Longitudinal Creep Behavior of Nanocrystalline Ni-NiZr Glass Nanocomposite

Md. Meraj and Snehanshu Pal
Department of Metallurgical and Materials Engineering
National Institute of Technology Rourkela,
Rourkela- 769008, Odisha, India

Abstract

Longitudinal creep behavior of nanocomposite for NC Ni-NiZr glass has been studied at various temperatures (from 1200 to 1400 K) at 1 GPa stress using MD simulations. A simulation box of the specimen 15.85 × 15.85 × 15.85 nm dimension (contains 312,924 atoms) is taken for performing MD simulation. Common neighbor analysis (CNA), Centro-symmetry parameter (CSP) analysis, Wigner–Seitz defect analysis and radial distribution function (RDF) have been carried out to investigate the structural evolution and deformation mechanism of nanocomposite specimen during creep process. Self-diffusion of nanocomposite specimen has been performed using MD simulation for interface region and whole specimen at different temperature.

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Presented by: **Md. Meraj**

Co-author: Prof. Snehanshu Pal

Department of Metallurgical and Materials Engineering

National Institute of Technology Rourkela,

Rourkela- 769008, Odisha, India

17th Edition of International Conference on

Emerging Trends in Materials Science and Nanotechnology (Nanomat- 2018), 26-27 April, 2018, Rome, Italy

What is Nanocrystalline Material?

Nanocrystalline (NC) materials are characterized by a grain size in the range of 1–100 nm.

What is special about Nanocrystalline Material?

It has unique mechanical, electrical, magnetic and optical properties with respect to its macroscopic counterpart, and also allows flexibility for producing micro and nano scale devices.

Mechanical Behaviour Perspective :

The high strength of NC material at room temperature (Gleiter, 2000)

Reason: It has higher volume fraction of grain boundaries (GBs) and triple junctions in comparison with conventional poly-crystalline materials .

But, the **strength** of Ultrafine grained (i.e. grain size less than 20–25 nm) **NC metal starts to decrease** due to softening phenomenon and such ultrafine grained NC metals follow an **inverse Hall-Petch relation** (Chokshi et. al., 1989).

Some literature survey

- In case of fine grain NC metals, creep deformation is mostly facilitated by grain boundary (GB) diffusion (Coble creep [Coble, 1963]) and/or lattice diffusion (Nabarro–Herring creep [1950]).

- Ni-Zr glass is considered for this study owing to its high thermal stability, ultra-high strength, excellent corrosion resistance and good ductility [Chen et al., 2007].

- In both NC and submicron-grained zirconia, grain boundary sliding is dominating factor during deformation of creep process via experimentally is reported by Ghosh and Chokshi, 2014.

- Understanding of mechanical behaviour of such glass reinforced metal composites is essential in order to broaden its application domain, actually studies carried out in this front are limited [Markó et al., 2014].

