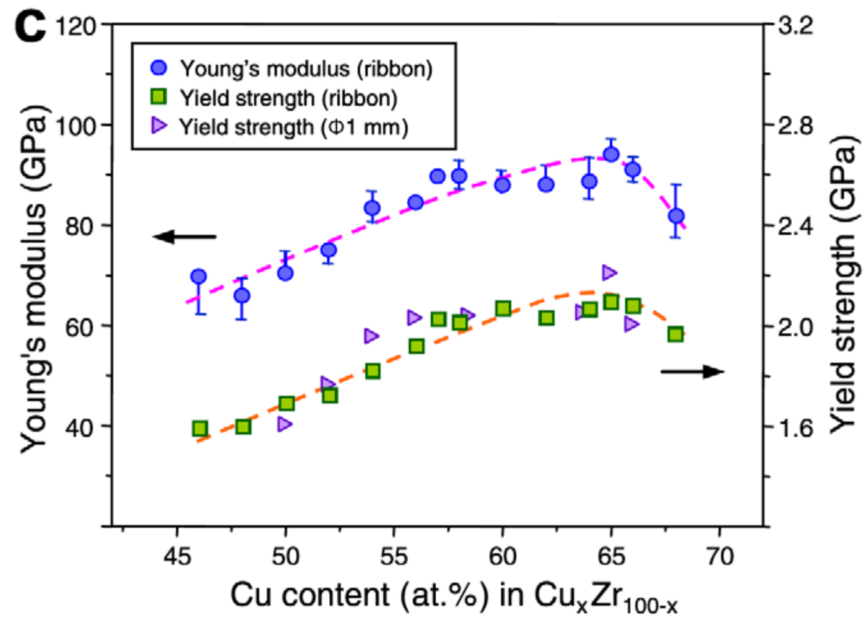
Atomic packing density and its influence on the properties of Cu–Zr amorphous alloys

Kyoung-Won Park,[a] Jae-il Jang,[b] Masato Wakeda,[c] Yoji Shibutani[c] and Jae-Chul Lee[a,*]

Investigate relationship between structural properties of MG and its properties

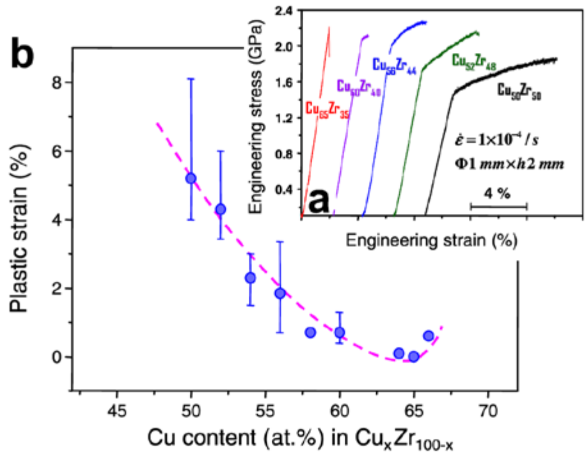


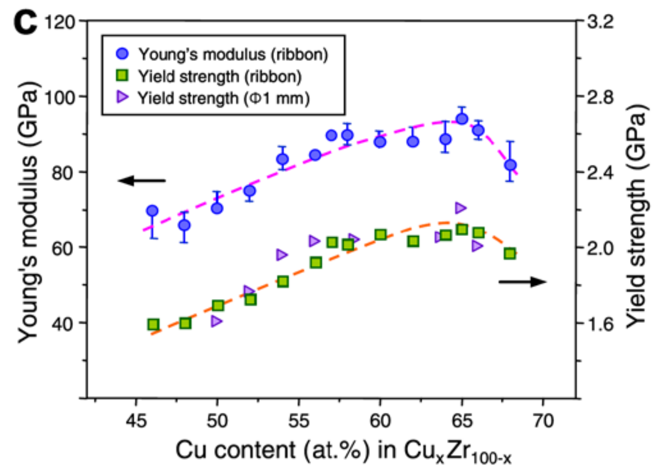


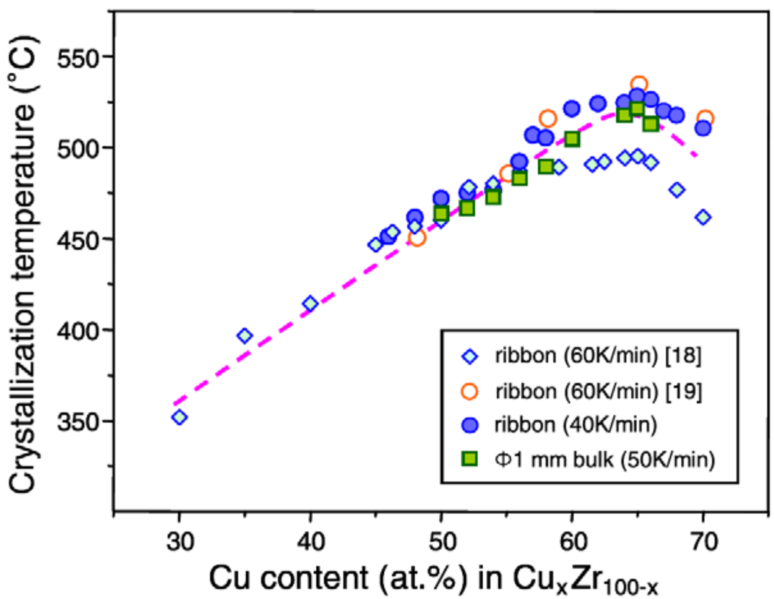
1. Using 14 ribbon samples (50µm thickness X 2mm width) with composition range from $Cu_{46}Zr_{54}$ to $Cu_{70}Zr_{30}$,
   Nanoindentation test → Hardness (converted to the yield strength, σ_y (MPa)=274H_N (GPa)), Young's modulus
2. Using 9 rod samples (φ1mm X 30mm height) with different composition ranging from $Cu_{46}Zr_{54}$ to $Cu_{70}Zr_{30}$,
   Room-temp. compression test → Stress-strain curve, Yield strength, Plastic strain,

