Structural signature in amorphous alloy formation and plastic deformation

Supported by the Key Project and the Fund for Creative Research Groups of the National Natural Science Foundation of China, Prof. WANG Weihua and his group from Institute of Physics, CAS, together with their cooperative partner Prof. LI Maozhi from Renmin University of China, adopted molecular dynamics simulations to carry out their research on structural and dynamical features for the glass forming ability (GFA) in a model CuxZr100-x metallic glass-forming systems. It is revealed that not only the 〈0,0,12,0〉 icosahedral clusters but also some Zr-centered clusters such as 〈0,2,8,6〉, 〈0,1,10,4〉 and 〈0,1,10,5〉 play a key role in slowing down the dynamics in CuZr system. While Zr-centered clusters fundamentally determine the stability and slow dynamics, they are further enhanced by 〈0,0,12,0〉. Due to the strong spatial correlation between 〈0,0,12,0〉 and these Zr-centered clusters, their relative population influences the dense packing and dynamics in metallic glasses, and further the GFA. The research, which was published in *Appl. Phys. Lett.* 96, 021901(2010) and highlighted by Nature Asian Materials website (http://www.natureasia.com/asia-materials/highlight.php?id=648), could provide deep understanding on some important issues of glass formation mechanism.

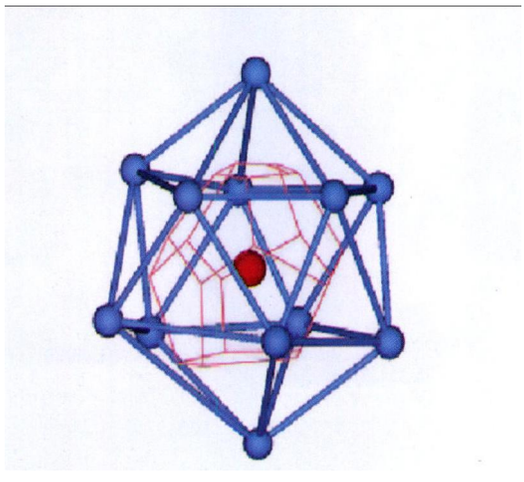

Fig. 1 A cluster in CuZr binary metallic glass. It is a distorted icosahedra and has close relation with the glass forming ability of alloys.

More recently, they have studied, with molecular dynamics simulations, the structural features of a model CuZr metallic glass during deformation. Spatially heterogeneous irreversible rearrangement is observed in terms of non-affine displacement. It is revealed that the regions with smaller non-affine displacement have more Voronoi pentagons, while in those with larger non-affine displacement other types of faces are more populated. They used the degree of local five-fold symmetry as the structural indicator to predict the plastic deformation of the local structures and found that the plastic events prefer to be initiated in the regions with less degree of local five-fold symmetry and propagate toward the region with more degree of local five-fold symmetry. The research, which was published in Phys. Rev. Lett. 106, 135503(2011), is of important significance to understand the long standing issues of plastic mechanism of amorphous materials.

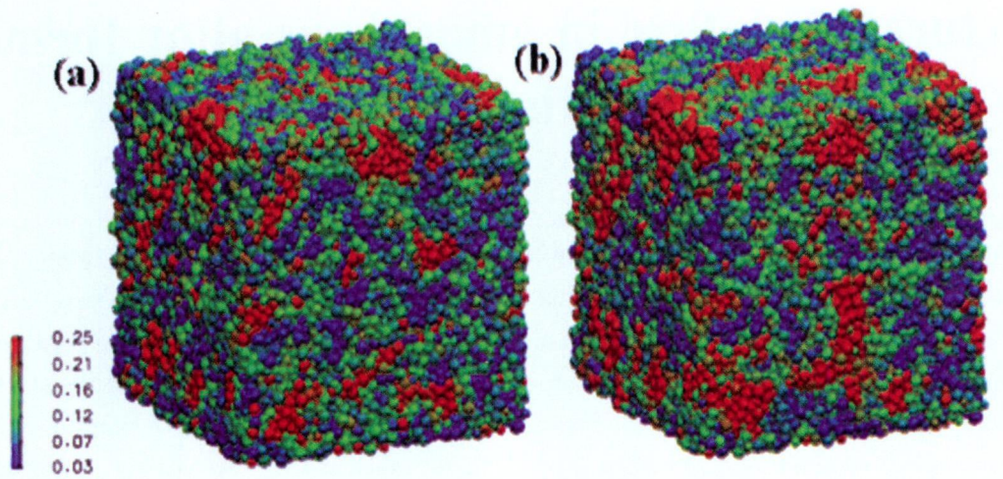

Fig. 2 The atomistic configurations of the non-affine displacement D2 illustrated by colors at the strain of 5% with time interval of = 10 ps (a) and 40 ps (b).

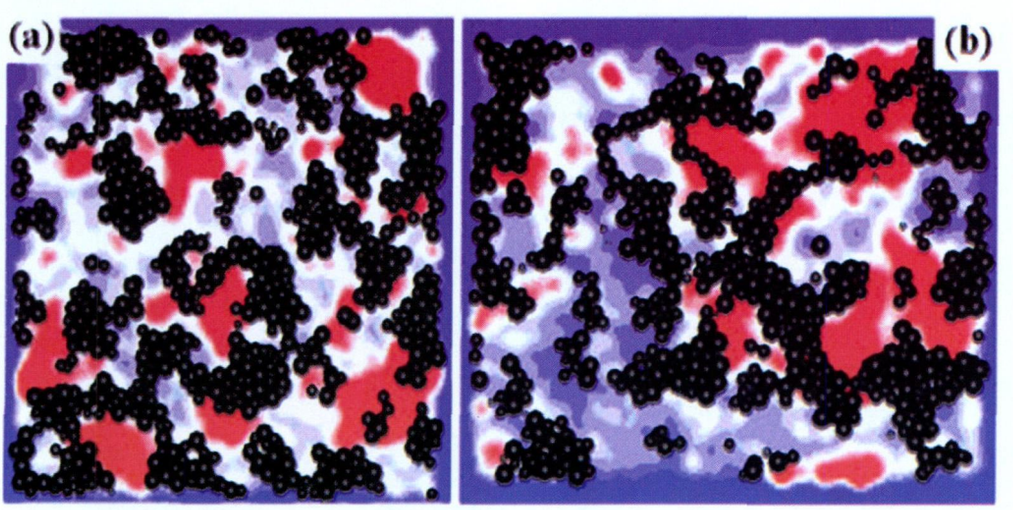

Fig. 3 The correlation between the structures having more degree of local five-fold symmetry and the irreversible rearrangement during deformation at the strain of (a) 5% and (b) 10%.