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Supporting information for article:

Investigation of short-range structural order in Zr69.5Cu12Ni11Al7.5 and Zr41.5Ti41.5Ni17 glasses, using X-ray absorption spectroscopy and *ab initio* molecular dynamics simulations

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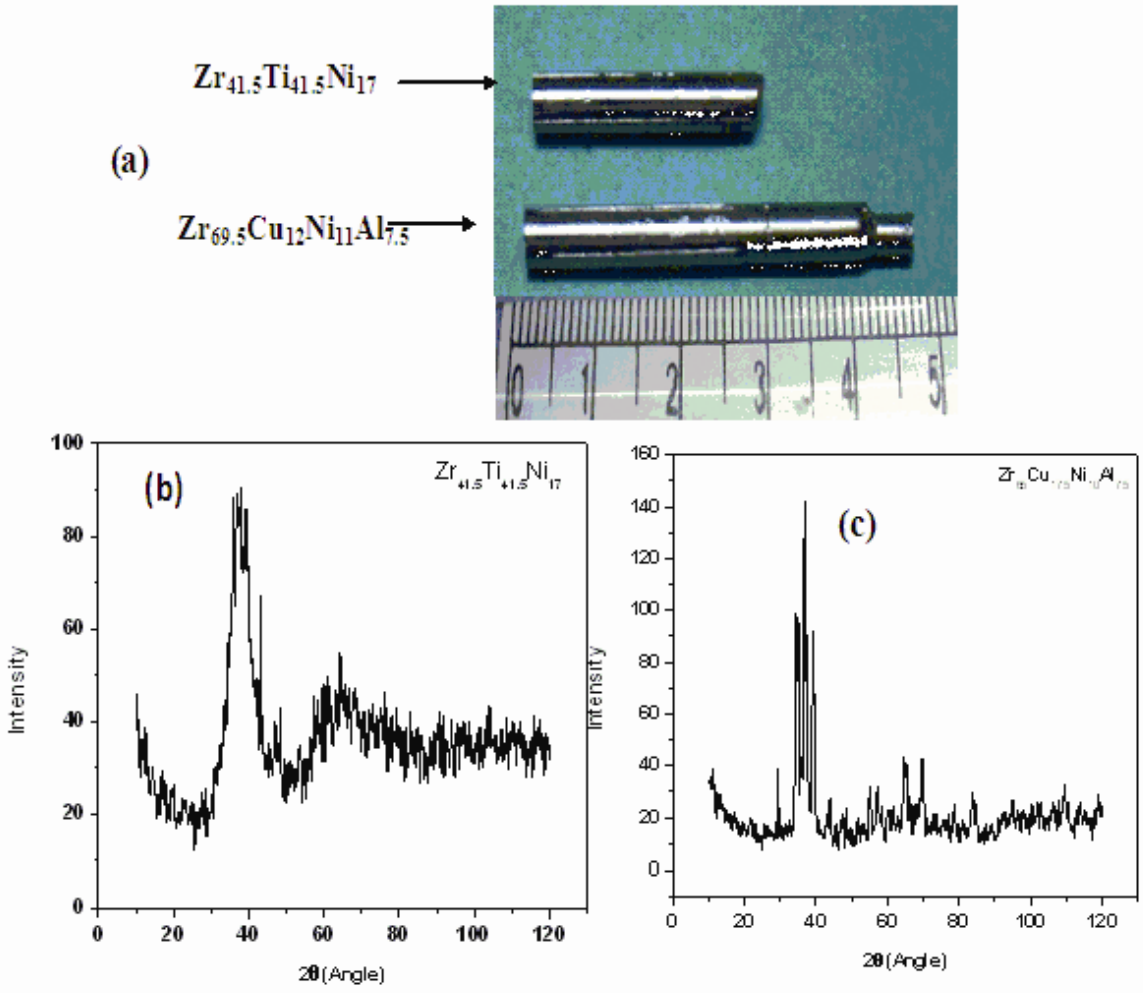

Figure S1

(a) Suction casted 3 mm diameter cylindrical rods of $Zr_{41.5}Ti_{41.5}Ni_{17}$, $Zr_{69.5}Cu_{12}Ni_{11}Al_{7.5}$ XRD pattern of (b) $Zr_{41.5}Ti_{41.5}Ni_{17}$ and (c) $Zr_{69.5}Cu_{12}Ni_{11}Al_{7.5}$ cylindrical rod.