"Atomic packing density and its influence…"

K.W. Park et al., Scripta Materialia, 57, 2007, 805-808







DSC measurement → crystallization temperature, T_x (cf. T_g)

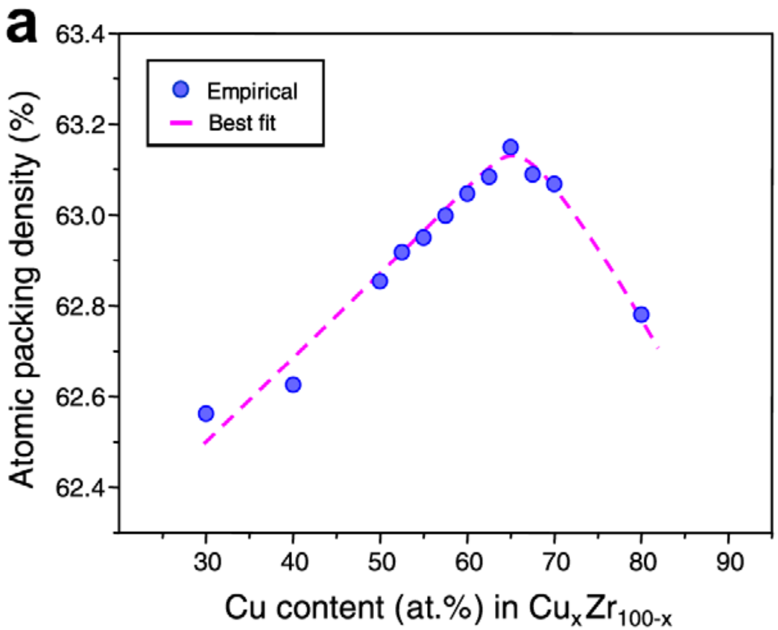
In this study, focus on composition of the highest T_x

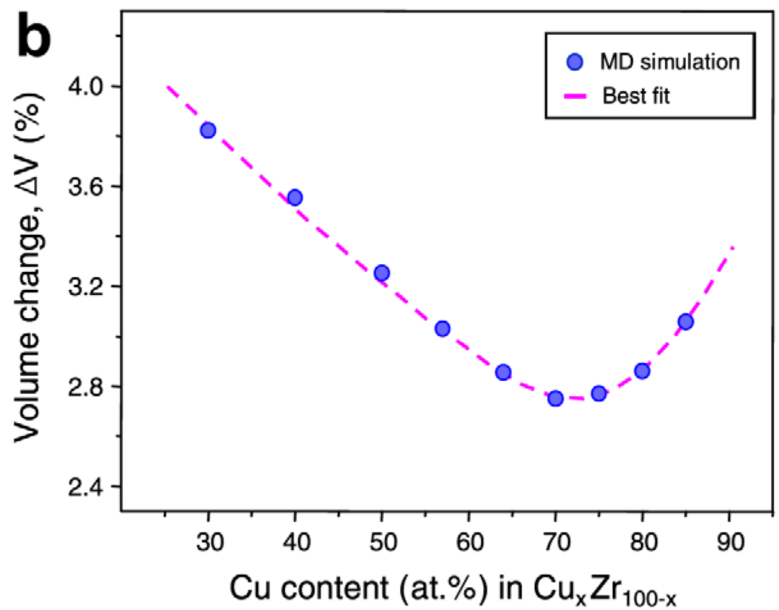
Any correlation of T_g or T_x with other properties?

“Atomic packing density and its influence…”

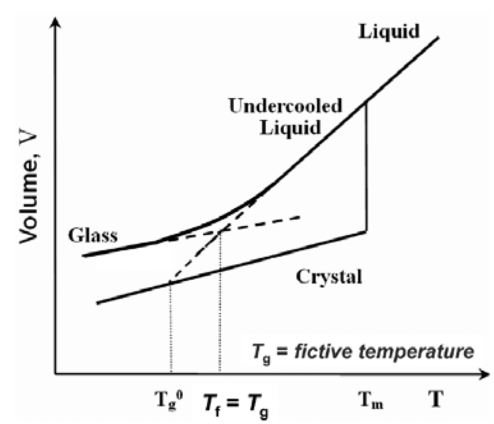
K.W. Park et al., Scripta Materialia, 57, 2007, 805-808

