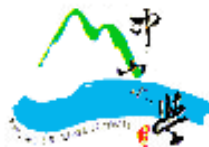




# The applications of MD simulation on the material properties

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國立中山大學

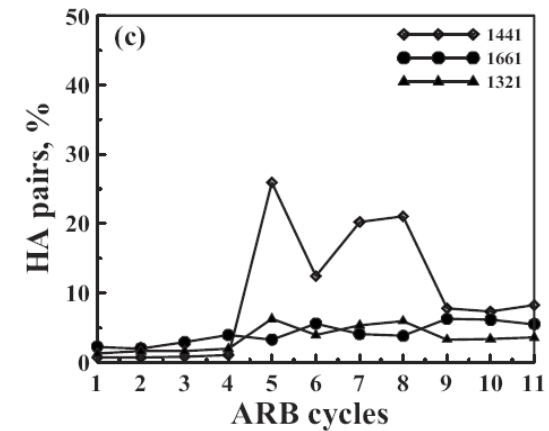
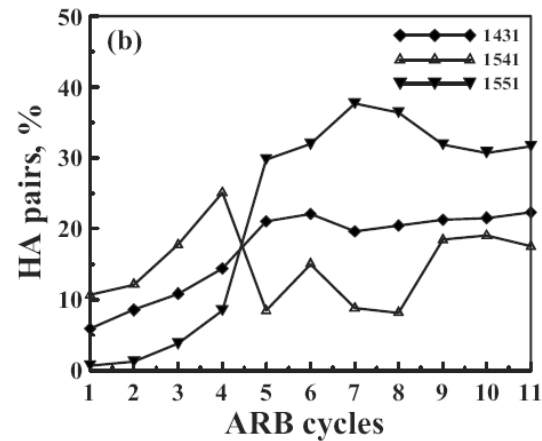
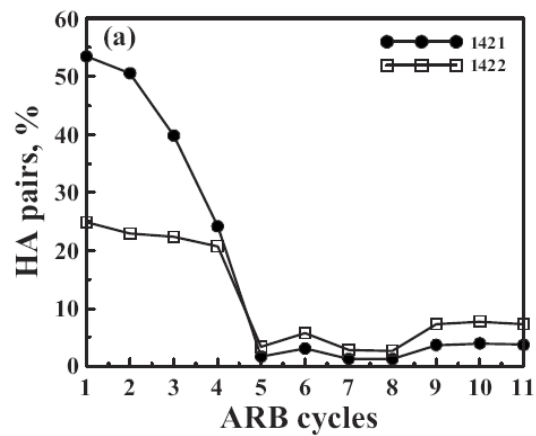
National Sun Yat-Sen University

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## ■ Current topics:

- The structural evolution from nanocrystalline to amorphous phases during ARB process.
  - Atomic Simulation of Vitrification Transformation in Mg-Cu Thin Film
  - cyclic loading fatigue on Zr-Cu bulk metallic glass
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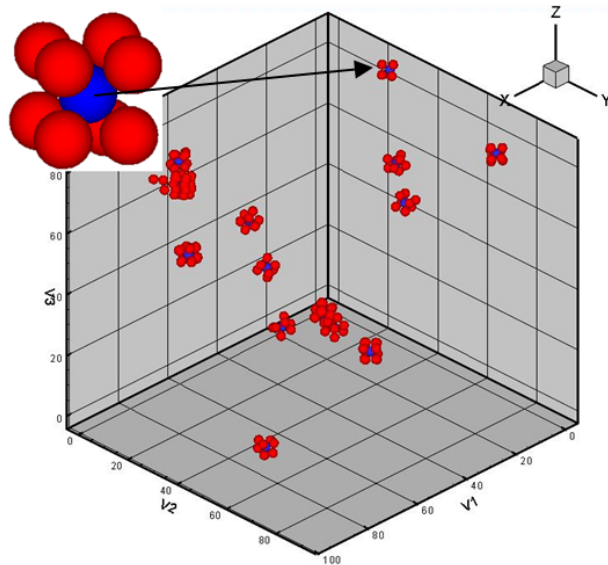
“Atomic structure evolution of Zr-Ni during severe deformation by HA pair analysis” PRB 2007



