Creep behavior study for ultra-fine grained nano-crystalline metallic systems using atomistic simulation

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Molecular dynamics (MD) simulation based study of creep behaviour nano crystalline metal and nano joint between two different nano-crystalline metal have been performed. Simulation of creep behaviour of nano crystalline metal is performed taking nano crystalline Nickel as a representative system. On the other hand, creep behaviour of nano joint between two different nano-crystalline metallic systems is investigated taking nano joint of nano-crystalline (NC) Ni and Fe-Ni-Cr alloy (18 at% Cr, 8 at% Ni and rest Fe) as representative case. MD simulation has been carried out using EAM (Embedded Atomic Method) potential. Centro-symmetry parameter (CSP) analysis, common neighbour analysis (CNA), radial distribution function (RDF), Wigner-Seitz defect analysis and Voronoi cluster analysis (VCs) have been performed to study structural evolution during creep process. The MD study reveals that the grain boundary diffusion is the governing mechanism of creep deformation in ultra-fine grained (< 10 nm) nano crystalline metallic systems. In case nano joint between two nano metallic systems, the atoms are observed to be displaced more which are nearer to the interface during creep.

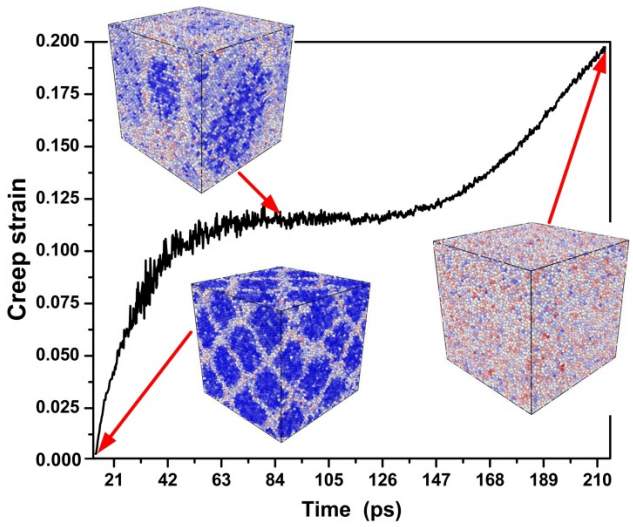

Fig.1: Creep curves of NC Ni with corresponding snapshots during deformation

Key words: Molecular dynamics; creep; nano-joining; nano-crystalline; nickel

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by

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What is Nanocrystalline Material?

Nanocrystalline 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).

Motivation for creep behaviour study of Nanocrystalline Materials

Due to the high volume fraction of GBs and triple junctions, ultrafine grained NC materials are sensitive to high temperature and have **lower strength at high temperature.**

Accordingly investigations on the creep properties of ultrafine grained NC materials is necessary for increase their utilization in high temperature application domain.

Some literatures on experimental creep studies for NC metals

- Segregating solutes at GB causes significant improvement in the strength of the NC materials (Vo et. al., 2011).
- In both NC and submicron-grained zirconia, grain boundary sliding is dominating factor during deformation of creep process (Ghosh and Chokshi, 2014).
- Effects of loading strain rate and stacking fault energy on nano--indentation creep behaviors of nanocrystalline Cu, Ni-20 wt.%Fe and Ni (Hu et. al., 2015).

To study creep behavior of nanocrystalline metallic system why atomistic simulation (molecular dynamics simulation)?

- Investigation of creep 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 indentifying deformation mechanism of creep for NC materials.

Some molecular dynamics simulation study of high temperature deformation of NC metallic system :

- Segregated Cu and Ag solute at grain boundary influence β-Sn grain boundary energy and shear stress according to MD simulation performed by Sellers et. al. 2011.

- The effect of yttrium on creep behaviour of NC magnesium at different temperature and stresses using MD has been investigated by Bhatia et. al., 2015.