General structural properties: atomic packing density, volume change





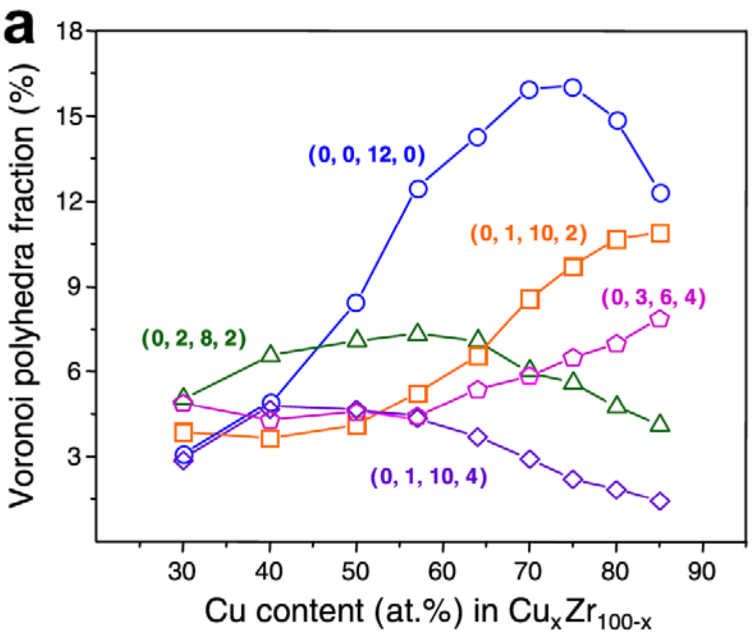
1. Not precise method, using just simple experimental method
   → Atomic packing density measured, mixture of φ4 and 5mm steel balls (relative size 1.250, similar with 1.254, atomic radius ratio of Cu and Zr)
2. Free volume evaluated based on MD simulations (using simple potential database, the Lennard-Jones potential)

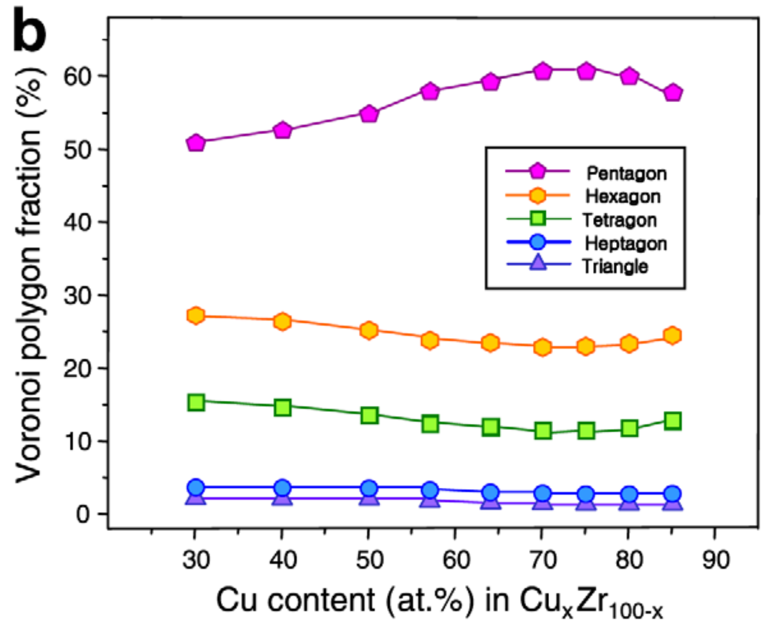


"Atomic packing density and its influence…"

K.W. Park et al., Scripta Materialia, 57, 2007, 805-808

Detail structural properties: SRO structure (3-D simulation, 2-D simulation)





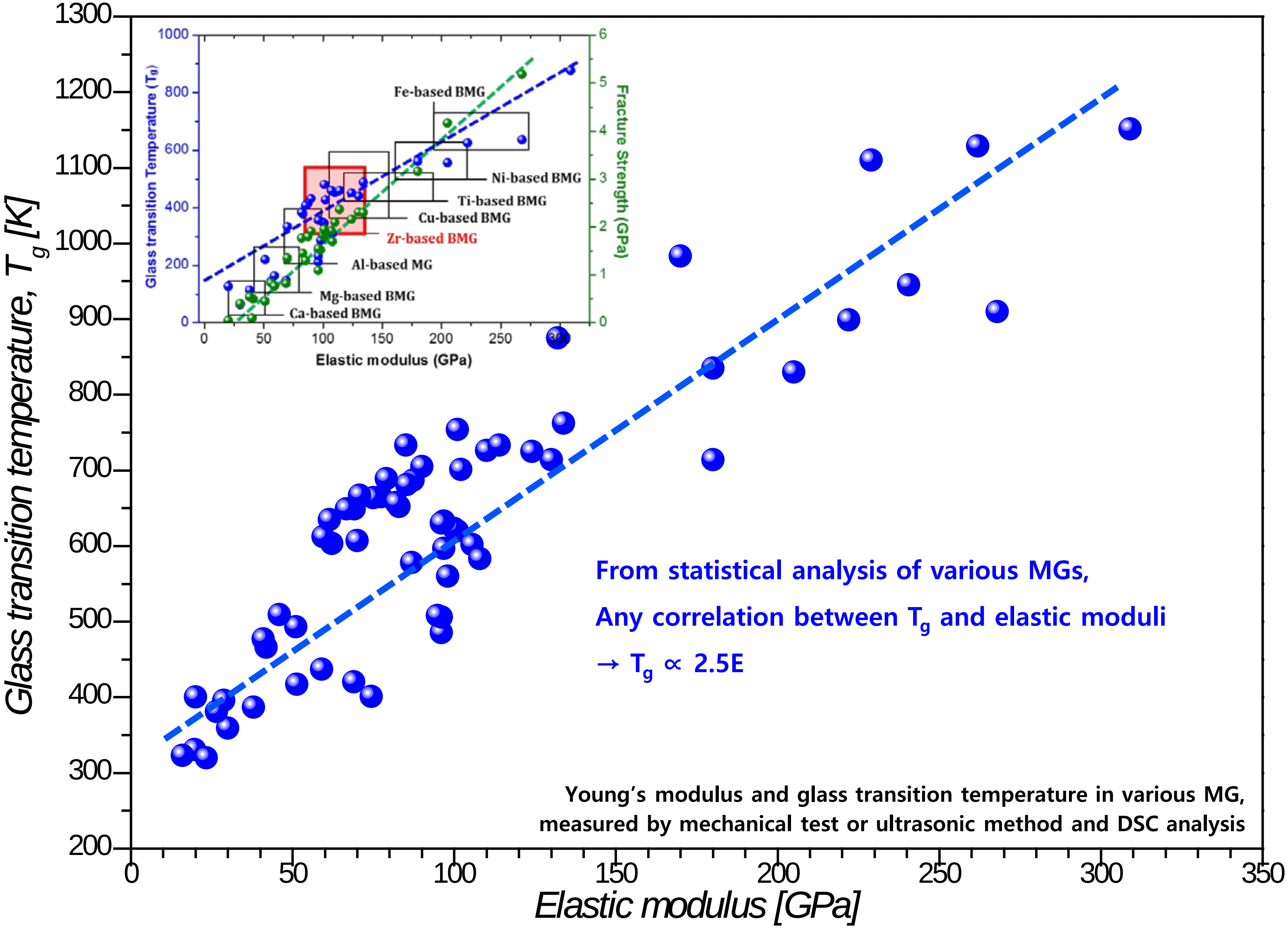
1. 3-D Voronoi polyhedral fraction → Dominant SRO structure, (0, 0, 12, 0) Icosahedron
2. For simple analysis, using 2-D Voronoi polygon fraction → Dominant SRO structure, Pentagon
   (fivefold symmetry exhibiting the densest packing with the highest shear resistance)

