INFLUENCE OF ZIRCONIUM ADDITION ON CREEP BEHAVIOUR OF NANO CRYSTALLINE NICKEL: A ATOMISTIC SIMULATION BASED STUDY

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Abstract

Objective: The aim of this work is to study the effect of Zr addition (i.e. Ni-3 at. % Zr, 6 at. % Zr, 12 at. % Zr) on structural evaluation and deformation features of nano crystalline (NC) Ni during creep process. In addition, the study of the variation in the effect between randomly distributed Zr and segregated Zr atoms at grain boundary on the creep behaviour of nano crystalline (NC) Ni has been performed.

Method: Three dimensional NC Ni specimen with and without Zr addition have been designed using modified Voronoi method. A 14nm x 14nm x 14nm simulation box is taken for performing MD simulation and the simulation box contains 240524 atoms. All the molecular dynamics calculations are performed using a large-scale atomic/molecular massively parallel simulator, LAMMPS with an embedded atom method potential, establish by Wilson and Mendelev applicable for Ni-Zr systems.

Result: All the simulated creep curves of NC Ni with and without presence Zr are observed to be consist short primary creep regime, very short secondary creep regime and wide tertiary creep regime. Quasi-uniform deformation mechanism is operative during creep process of NC Ni and Ni-Zr systems. Calculated dislocation density almost becomes nil just after primary regime of creep curve. It is observed that segregated Zr atoms at grain boundaries of NC Ni shows better creep properties compared randomly distributed Zr atoms in NC Ni.

Conclusion: The presence of segregated Zr atoms at grain boundaries improves the creep properties of NC Ni.

Keywords: Creep; Nano-crystalline; Molecular dynamics; Segregation; Ni-Zr alloy





BEHAVIOUR OF NANO CRYSTALLINE NICKEL: A ATOMISTIC SIMULATION BASED STUDY

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

Understanding creep mechanisms for ultrafine grained NC metals and alloys at atomistic level is hugely vital for designing mechanically and thermodynamically stable NC material applicable over a wide range of temperature.

The detail understanding of influence of alloying element on structural evaluation and deformation features at atomic-scale during diffusional creep for NC metal and alloys is still far from conclusion.

Objective:

Influence of Zr addition (done in two fashion such as GB segregation and randomly distributed in the specimen) on creep behaviour of ultrafine grained NC Ni.

Study the nanocrystalline Ni-Zr alloy system

Atomic configuration snapshots of NC Ni and NC Ni-Zr alloy system



Specimens highlighting particle types (a) NC Ni, (b) Ni-3 at.% Zr alloy, (c) Ni-6 at.% Zr alloy, (d) Ni-12 at.% Zr alloy, (e) Ni-3 at.% Zr alloy, (f) Ni-6 at.% Zr alloy and (g) 3-D specimen according to CSP.

Creep curves of NC Ni and NC Ni-Zr alloy specimens



(a) NC Ni and different at.% of Zr atoms with Ni alloy, (b) NC Ni and different at.% of Zr atoms with Ni alloy, (c) Ni-3 at.% Zr alloy and (d) Ni-6 at.% Zr alloy.

Creep rate vs. time plots of NC Ni and NC Ni-Zr alloy specimen



(a) NC Ni and different at.% of Zr atoms with Ni alloy, (b) NC Ni and different at.% of Zr atoms with Ni alloy, (c) Ni-3 at.% Zr alloy and (d) Ni-6 at.% Zr alloy.

