Supplementary Information 13

To study the effect of temperature on the compression yield strength, σ_y, we performed uniaxial compression test at different temperatures using a $Cu_{60}Zr_{40}$ metallic glass sample of the dimensions of 10x5x20 nm^3 (in the *x*, *y* and *z* directions, respectively) with PBCs in all dimensions resembling the bulk state of the material. The typical engineering stress-strain curves are presented in Fig. S1(a) for the temperature range of 50 K (~ 0.06 T_g) to 480 K (~ 0.6 T_g). Fig 1(a) clearly shows that the peak stress (*i.e.* the yield strength, σ_y) of the MG sample reduces by increasing the temperature. It is understood that[2-4] the mechanical failure of bulk metallic glasses at temperatures lower than the glass transition temperature (T_g) arises from the result of localized shearing induced by the applied stress.[3] Indeed, the applied stress biases the local energy landscape by making some relatively unstable atomic clusters undergo shearing to form shear transformation zones (STZs),[2] which in turn leads to initiation and propagation of shear bands (SBs) along the principle shear direction. In the formation of STZs, the applied stress and temperature collaborate, that is, increasing the temperature facilitates the formation of STZs at lower applied stresses.[2, 5] Consequently, increasing the temperature reduces the mechanical strength of the glass. Fig. 2(b) shows the variation of yield strength against temperature obtained from our simulations (the scattered dots), as well as the linear approximation (dashed-line) employed in the discussion of our experimental results. It can be seen that in the temperature range of our experiments (130 K to 300 K), the MD results confirm the linear dependence (slope ~ $3x10^{-3}$) of the compressive yield strength on the temperature.

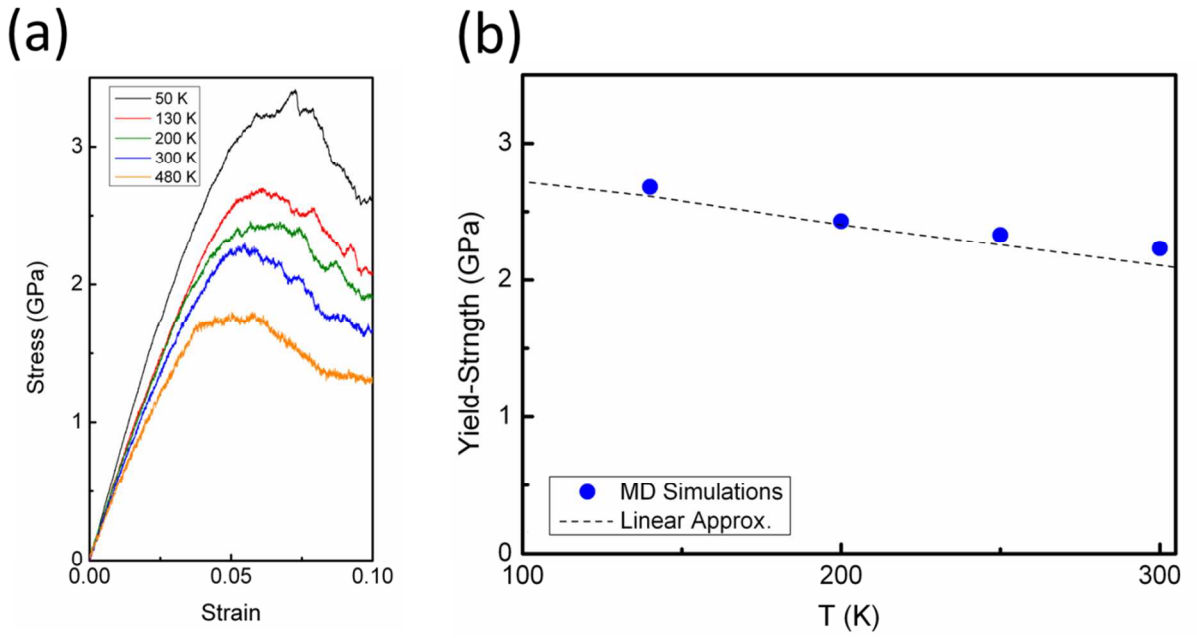

Fig. S1| (a) Engineering stress-strain curves for the $Cu_{60}Zr_{40}$ metallic glass under uniaxial compression test at different temperatures from 50 K to 480 K. **(b)** Variation of yield strength, σ_y, with temperature at the temperature range of our experiments (130 K-300 K) obtained from molecular dynamics (scattered dots) and the suggested linear approximation to explain the experimental results (dashed-line).