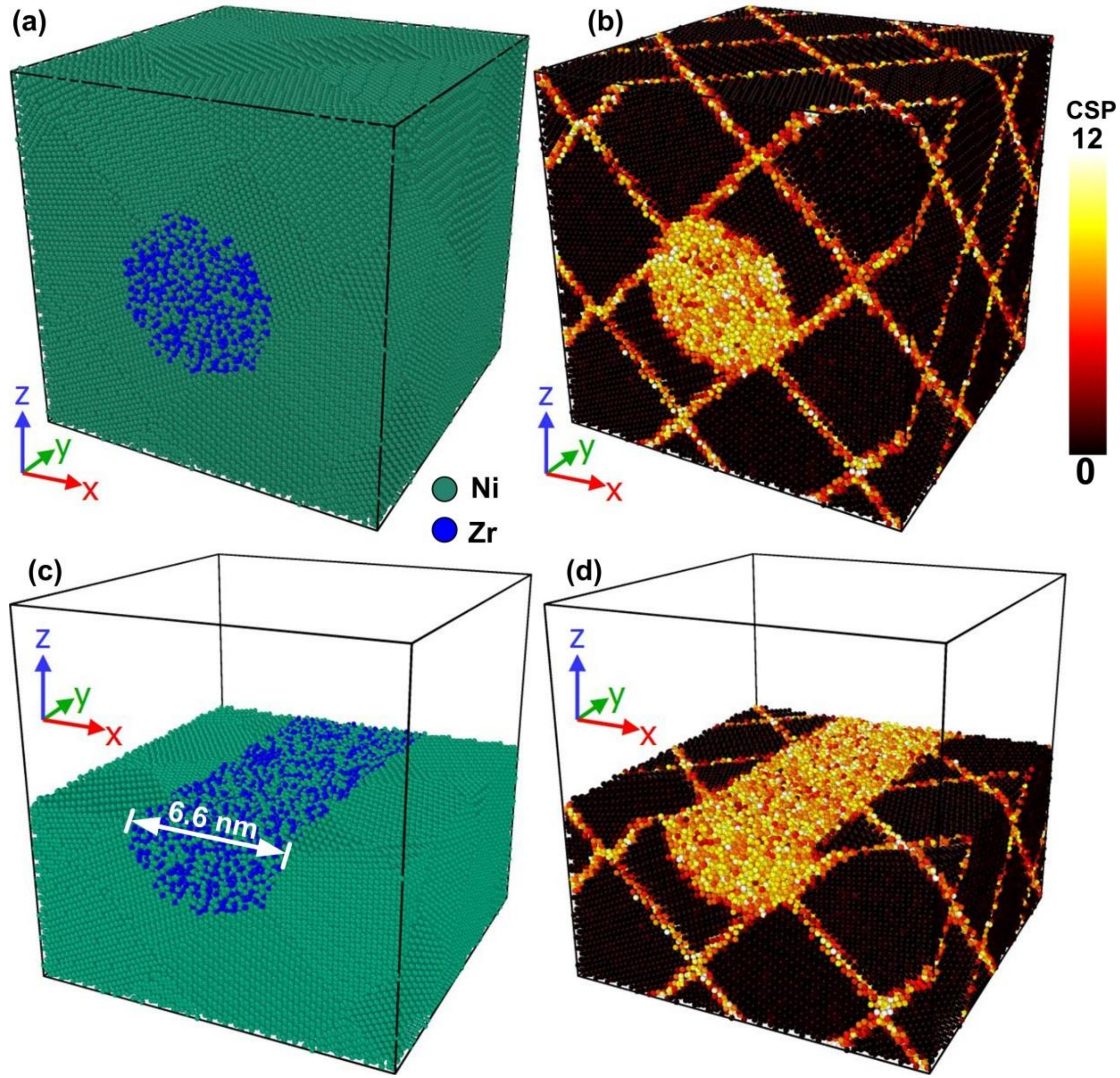
- Investigation of creep properties of glass reinforced metal composites is crucial for enhancing their high temperature application.

To study mechanical behavior of NC metallic system why atomistic simulation (molecular dynamics simulation)?