"조성에 따라 특정 structural feature에 변화가 생기고, mechanical 혹은 thermal property에 영향을 줌."
단, 조성 변화가 structural feature에 끼치는 영향에 대해서는 언급이 없음.

3. Correlation between elastic moduli and T_g

Correlation between elastic modulus and T_g

W.H. Wang, Journal of Non-Crystalline Solids, 351, 2005, 1481-1485
W.H. Wang, Journal of Applied Physics, 99, 2006, 093506
W.H. Wang, Progress in Materials Science, 57, 2012, 487-656



“Atomic packing density and its influence…”

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Atomic packing density and its influence on the properties of Cu–Zr amorphous alloys

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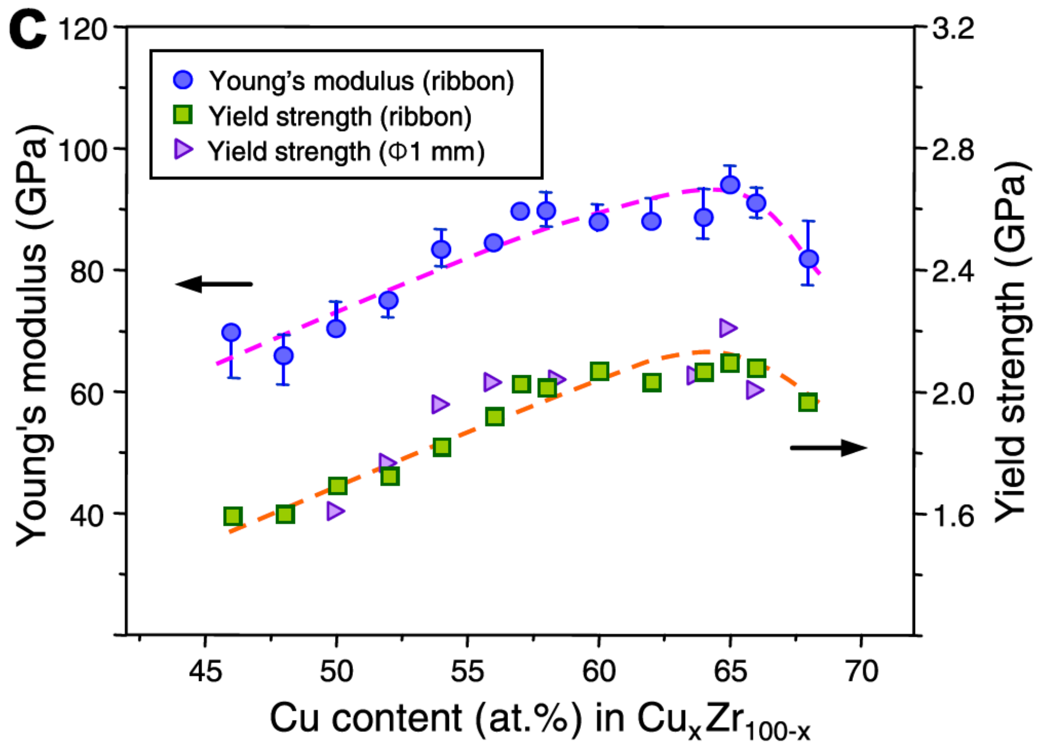
Investigate relationship between structural properties of MG and its properties



