Thermal Expansion of Metallic Glasses Studied by Real-Space Distribution Functions Obtained from X-ray Diffractometry Investigations

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Bulk metallic glasses defined as 3-dimentional massive glassy (amorphous) articles with a size of not less than 1 mm in any dimension have been widely studied since early 1990s [1].

At the same time the structure of metallic glasses and thermal expansion mechanisms are not completely understood yet.

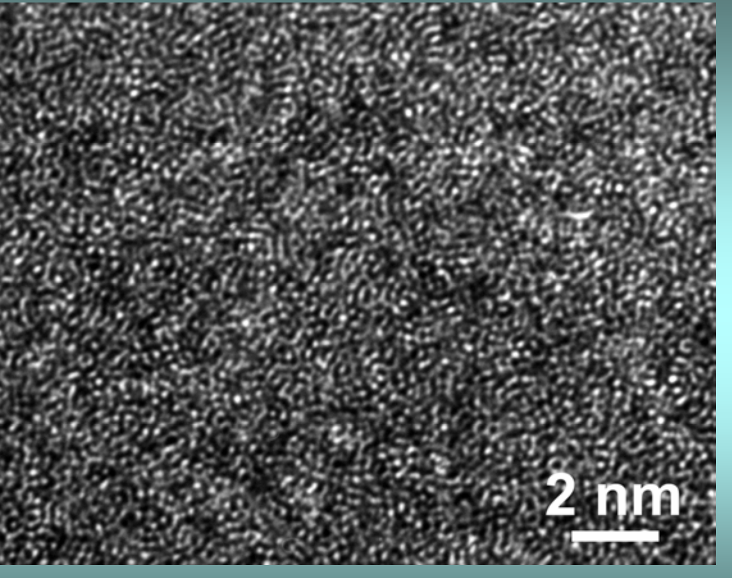
Following pioneering works of Yavari and his colleagues [2,3] on thermal expansion of metallic glasses studied by synchrotron-radiation diffractometry using reciprocal-space functions we continued these studies using real-space distribution functions [4].

[1] - A. Inoue, Acta Mater. 48, 279, (2000).

[2] - A. R. Yavari, S. Pang, D.V. Louzguine, A. Inoue, N. Lupu, N. Nikolov, G. Heunen, Mater. Sci. Forum/J. Metast. Nanocrys. Mater. 15-16, 105 (2003).

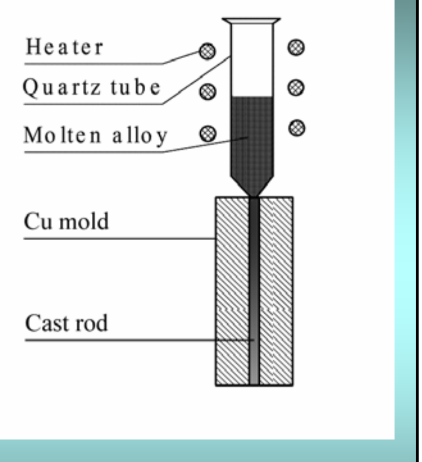
[3] - A. R.Yavari, A. Le Moulec, A. Inoue, N. Nishiyama, N. Lupo, E. Matsubara, W. J.Botta F., G. Vaughan, M. di Michiel, A. Kvick, Acta Materialia, 53, 1611 (2005).

[4] - D. V. Louzguine-Luzgin, A. Inoue, A. R. Yavari, and G. Vaughan Appl. Phys. Lett. 88, 121926 (2006).



Structure of a glassy alloy. High-resolution TEM.

Casting procedure for bulk (massive) glassy alloys



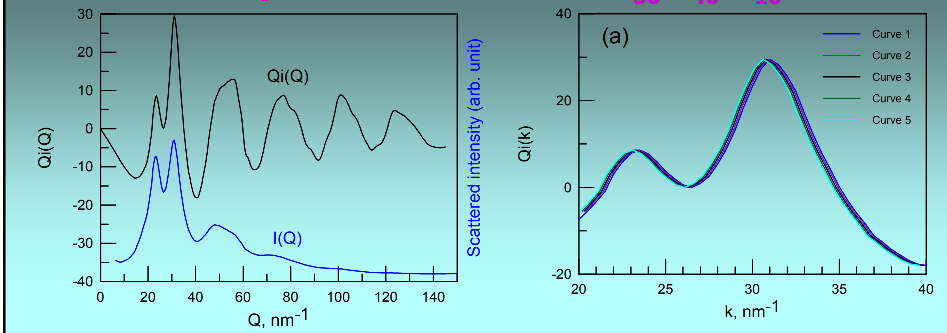
Bulk Glassy Alloys
size **> 1 mm** in any dimension