3-D atomic configuration snapshots after different time period during creep process for NC Ni



(a) $\rightarrow 0$ ps, (b) $\rightarrow 1$ ps, (c) $\rightarrow 5$ ps, (d) $\rightarrow 25$ ps, (e) $\rightarrow 50$ ps, (f) $\rightarrow 100$ ps and (g) $\rightarrow 200$ ps (colored according to CSP values)

3-D atomic configuration snapshots after different time period during creep process for NC Ni-12 at. % Zr alloy having Zr atoms randomly distribution in the specimen



(a) $\rightarrow 0$ ps, (b) $\rightarrow 1$ ps, (c) $\rightarrow 5$ ps, (d) $\rightarrow 25$ ps, (e) $\rightarrow 50$ ps, (f) $\rightarrow 100$ ps and (g) $\rightarrow 200$ ps (colored according to CSP values)

3-D atomic configuration snapshots after different time period during creep process for NC Ni-3 at. % Zr alloy having Zr atoms segregated at grain boundary in the specimen



(a) $\rightarrow 0$ ps, (b) $\rightarrow 1$ ps, (c) $\rightarrow 5$ ps, (d) $\rightarrow 25$ ps, (e) $\rightarrow 50$ ps, (f) $\rightarrow 100$ ps and (g) $\rightarrow 200$ ps (colored according to CSP values)

3-D atomic configuration snapshots after different time period during creep process for NC Ni-6 at. % Zr alloy having Zr atoms segregated at grain boundary in the specimen



(a) $\rightarrow 0$ ps, (b) $\rightarrow 1$ ps, (c) $\rightarrow 5$ ps, (d) $\rightarrow 25$ ps, (e) $\rightarrow 50$ ps, (f) $\rightarrow 100$ ps and (g) $\rightarrow 200$ ps (colored according to CSP values)

RDF plots of NC Ni and NC Ni-Zr alloy specimens during creep process



(a) NC Ni, (b) Ni-3 at.% Zr alloy (Zr atoms randomly distributed), (c) Ni-6 at.% Zr alloy (Zr atoms randomly distributed), (d) Ni-12 at.% Zr alloy (Zr atoms randomly distributed), (e) Ni-3 at.% Zr alloy (Zr atoms segregated at GBs) and (f) Ni-6 at.% Zr alloy (Zr atoms segregated at GBs).

Number of cluster vs. time plots during creep process



Coordination number of atoms and corresponding population fraction after different time period during creep process



(a) NC Ni, (b) Ni-12 at.% Zr alloy (Zr atoms randomly distributed).

Coordination number of atoms and corresponding population fraction after different time period during creep process



(a) Ni-6 at.% Zr alloy (Zr atoms randomly distributed) and (e) Ni-6 at.% Zr alloy (Zr atoms segregated at GBs).

Voronoi polyhedra index and their populations after different time period during creep process



(a) NC Ni, (b) Ni-3 at.% Zr alloy (Zr atoms randomly distributed), (c) Ni-6 at.% Zr alloy (Zr atoms randomly distributed), (d) Ni-12 at.% Zr alloy (Zr atoms randomly distributed), (e) Ni-3 at.% Zr alloy (Zr atoms segregated at GBs) and (f) Ni-6 at.% Zr alloy (Zr atoms segregated at GBs).

Number of vacancies for NC Ni and NC Ni-Zr alloy specimen during creep process



(a) NC Ni and different at.% of Zr atoms with Ni alloy, (b) NC Ni and different at.% of Zr atoms with Ni alloy, (c) Ni-3 at.% Zr alloy and (d) Ni-6 at.% Zr alloy.

Evaluated dislocation density of NC Ni and NC Ni-Zr alloy system during creep process



(a) NC Ni and different at.% of Zr atoms with Ni alloy, (b) NC Ni and different at.% of Zr atoms with Ni alloy, (c) Ni-3 at.% Zr alloy and (d) Ni-6 at.% Zr alloy

Conclusions

- □ The creep properties of NC Ni-Zr alloy having segregated Zr atoms at GB is superior compared to that of both NC Ni and NC Ni-Zr alloy having randomly distributed Zr atoms.
- □ Creep curves at primary creep regime for NC Ni and Ni-Zr alloy having Zr atoms randomly distributed exhibit similar trends whereas significant deviation is found in nature of their creep curves at secondary creep regime.
- ❑ Aamorphization process becomes faster during creep deformation of NC Ni as amount of Zr addition increases in NC Ni.
- Dislocation is observed to be present longer time during creep process in case of NC Ni with segregated Zr atoms at GBs compared to NC Ni with randomly distributed Zr atoms.

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Thank you