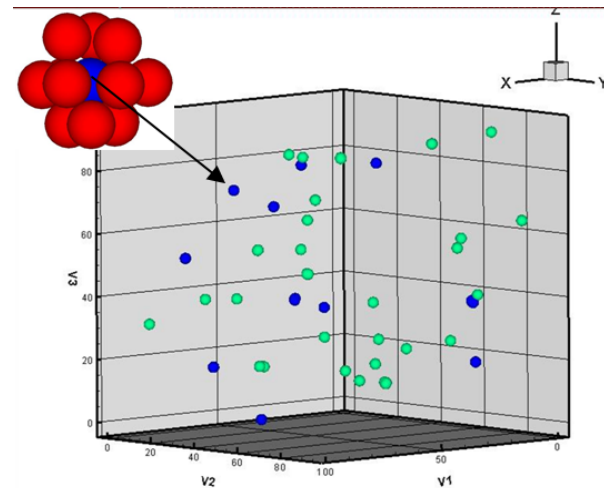
The current simulation results reveal that the short-range icosahedra structures always play an important role during the course of crystalline-to-amorphous transition, both during the solid state strain-induced severe deformation and rapid cooling processes.

An investigation of cyclic loading fatigue on ZrCu bulk metallic glass (BMG) by MD simulation. Some interesting results of this topic are shown in the below figures:

(a)

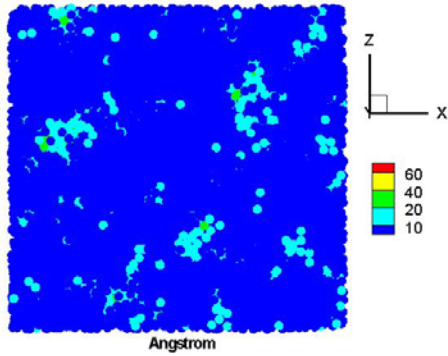


(b)

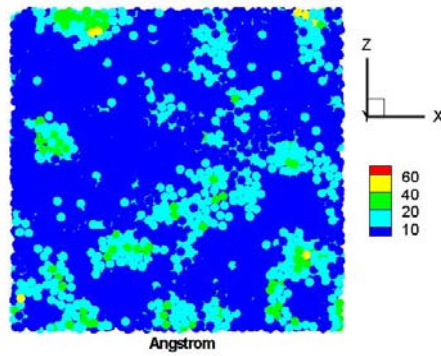


The scheme of the superimposed projections of the ordered atoms during the stress-control mode at  $\sigma_{\max} = 2$  GPa. The blue circles represent the central atoms, and red circles represent the surrounding atoms of a B2 structure. Note that this scheme represents the superimposition of all occurrences of the atoms that have occurred over the whole 50 cycles. (a) B2 clusters (b) FCC or HCP clusters.

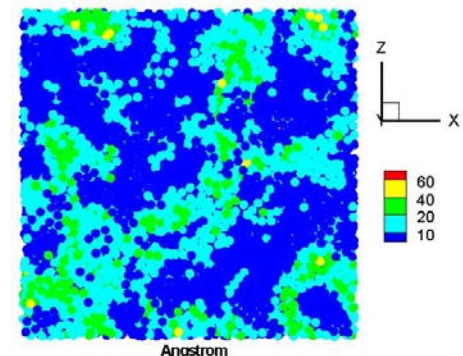
# The local strain distribution of tension mode fatigue at different cycles (stress control mode)