Injection casting

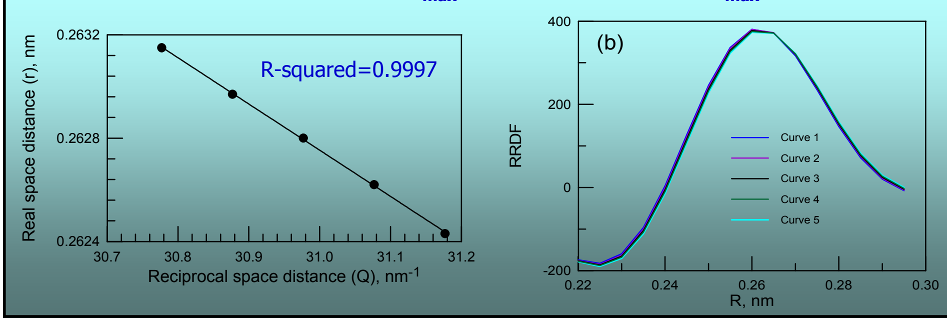
Synchrotron radiation X-ray diffraction in transmission was carried out during *in situ* heating using a high energy monochromatic beam on the ID15 beam line of the European Synchrotron Radiation Facility (ESRF)[1] equipped with a nitrogen-cooled double-silicon monochromator. The photon energy was 88.5 keV. The temperature was measured by thermocouple of a commercial Linkam hot stage.
After correction for air scattering, polarization, absorption,[2] and Compton scattering,[3] the measured intensity was converted to electron units per atom with the generalized Krogh-Moe-Norman method,[4] using the X-ray atomic scattering factors and anomalous dispersion corrections[5]. The total structure factor S(Q) and the interference function Qi(Q) have been obtained from the coherent scattering intensity by using atomic scattering factors[6]. The values of Qi(Q) less than 10 nm^{-1} were smoothly extrapolated to Q=0. The radial distribution RDF(r) and pair distribution PDF(r) functions have been obtained by the Fourier transformation of Qi(Q)[6].

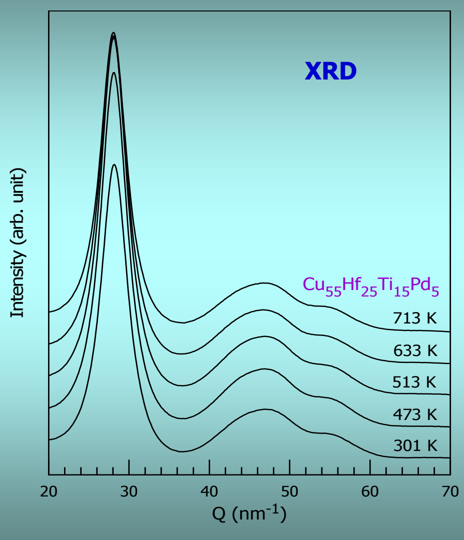
[1] A. R. Yavari, A. LeMoulec, A. Inoue, W. J. Botta, G. Vaughan, and A. Kvick, Mater. Sci. Eng. A 304-306, 34 (2001).
[2] C. N. J. Wagner J. Non-Cryst. Solids 31, 1 (1978).
[3] D. T. Cromer J. Chem. Phys. 47, 4857 (1969).
[4] C. N. J. Wagner, H. Ocken, and M. L. Joshi, Z. Naturforsch. 20a, 325 (1965).
[5] *International tables for X-ray Crystallography*, ed. J. A. Ibers and W. C. Hamilton, Kynoch, Birmingem, 1974, Vol. 4, p.1.
[6] Y. Waseda, *The Structure of Non-Crystalline Materials,* McGraw-Hill, New York, 1980, p. 26.