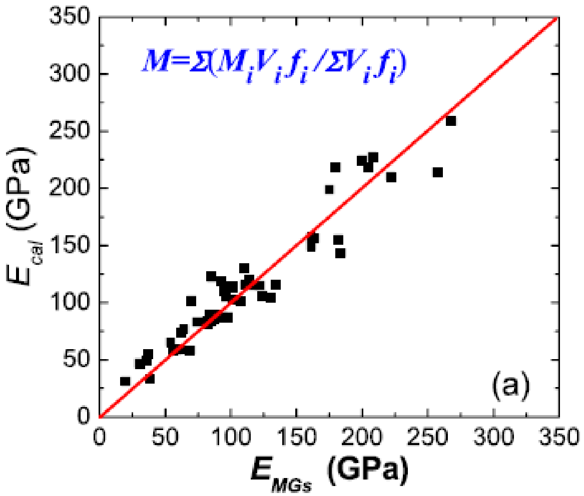
“Properties inheritance in metallic glasses”

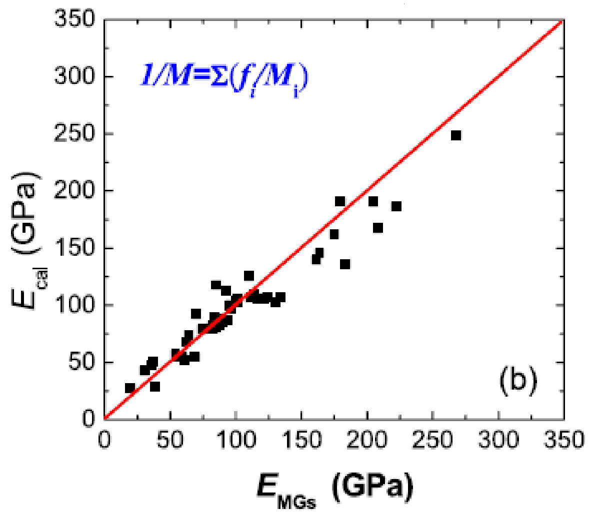
JOURNAL OF APPLIED PHYSICS **111**, 123519 (2012)

W.H. Wang, Progress in Materials Science, 57, 2012, 487-656

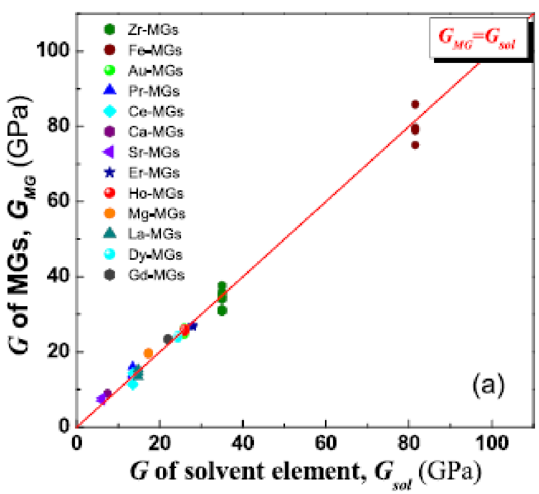
Properties inheritance in metallic glasses

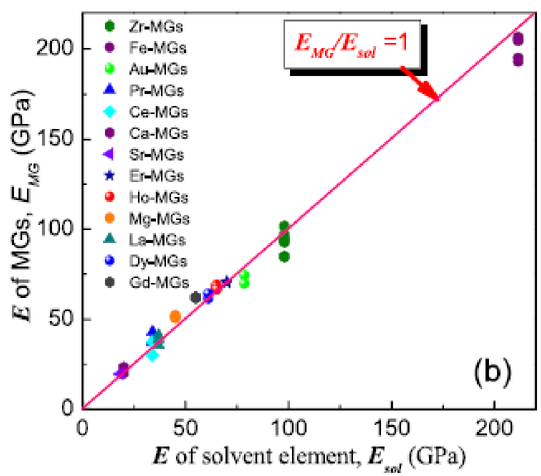
Wei Hua Wang (汪卫华)[a)]
Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China





The structural features of MG (similar structure as liquid, determined by constituent elements)