Table S1 Glass-forming-ability parameters

	$Zr_{69.5}Ni_{11}Cu_{12}Al_{7.5}$	$Zr_{41.5}Ti_{41.5}Ni_{17}$
Transition Temperatures (^{o}C)		
Glass (T_g)	368	423
Crystallization (T_x)	421	522
Melting (T_m)	850	800
GFA (γ)		
$\gamma = \left(T_g / T_m \right)$	0.427	0.533
$\gamma = \left(\frac{T_x}{T_m + T_g} \right)$	0.343	0.429
$\gamma = \left(\frac{2T_x - T_g}{T_m} \right)$	0.551	0.782

S1. Method of Ni K-edge XAFS fitting for Zr-Cu-Ni-Al, based on AIMD model

From AIMD distribution in Fig. 5b, we observe that Ni-Ni has narrow distribution $\left(2\sigma = 0.28\text{Å}\right)$ [*i.e.* $\left(\sigma^2_{NiNi} = 0.019\,\text{Å}^2\right)$]. For XAFS fitting, we could represent Ni-Ni/Cu with single scattering path centered around $\left(R_{NiNi} \approx 2.7\text{Å}\right)$ and conventionally fit this path with $\left(N, \sigma^2, R\right)_{NiNi}$ variables.

On the other hand, Ni-Zr peak is significantly broadened $\left(2\sigma = 0.44\text{Å}\right)$ [*i.e.* $\left(\sigma^2_{NiZr} = 0.048\,\text{Å}^2\right)$]. For fitting, we generated different Ni-Zr bond-lengths (in intervals of 0.1 Å) centered at peak maxima $\left(R_0 \approx 2.67\text{Å}\right)$ and covering the theoretical peak spread viz. 2.47-3.27 Å (Fig. 5b). [For XAFS fit range ($R = 1.5 - 3\text{Å}$), contribution from paths beyond 3.27 Å is negligible.] Accordingly, we split NiZr path in feffit.inp file into sub-paths *(i)* with their respective bond-lengths $\left(R_i\right)$ defined *wrt* $\left(R_0\right)$ (Table S2). [R_0 corresponds to path $\left(i = 0\right)$]. During fitting, we varied $\left(R_0\right)$ which automatically fixed $\left(R_i\right)$ for all the sub-paths.

To define CN of each path, we generated normalized coordination (CN) viz. $\left(N_i^{nor}\right)$, from Fig. 5b (Table S2). Normalization was performed *wrt* peak maxima amplitude (at R_0) *i.e.* $\left(N_{i=0}^{nor} = 1\right)$; this constrains CN of each path *wrt* $\left(i = 0\right)$ path. During fitting, we used common scaling factor "A" (variable) to generate the actual CN of each sub- path *i.e.* $\left(N_i\right) = A \times \left(N_i^{nor}\right)$. Average CN for NiZr is deduced from cumulative contribution of all these sub-paths $N_{NiZr} \propto \left(\sum_i N_i\right)$, normalized *wrt* number of Ni atoms in the configuration.

After defining these scattering path constraints in feffit.inp, we fitted the data by varying $\left(R_0, A\right)$ and common DWF for each of these paths. We obtained good fit (shown in Fig.8a) Our fit results: $R_{NiZr} = R_0 = 2.67\text{Å}$; $N_{NiZr} = 4.1 \pm 0.6$. [DWF of each sub-path was low and consistent with bond-length separation of 0.1 Å.] Total CN around Ni (including Ni/Cu and Zr neighbors): $N_{Ni}^{XAFS} = 4.5$.

[Note that we have also verified AIMD model by fitting with (constraining): $N_{NiZr} = 8$ (as obtained directly from AIMD distribution average) and $\left(\sigma^2_{NiZr}\right)$ as variable. $\left(N = 8, \sigma^2 = 0.06\,\text{Å}^2\right)_{NiZr}$ yielded good fit quality and consistent with AIMD distribution.]

Table S2 Parameters defined *wrt* $\boldsymbol{R_0 = 2.67\text{Å}}$ and input into feffit.inp

$\boldsymbol{i =}$	$\boldsymbol{-2}$	$\boldsymbol{-1}$	$\boldsymbol{0}$	$\boldsymbol{1}$	$\boldsymbol{2}$	$\boldsymbol{3}$	$\boldsymbol{4}$	$\boldsymbol{5}$	$\boldsymbol{6}$
$\boldsymbol{(R_i - R_0)}$	**−0.2**	**−0.1**	**0**	**0.1**	**0.2**	**0.3**	**0.4**	**0.5**	**0.6**
$\boldsymbol{(N_i^{nor})}$	**0.396**	**0.901**	**1**	**0.8**	**0.562**	**0.419**	**0.301**	**0.239**	**0.213**