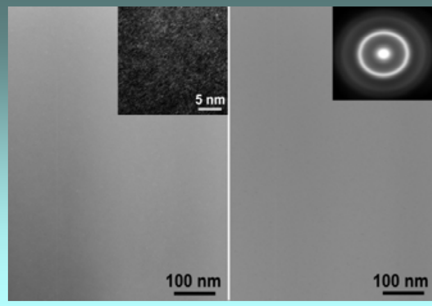
Computer simulation for $Ge_{50}Al_{40}Cr_{10}$



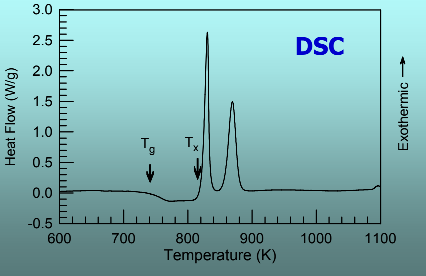
Real space R_{max} vs. reciprocal space Q_{max}



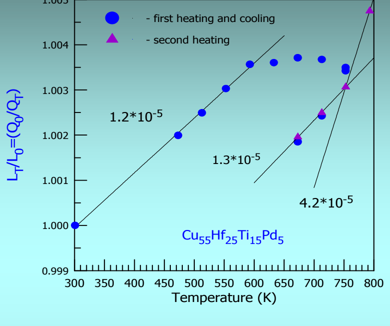


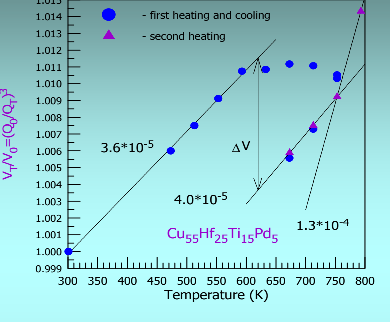


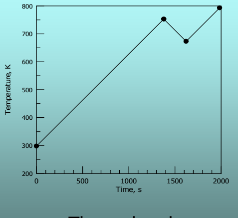
BF TEM DF



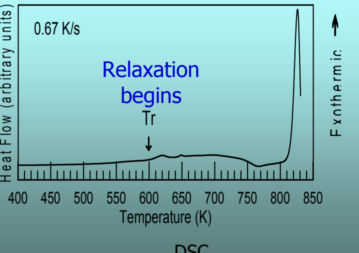
Q_0/Q and $(Q_0/Q)^3$ values related to L_T/L_0 and V_T/V_0, respectively, versus temperature for Bulk Glass Formers (Thermal expansion coefficients are given in K^{-1})



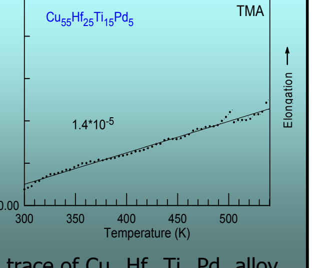




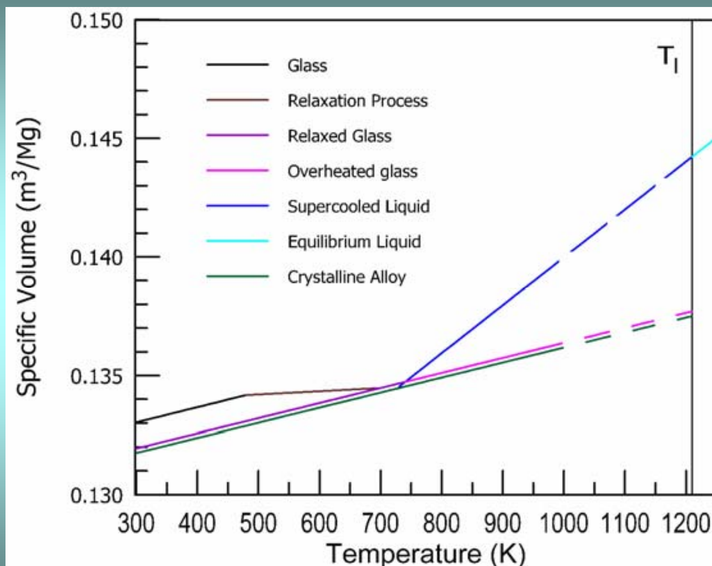
Thermal cycle
$Cu_{55}Hf_{25}Ti_{15}Pd_5$