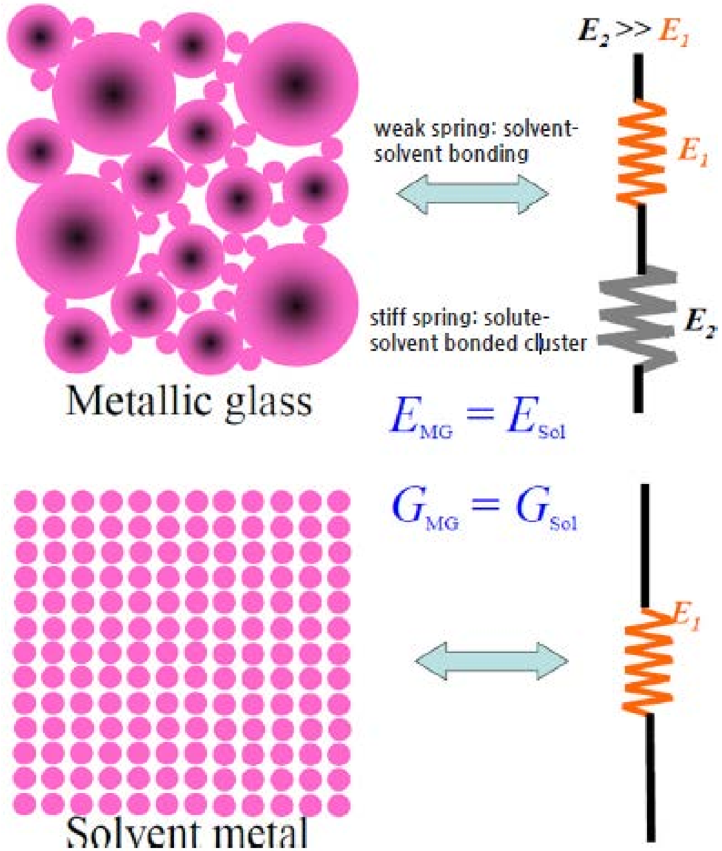


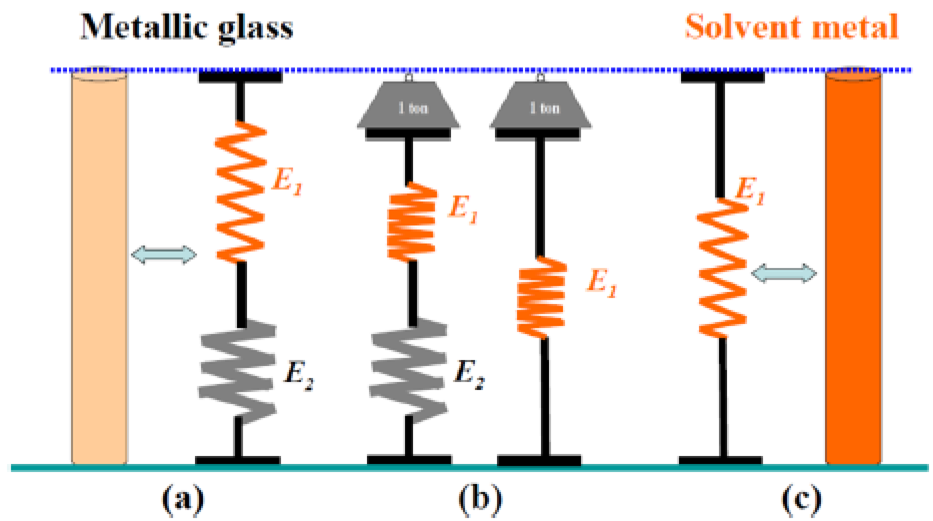


Not from all constituent elements, *its solvent component* *(or base component)*

“Properties inheritance in metallic glasses”

W.H. Wang, Journal of Applied physics, 111, 2012, 123519





Simple model of MG with a stiff spring (solute-solvent bonding) and less stiff spring (solvent-solvent bonding)

"Elastic moduli inheritance and the weakest link in bulk metallic glasses"

PRL 108, 085501 (2012) PHYSICAL REVIEW LETTERS week ending 24 FEBRUARY 2012

Elastic Moduli Inheritance and the Weakest Link in Bulk Metallic Glasses

D. Ma,[1] A. D. Stoica,[1] X.-L. Wang,[1,*] Z. P. Lu,[2] B. Clausen,[3] and D. W. Brown[3]

TABLE I. Experimental Young's modulus (E) and shear modulus (G) for BMGs and their solvent elements (Sol). Also listed are the ratios of BMG to solvent in terms of E and G, respectively. Data for solvents were taken from [6].

BMGs	Sol	E (GPa)			G (GPa)			Ref.
		BMG	Sol	Ratio	BMG	Sol	Ratio	
$Zr_{55}Cu_7Co_{19}Al_{19}$	Zr	101.7	98.0	1.04	37.6	35.0	1.07	[1]
$Zr_{41.2}Ti_{13.8}Ni_{10}Cu_{12.5}Be_{22.5}$	Zr	97.2	98.0	0.99	35.9	35.0	1.03	[1]
$Zr_{48}Nb_8Cu_{12}Fe_8Be_{24}$	Zr	95.7	98.0	0.98	35.2	35.0	1.01	[7]
$Zr_{48}Nb_8Cu_{14}Ni_{12}Be_{18}$	Zr	93.9	98.0	0.96	34.3	35.0	0.98	[7]
$Zr_{46}Cu_{46}Al_8$	Zr	93.7	98.0	0.96	34.3	35.0	0.98	[8]
$Zr_{50.6}Ti_{5.1}Cu_{18.9}Ni_{11.1}Al_{14.3}$	Zr	92.7	98.0	0.95	34.0	35.0	0.97	[7]
$Zr_{50}Cu_{50}$	Zr	85.0	98.0	0.87	31.3	35.0	0.89	[8]
$Zr_{55}Ti_5Cu_{20}Ni_{10}Al_{10}$	Zr	85.0	98.0	0.87	31.0	35.0	0.89	[8]
$Zr_{57.5}Nb_5Cu_{15.5}Ni_{12}Al_{10}$	Zr	84.7	98.0	0.86	30.8	35.0	0.88	[7]
$Er_{50}Y_6Al_{24}Co_{20}$	Er	71.1	70.0	1.02	27.0	28.0	0.96	[8]
$Ho_{39}Al_{24}Co_{20}Y_{12}Zr_5$	Ho	69.3	65.0	1.07	26.2	26.0	1.01	[9]
$Ho_{39}Al_{25}Co_{20}Y_{16}$	Ho	69.1	65.0	1.06	26.2	26.0	1.01	[9]
$Dy_{46}Y_{10}Al_{24}Co_{18}Fe_2$	Dy	64.2	61.0	1.05	24.4	25.0	0.98	[10]
$Mg_{65}Cu_{25}Gd_{10}$	Mg	49.1	44.7	1.10	18.6	17.3	1.08	[1]
$La_{55}Cu_{10}Ni_5Co_5Al_{25}$	La	41.9	37.9	1.11	15.6	14.9	1.05	[8]
$La_{66}Cu_{10}Ni_{10}Al_{14}$	La	35.7	37.9	0.94	13.4	14.9	0.90	[8]
$La_{62}Cu_{11.7}Ag_{2.3}Ni_5Co_5Al_{14}$	La	35.0	37.9	0.92	13.0	14.9	0.87	[11]
$Pr_{60}Ni_{10}Al_{10}Cu_{20}$	Pr	37.2	37.0	1.01	13.6	15.0	0.91	[10]
$Ce_{68}Cu_{20}Nb_2Al_{10}$	Ce	31.0	33.5	0.93	12.0	13.5	0.89	[12]
$Ce_{68}Cu_{20}Fe_2Al_{10}$	Ce	30.8	33.5	0.92	11.8	13.5	0.87	[8]
$Ce_{70}Cu_{10}Ni_{10}Al_{10}$	Ce	30.3	33.5	0.90	11.5	13.5	0.85	[10]
$Fe_{61}Mn_{10}Cr_4Mo_6Er_1C_{15}B_6$	Fe	193	211.4	0.91	75	81.6	0.92	[13]
$Fe_{53}Cr_{15}Mo_{14}Er_1C_{15}B_6$	Fe	195	211.4	0.92	75	81.6	0.92	[13]
$Au_{49.5}Ag_{5.5}Pd_{2.3}Cu_{26.9}Si_{16.3}$	Au	74.4	78.5	0.95	26.5	26	1.02	[14]
$Au_{55}Cu_{25}Si_{20}$	Au	69.8	78.5	0.89	24.6	26	0.95	[14]
Mean				0.97			0.96	
Standard Deviation				0.07			0.07	