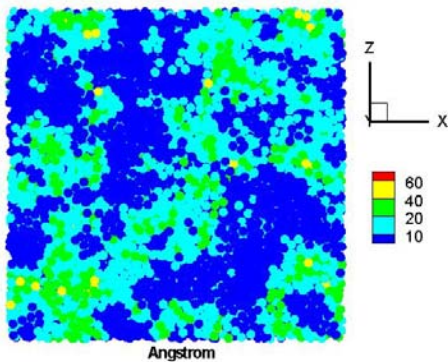
Cycle one



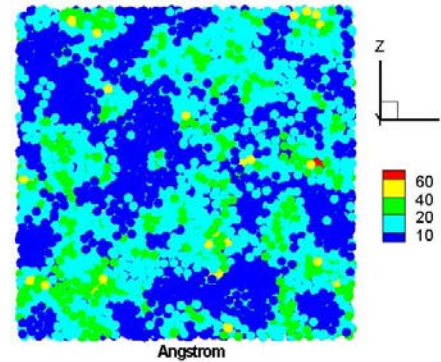
Cycle ten



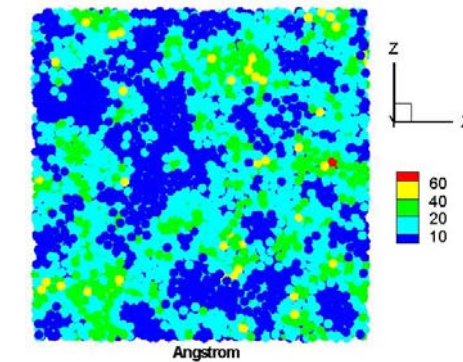
Cycle thirty



Cycle sixty

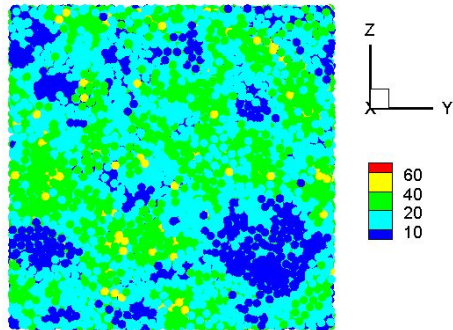


Cycle eighty

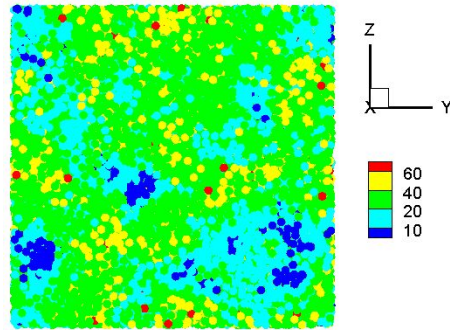


Cycle one hundred

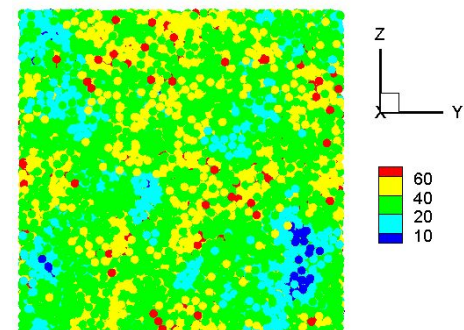
# The local strain distribution of tension mode fatigue at different cycles (strain control mode)