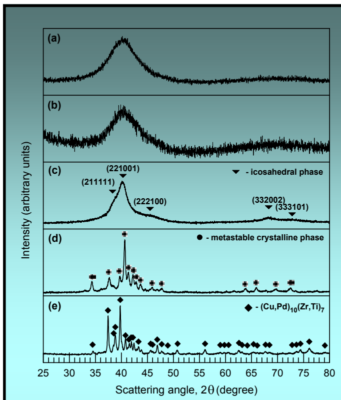


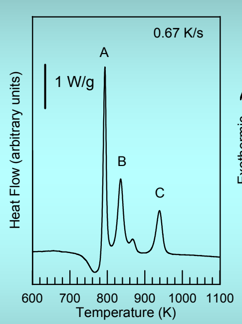
DSC

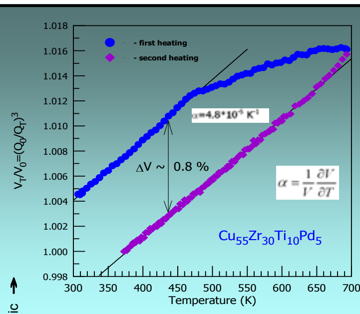


TMA trace of $Cu_{55}Hf_{25}Ti_{15}Pd_5$ alloy



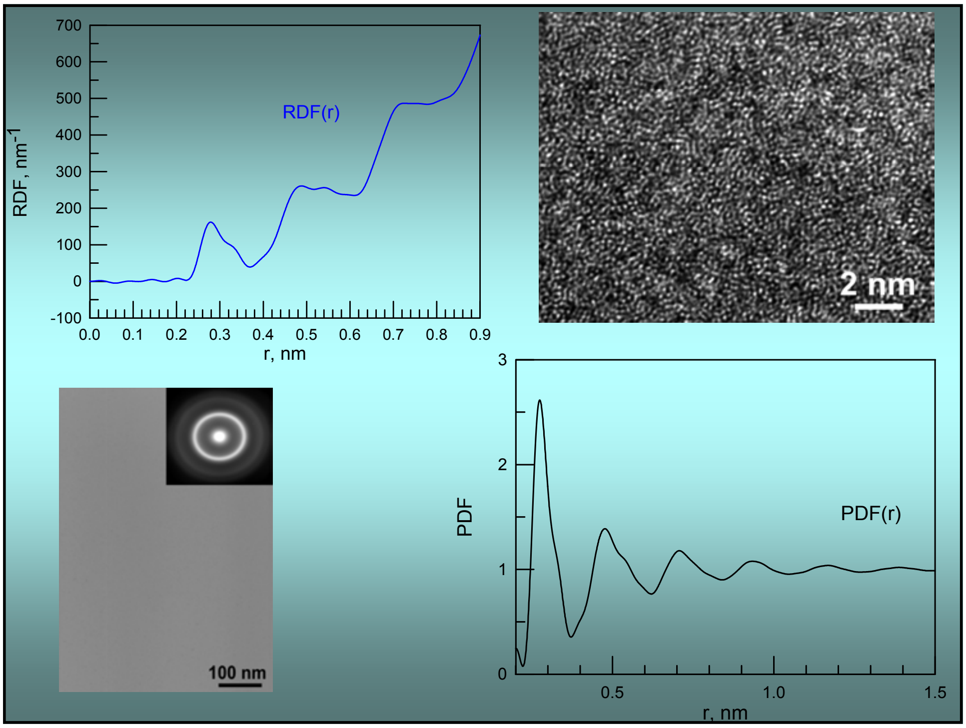


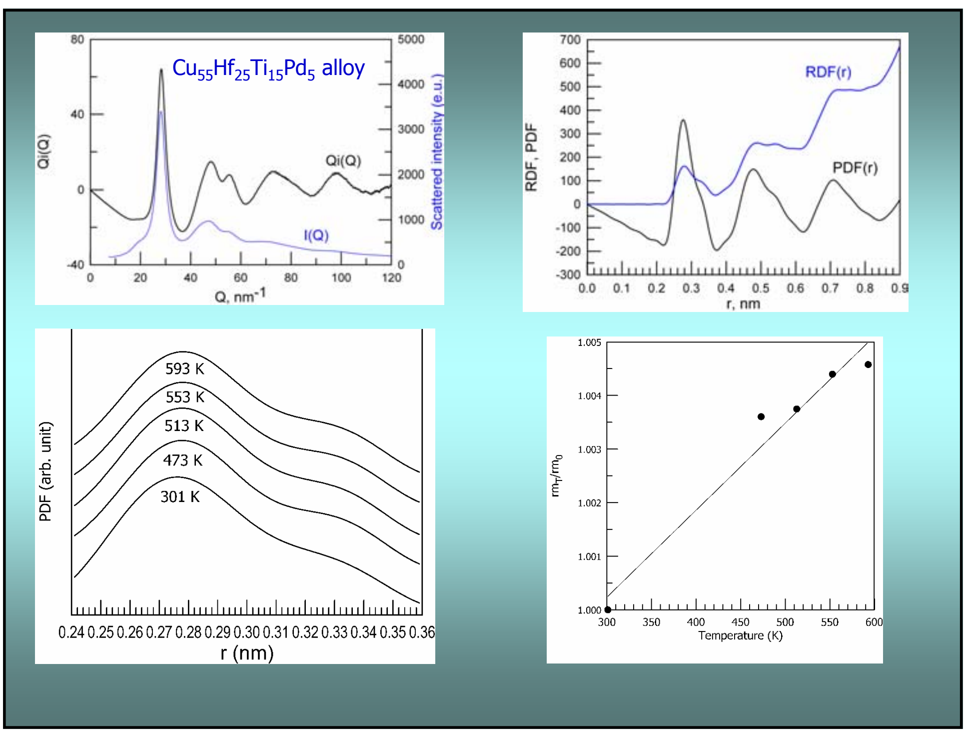


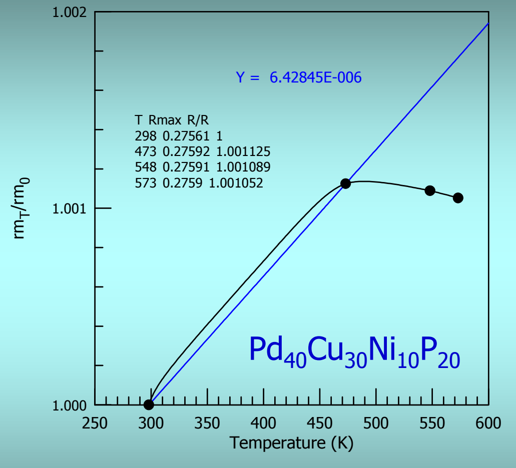


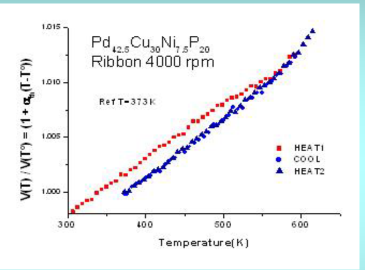
$Cu_{55}Zr_{30}Ti_{10}Pd_5$ alloy

Parameter	As-prep. Glass	Relaxed Glass 740 K, 120 s	Peak 1 I-ph. 785 K, 300 s	Peak 2 MIMC 850 K, 180 s	Peak 3 SIMC 993 K, 300 s
ρ, Mg/m^3	7.518	7.580	7.592	7.650	7.591
ΔV, %	0rigin	-0.8	-1.0	-1.8	-1.0


RDF(r)
RDF, nm-1
r, nm
2 nm
100 nm
PDF(r)
PDF
r, nm


Cu55Hf25Ti15Pd5 alloy
Qi(Q)
I(Q)
Scattered intensity (e.u.)
Q, nm-1
RDF(r)
PDF(r)
RDF, PDF
r, nm
593 K
553 K
513 K
473 K
301 K
PDF (arb. unit)
r (nm)
Temperature (K)





Conclusions

Thermal expansion of glassy alloys studied by using reciprocal space functions is verified using a real-space pair distribution function in the present work. The experimental results obtained by real-time diffraction during heating in a synchrotron beam and their Fourier transformation processing to derive radial distribution functions indicate that both reciprocal and real-space distribution functions give good agreement in the calculation of thermal expansion data. In addition to providing structural information, these findings indicate that the change in the average atomic nearest neighbor distance evaluated from the variation of the position of the main broad diffraction maximum can provide good thermal expansion data for metallic glasses.