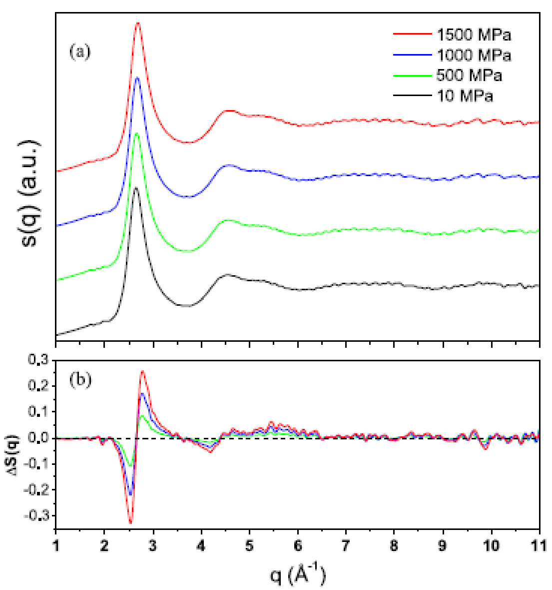
"Conventionally, the elasticity of a glass is viewed as what takes place in an isotropic solid, i.e., elastic bond stretching and uniform straining at all scales."

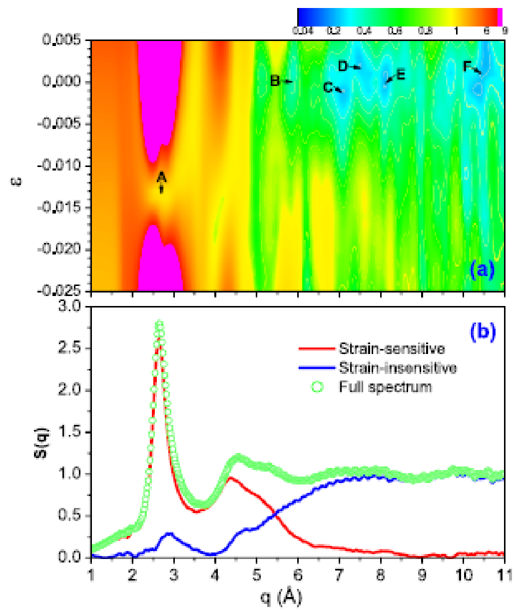
"In this letter, we set out to investigate the elasticity … adopt the moduli of their solvent components"

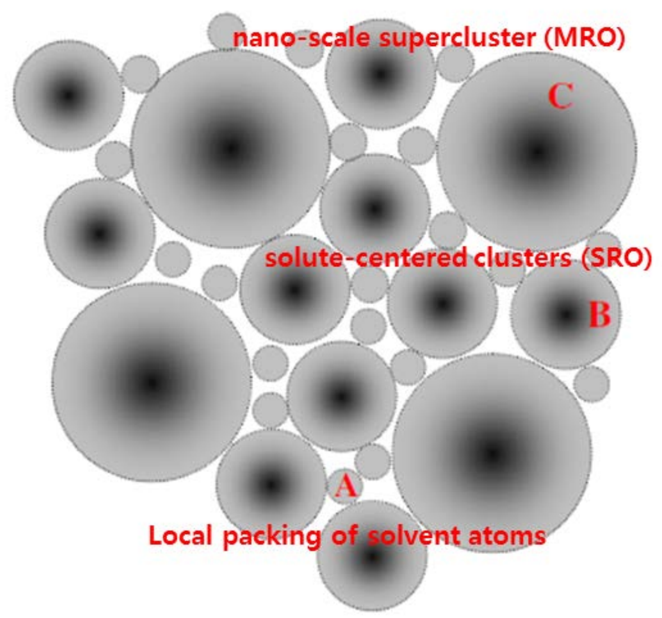
"Since the elastic modulus reflects the inherent stiffness of atomic bonds, Table 1 suggests that solvent-solvent bonds are essentially responsible for the elasticity of BMGs"

