Indian Institute of Technology Kanpur, Kanpur-208016, U.P., India.
Nov 11-14, 2016

The effect of porosity on creep behavior of nickel single crystal: An atomistic simulation based study

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ABSTRACT

Tensile creep behavior of single crystal Ni with and without presence of porosity in various atom percent (i.e. 0, 10 and 18 at. %) has been studied using a molecular dynamic (MD) simulation with an embedded atom method (EAM) potential. A10 nm x 10 nm x 10 nm cubic simulation box is taken for performing MD simulation which contained 92597 atoms for 0 at % porosity, 83387 atoms for 10 at % porosity and 75948 atoms for 18 at % porosity. MD simulation of creep for this single crystal has been carried out at 907 ^{o}C, 917 ^{o}C, 927 ^{o}C and 936 ^{o}C temperatures and constant 1.0 GPa stress. The increase in porosity has strong influence on creep behaviour as revealed from the simulated creep curves. Centro symmetry parameter (CSP) evaluation, common neighbour analysis (CNA), Voronoi clusters (VCs) analysis, radial distribution function (RDF) plots study and Wigner Seitz defect analysis have been carried out to investigate structural evolution of the specimen during creep. It is evident that amorphization during creep deformation process become faster and intensified as atomic fraction of porosity increases.

Simulated creep curve with corresponding 3-D snapshots at 907^{o}C temperature and 1.0 GPa stress for 18 at. % porosity in single crystal Ni specimen is represented in **Figure. 1**. It is found that nano-materials have faster diffusibility of the atoms for 18 at. % porosity of single crystal Ni specimen than 0 and 10 at. % porosity. **The effect of porosity variation (0 to 18 at. % porosity) is prominent on creep process.** The creep curves of specimen are observed to be shifted towards higher creep strain during secondary part of creep with increase of porosity from 0 to 18 at. %.

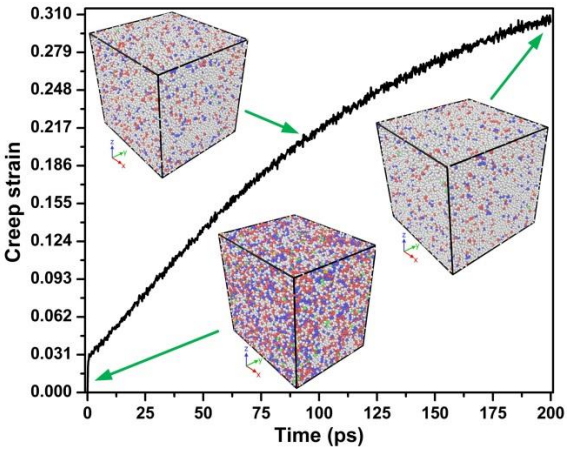

Figure 1. Simulated creep curve with corresponding 3-D snapshots at 907^{O}C temperature and 1 GPa stress for 18 at. % porosity in single crystal Ni specimen.

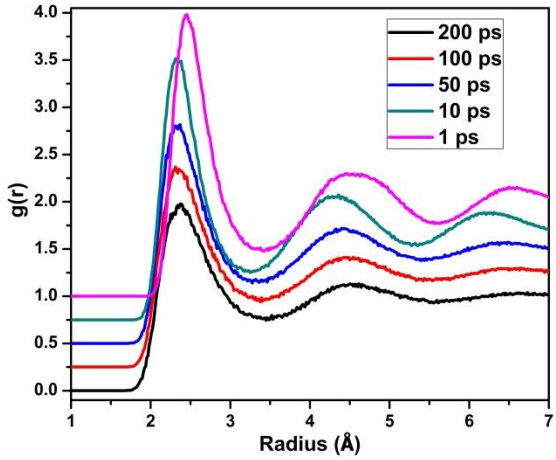

Figure 2. Radial distribution function plots at 907^{o}C temperature and 1 GPa stress for different time step of 18 at. % porosity in single crystal Ni specimen.

Keywords: Molecular dynamics; Creep; Single crystal; Porosity;

References:

[1] S. J. Plimpton, Comp. Phys., 117 (1995) 1-19.
[2] A. Stukowski, Modelling Simul. Mater. Sci. Eng., 18 (2010) 015012.
[3] M. I. Mendelev, M. J. Kramer, S. G. Hao, K. M. Ho, C. Z. Wang, Phil. Mag., 92 (2012) 4454-4469.

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Abstract

Tensile creep behavior of single crystal Ni with and without presence of porosity in various atom percent (i.e. 0, 10 and 18 at. %) has been studied using a molecular dynamic (MD) simulation with an embedded atom method (EAM) potential. A 10 nm x 10 nm x 10 nm cubic simulation box is taken for performing MD simulation which contained 92597 atoms for 0 at. % porosity, 83387 atoms for 10 at. % porosity and 75948 atoms for 18 at. % porosity. MD simulation of creep for this single crystal has been carried out at 907 ^{o}C, 917 ^{o}C, 927 ^{o}C and 936 ^{o}C temperatures and constant 1.0 GPa stress. The increase in porosity has strong influence on creep behaviour as revealed from the simulated creep curves. Centro symmetry parameter (CSP) evaluation, Voronoi clusters (VCs) analysis, radial distribution function (RDF) plots study and Wigner Seitz defect analysis have been carried out to investigate structural evolution of the specimen during creep. It is evident that amorphization during creep deformation process become faster and intensified as atomic fraction of porosity increases.

