## Atomic structure of Co92-xBxTa8 glassy alloys studied by ab initio molecular dynamics simulations

Di Ma<sup>1</sup>, Jing Zhang<sup>1</sup>, Yaxin Di<sup>1</sup>, Jianfeng Wang<sup>1</sup>, Shaokang Guan<sup>1</sup>, and Tao Zhang<sup>2</sup>

<sup>1</sup>Zhengzhou University <sup>2</sup>Beihang University

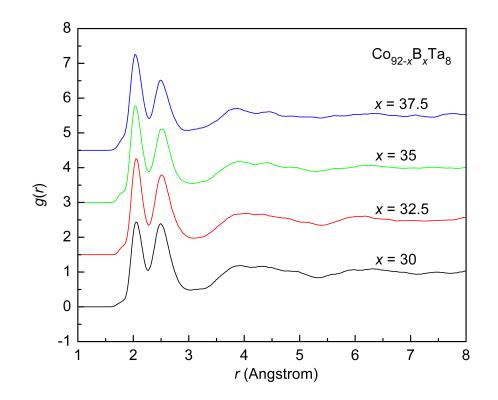
April 28, 2020

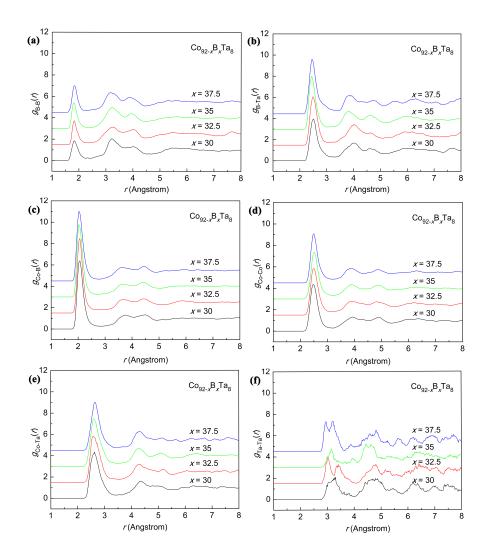
## Abstract

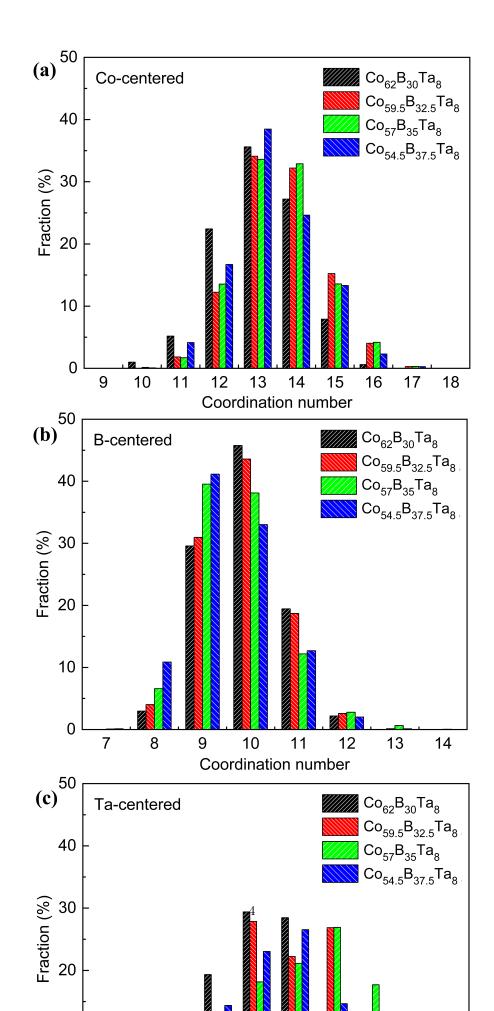
The ab initio molecular dynamics simulations are performed to study the atomic structures of Co92-xBxTa8 (x = 30, 32.5, 35, 37.5, at.%) glassy alloys. The result shows that the local packing of B-centered clusters is more efficient than that for Coand Ta-centered clusters. It is also found that B-centered clusters are the primary structure-forming clusters. The Kasper polyhedra with a Voronoi index of <0.360 and <0.280 are dominant in B-centered clusters. Specially, the <0.360 clusters can form a robust network structure, which plays a key role in mechanical properties. Such a network structure has a higher activation barrier for structural rearrangement and a better resist to plastic flow. Thus, the increase in the fraction of <0.360 with B content would result in an increase in yield strength as well as a sharp decrease in compression plasticity.

## Hosted file

Manuscript.docx available at https://authorea.com/users/306862/articles/437975-atomic-structureof-co92-xbxta8-glassy-alloys-studied-by-ab-initio-molecular-dynamics-simulations







Posted on Authorea 30 Mar 2020 — CC BY 4.0 — https://doi.org/10.22541/au.158557474.40133509 — This a preprint and has not been peer reviewed. Data may be preliminary.