D. Ma, et al., Physical Review Letters, 108, 2012, 085501

To explore evidence of the structural origin from solvent component, in-situ neutron diffraction study of Φ6mm Zr-based BMG ($Zr_{52.5}Cu_{17.9}Ni_{14.6}Al_{10}Ti_5$) under compressive stress (10MPa, 500MPa, 1000MPa, 1500MPa)



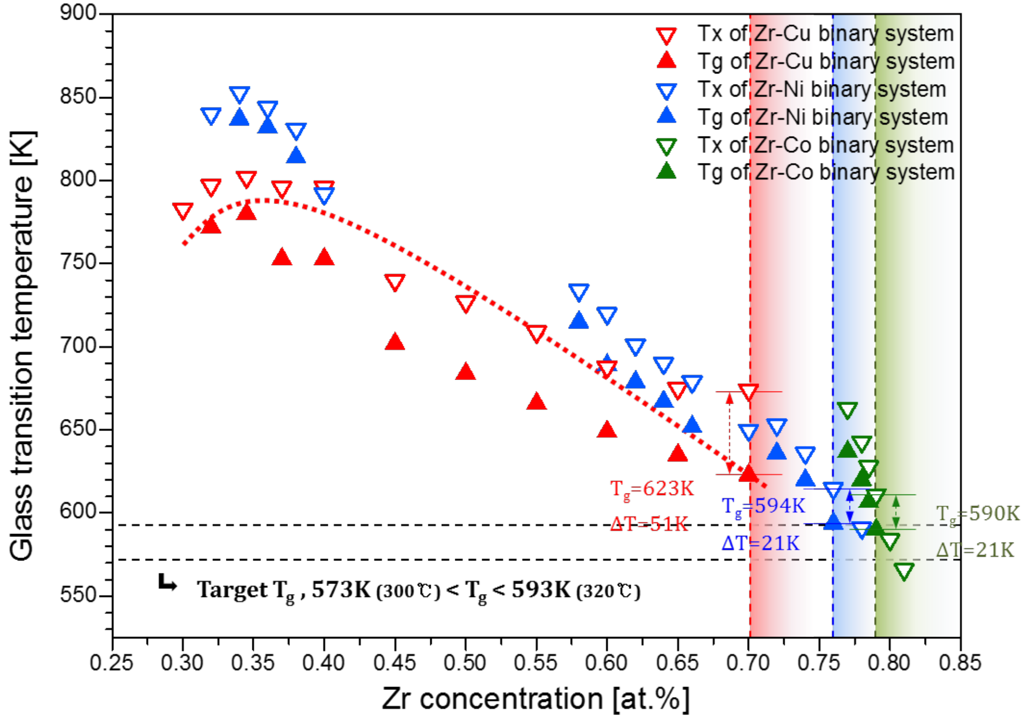


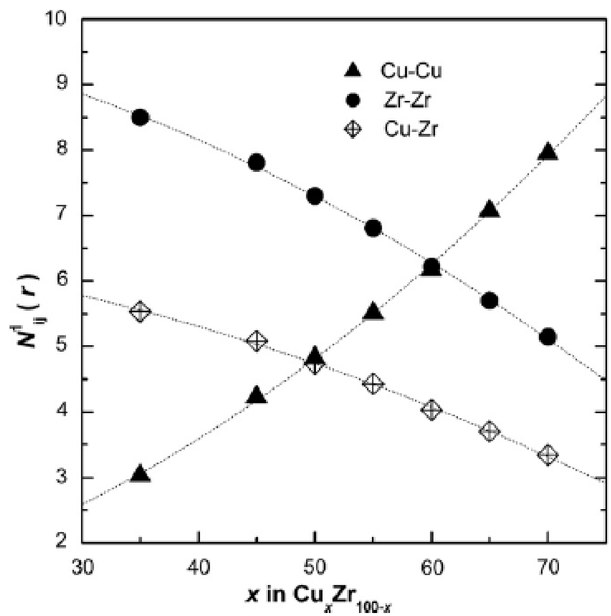


Strain-sensitive region → Junction among the solute-centered clusters and/or the superclusters by excess solvent atoms

Conclusion

N. Mattern et al., Journal of non-crystalline solids, 354, 2008, 1054-1060





Element	E (GPa)	G (GPa)	K (GPa)	T_m (K)
Zr	68	33	–	1125
Ti	116	44	110	1941
Cu	130	48	140	1356
Ni	200	76	180	1726
Nb	105	38	170	2741
Mg	45	17	45	922
Fe	211	82	170	1808
Al	70	26	76	933
Zn	108	43	70	692
Co	209	75	180	1768

Decrease of T_g depending on Zr content ?

→ First, increase fraction of solvent-solvent bonding

→ Second, T_g degree determined by sort of solvent element

Thank you for

Your Kind Attention