Introduction

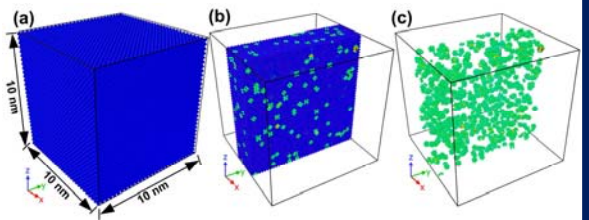
- Utility of nano materials is significant in case of high temperature applications and accordingly the study of creep behaviour of nano materials is highly necessary.
- Creep is known as a time-dependent plastic deformation phenomenon at constant stress and high temperature.
- Experimental study of creep properties of nano materials is difficult, so less numbers of experimental investigations on creep deformation behaviour of nano materials is reported.
- A molecular level study is an efficient tool to understand the mechanism of creep process.
- Creep behaviour study of porous single crystal material using atomistic simulation is not reported so far as per authors' knowledge.

Objective

- To study the effect of porosity on creep behavior of nickel single crystal using molecular dynamics simulation.

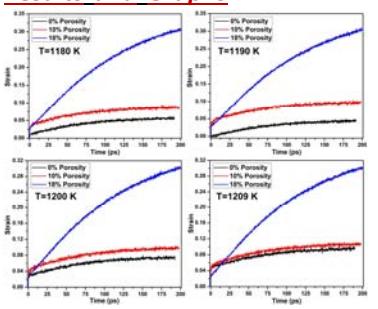
Simulation details

- Single crystal Ni specimen of dimension 10 nm x 10 nm x 10 nm has been taken for performing MD simulation which contained 92597 atoms for 0 at % porosity, 83387 atoms for 10 at % porosity and 75948 atoms for 18 at % porosity.
- MD simulation of creep for this single crystal has been carried out at 1180K, 1190K, 1200K and 1209K temperatures and constant 1.0 GPa stress.
- Energy minimization have been performed by using conjugate gradient algorithm and equilibration has been carried out using NVT ensemble.
- After that the specimens are subjected to uniaxial tensile loading along Y-direction [010] up-till attainment of 1 GPa stress. Then specimens are allowed to deform under constant stress (i.e. 1 GPa).
- Time step is taken as 0.002 ps and boundary conditions applied is periodic in all three directions.
- All the MD simulations have been performed using LAMMPS with an EAM potential.
- CSP, RDF analysis, Wigner Seitz defect analysis, VCs, and CN has been performed during compression using OVITO software.

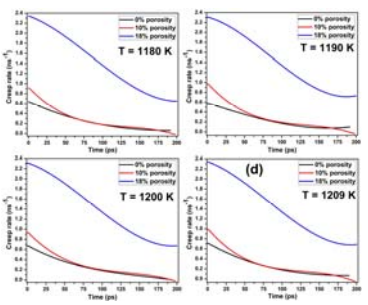


(a) Single crystal (SC) Ni, (b) slice view of 10 at. % porosity SC Ni and (c) only porous surrounded atoms

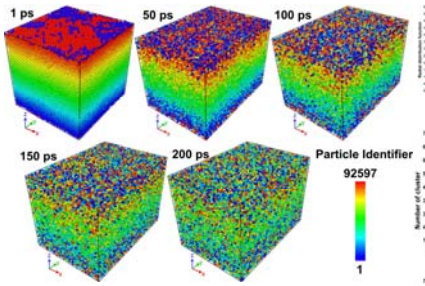
Results and Graphs



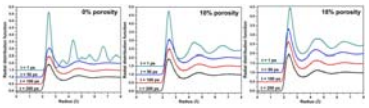
Creep curve with and without porous SC Ni at different temperature



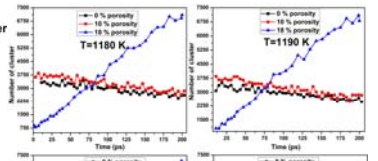
Creep rate vs. time plots with and without porous SC Ni at different temperature



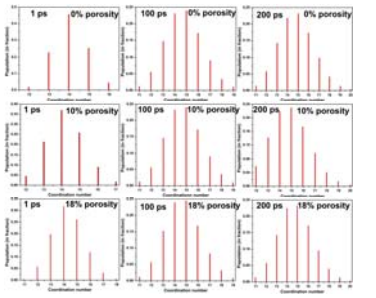
Atomic snapshot of SC Ni for different time step at 1180 K during creep process



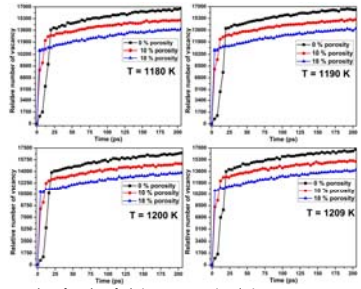
RDF plots for different % porosity at 1180 K temperature.



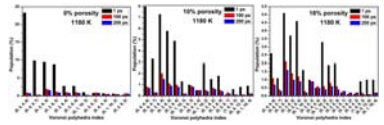
Plots of number of cluster vs. time during creep process



CN of atoms and corresponding population fraction for different time step at 1180 K.



Plots of number of relative vacancy vs. time during creep process



Voronoi polyhedra index and their populations at different time step at 1180 K.

Conclusion

- The MD simulation has been performed to study the effect of porosity on creep behavior of nickel single crystal.
- It has been found that the effect of porosity variation (0 to 18 at. % porosity) is prominent on creep process.
- The creep curves of specimen are observed to be shifted towards higher creep strain during secondary part of creep with increase of porosity from 0 to 18 at. %.
- It is found that nano-materials have faster diffusibility of the atoms for 18 at. % porosity of single crystal Ni specimen than 0 and 10 at. % porosity.

Reference

- S. J. Plimpton, Comp. Phys., 117 (1995) 1-19.
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Presented at 54th National Metallurgists' Day (NMD) celebration and the 70th Annual Technical Meeting (ATM) IIT Kanpur, November 11 – 14, 2016, India