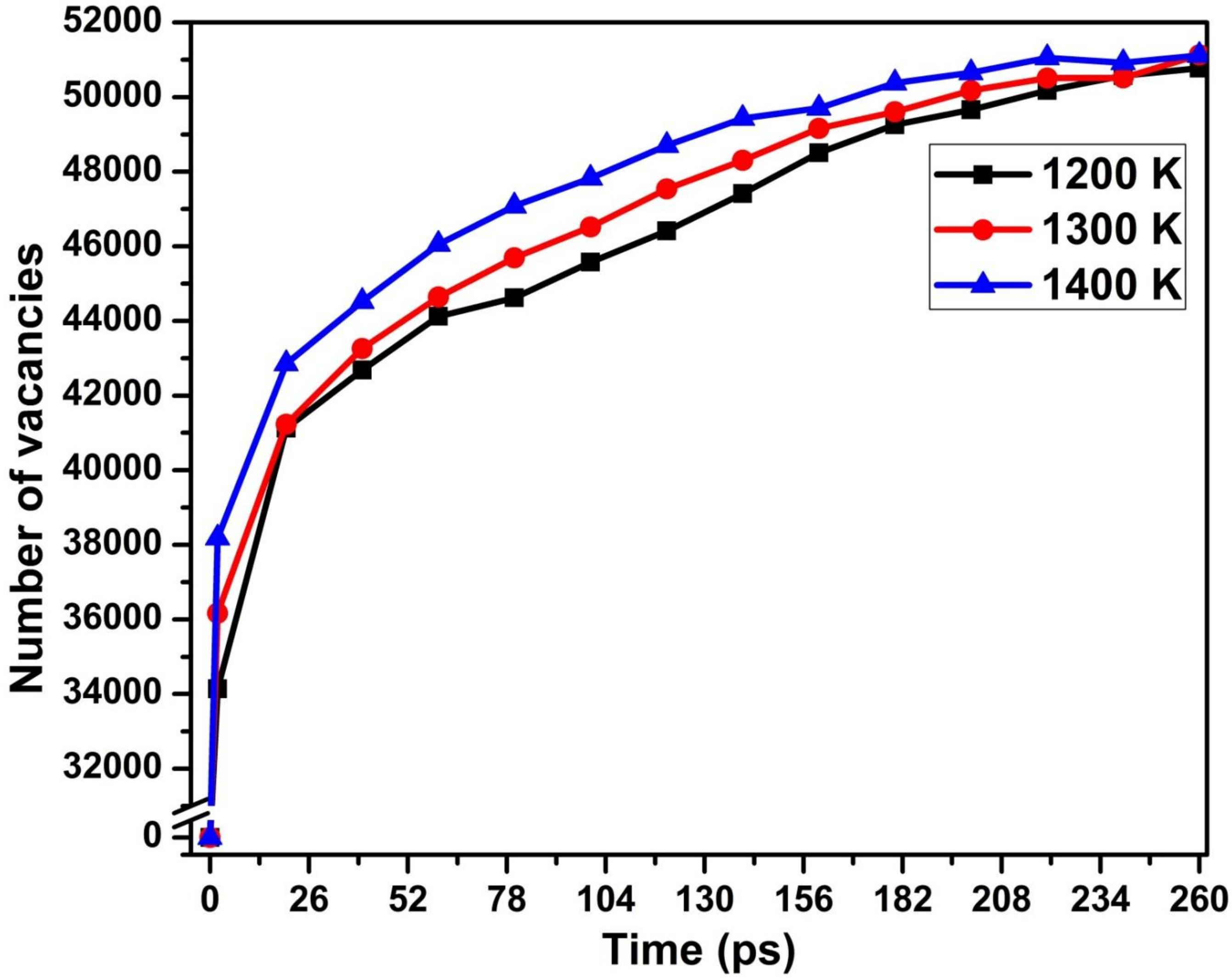
- Investigation of mechanical properties of nano-materials through experimentation is very difficult to perform as well as expensive.

- Molecular Dynamics (MD) simulation become already a useful and reliable tool to identify the underlying deformation mechanism at nano-scale. Currently is also becoming potential way for simulating creep deformation and identifying deformation mechanism of creep for NC materials.

3D atomic configuration snapshots NiZr glass reinforced Ni nano-composite specimen



Plots of evaluated number of vacancy vs. time for nano-composite specimen during creep process



Number of vacancy vs. time plots

Conclusions

- It is found from creep curves that primary and secondary creep regime is reduced with increasing creep temperature.
- Creep rate for nano-composite specimen is observed to be shifted downward with increasing creep temperature after 180 ps time period.

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THANK YOU