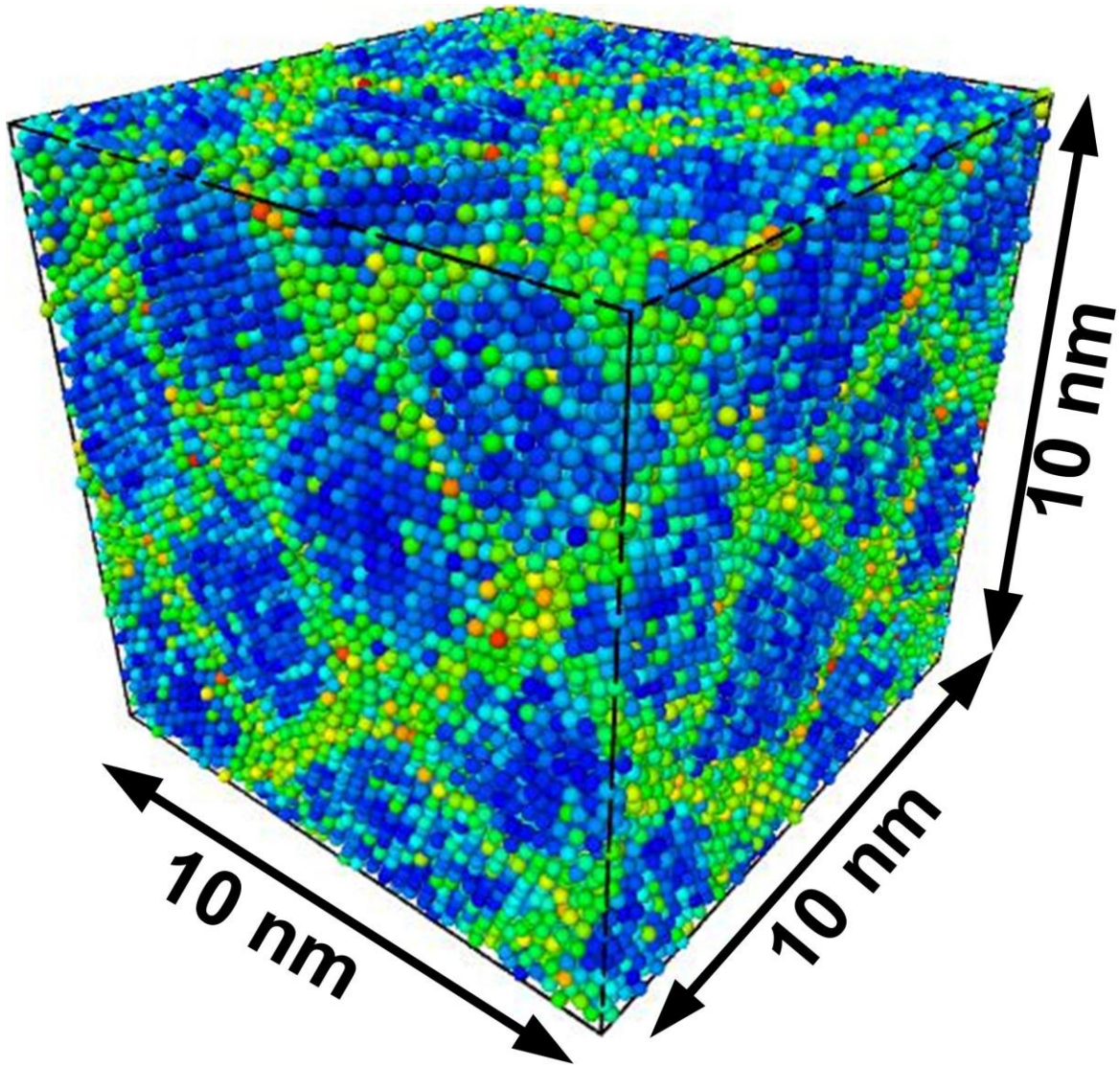
Motivation for studies on creep behavior of ultra fine grained NC metallic system using molecular dynamics simulation :

- The effect of defects on the creep behaviour of NC metallic having ultrafine grain ($d \leq 10$ nm) is needed to be performed.
- Investigation on structural evaluation and deformation features of interface of joint between two ultra-fine-grained nano-crystalline metals at high temperature is due.

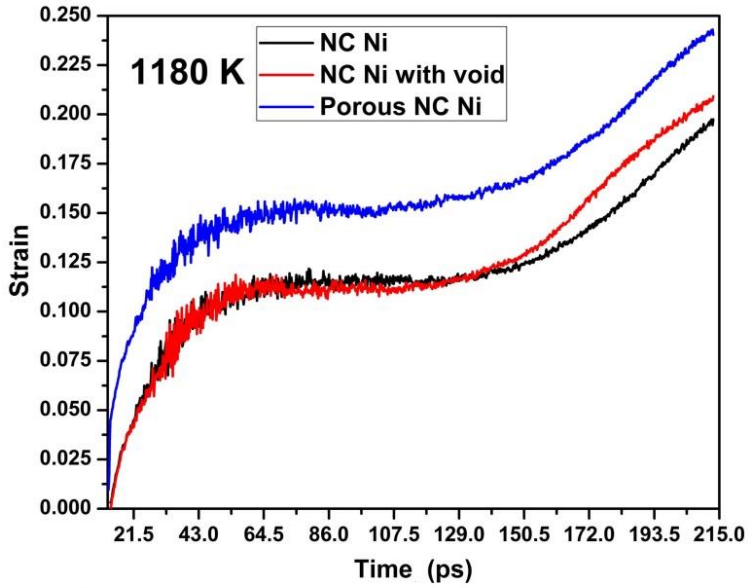
In this talk, following thing will be discussed :