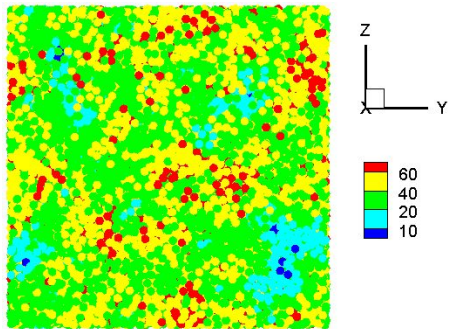
Cycle one



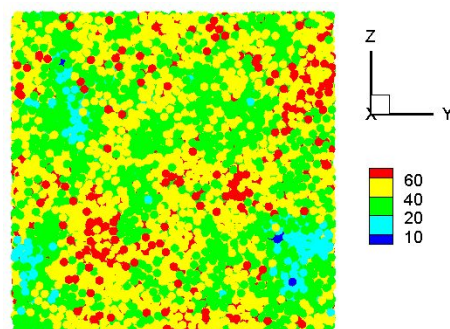
Cycle four



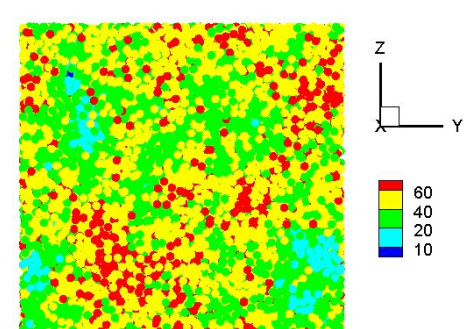
Cycle nine



Cycle fifteen

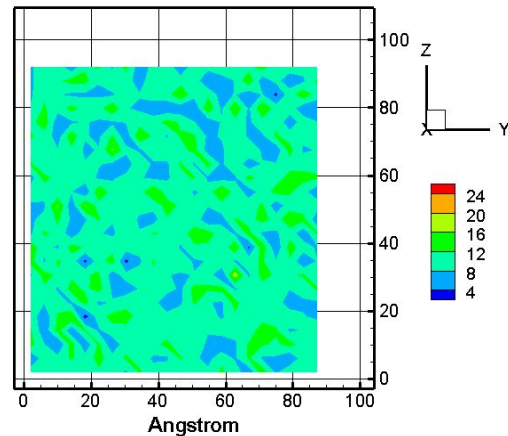


Cycle twenty

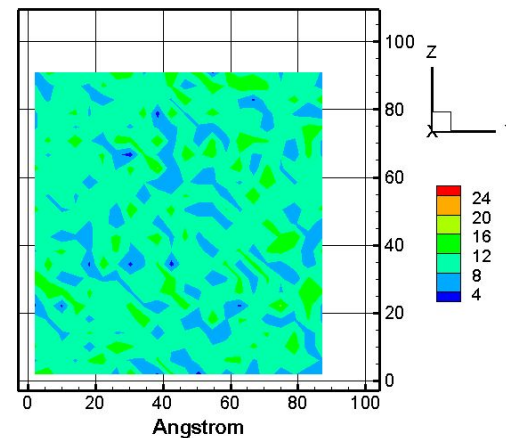


Cycle twenty-five

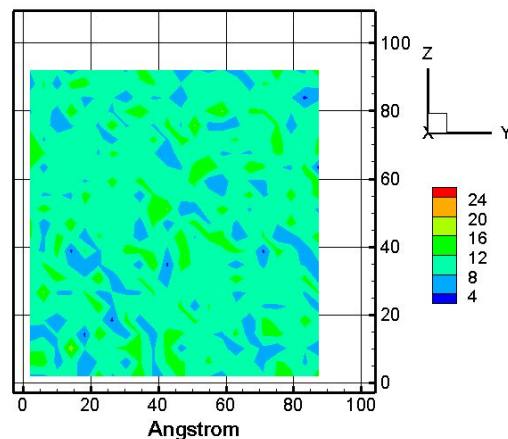
## Density profile of tension mode fatigue at different cycles



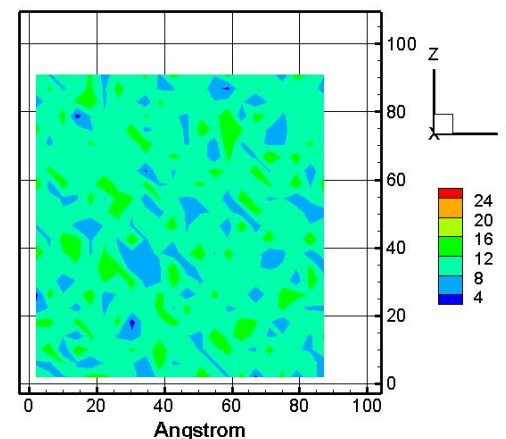
(a) cycle twelve, loading



(b) cycle twelve, unloading



(c) cycle twenty-five, loading



(d) cycle twenty-five, unloading

Density profile of the strain-control fatigue at different cycles. The blue color represents the lower density (as the regions with the free volume). The numbers of the horizontal and vertical axes are in the unit of angstrom.

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## Extending topics can be studied in the future

- Crack growth under cyclic loading in the MGs
  - Re-crystallization in the cyclic loading/fatigue.
  - reversible and irreversible plastic events in fatigue.
  - The modeling study of shear transformation zone in the MGs fatigue.
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