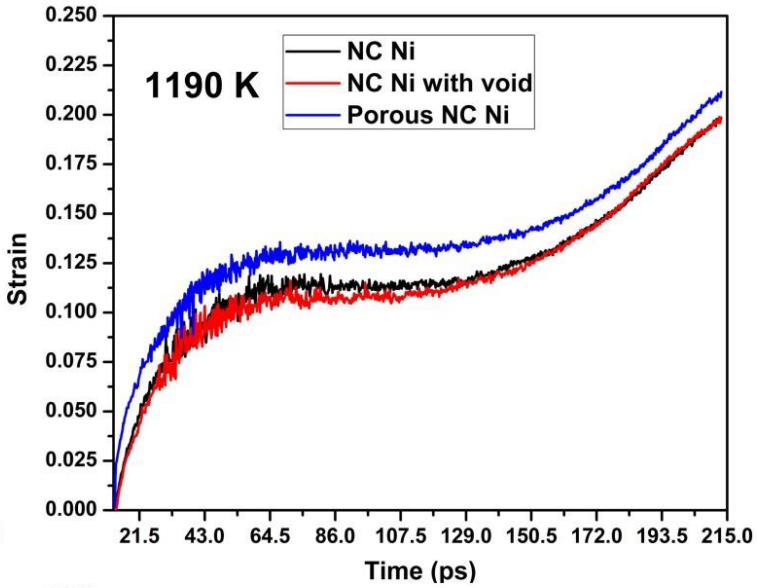
Effect of porosity and void on creep behavior of ultra fine grained NC Ni.

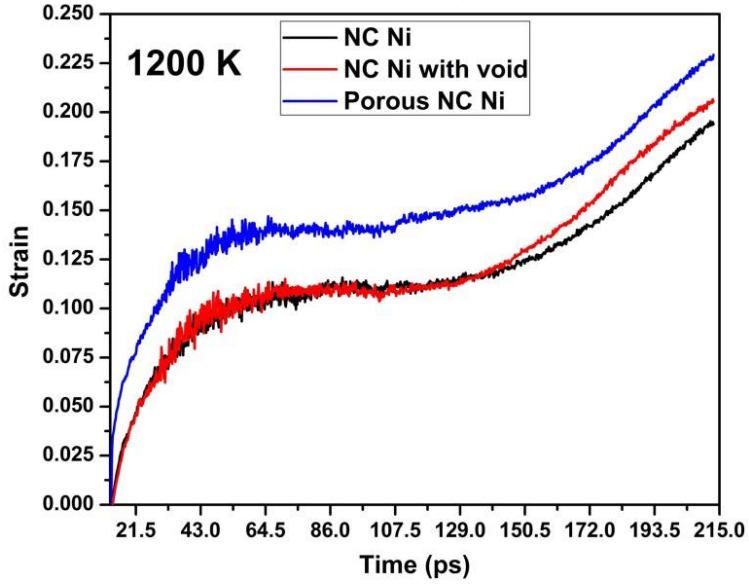
Initial atomic configuration of NC Ni specimen

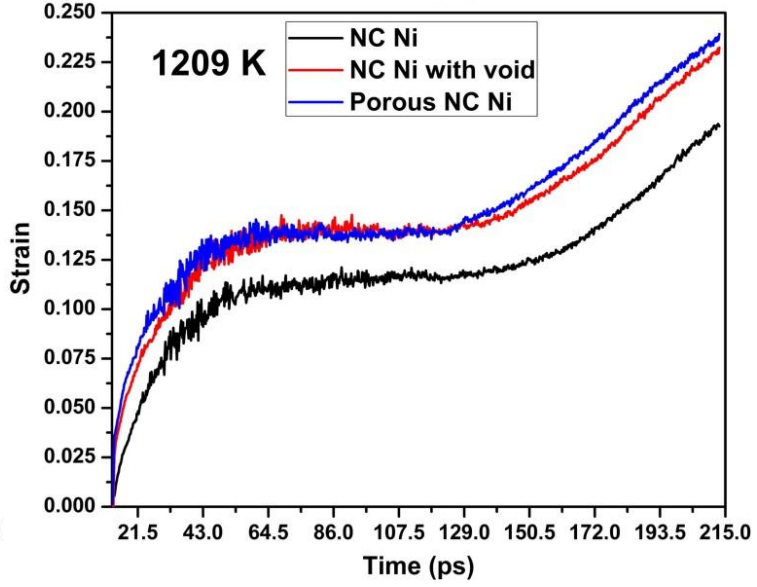


Creep curves of NC Ni with and without defect specimens









Conclusions

Coble creep mechanism is dominant in case of ultra-fine (~4 nm) grained NC Ni, and the porous NC Ni exhibits very poor creep properties compared to perfect NC Ni and NC Ni with single void.

Thank you