Creep behavior study of join of nano crystalline Stainless steel and nano-crystalline Nickel using molecular dynamics simulation

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ABSTRACT:

Creep properties of a join between fine grained (grain size ~ 6 nm) nano crystalline (NC) dissimilar materials such as 304 stainless steel and Ni is studied using molecular dynamics (MD) simulation for a constant stress 1 GPa and different temperatures (e.g. 1209K ,1309K, and 1409 K) using embedded atom method (EAM) potential. This join between two dissimilar nano-crystalline materials is prepared by heating the interfacial region to 500K and hold at that temperature for 50 ps, then cooled to room temperature (i.e. 300K). Uniaxial tensile creep simulation has been carried out up till 200ps. All the simulated creep curves have extensive and significant tertiary creep regime but primary creep and steady state creep deformation are very short. Mean square displacement (MSD) is also determined for different temperatures (e.g. 1209K, 1309K, and 1409 K) for estimating diffusivity. This MD simulation work shows that the creep deformation of the join of NC materials is significantly governed by atomic diffusion. Diffusivity of Nickel is observed to be more compared to iron and Chromium. The joined sample becomes amorphous at the end stage of tertiary regime of creep deformation.

Keywords: Molecular dynamics; Creep; Nano joining; Nano crystalline;

1.0 INTRODUCTION

Nano-materials are presently important concern for scientific and technological community due to its unique properties compared to conventional bulk materials [1, 2]. Nano-crystalline (NC) materials usually possess grain size ranging from 1 to 100 nm and accordingly volume of grain boundary is also more in case of nano crystalline materials [3-5]. Application of nano material for intricate purpose requires joining between to nano materials. A joining is actually leading to formation of permanent bonds between the atoms present at two joining surfaces of metals [6]. Metallurgical bonding is required in case of nano metal or nano-metallic alloys.

It is well known if two consummately clean and flat solid surfaces are situated closely, bonds between atoms presented both of the surfaces will formed spontaneously through interatomic forces. In reality, most material surfaces are not clean and flat enough for such kind of spontaneous joining, consequently the energy in the form of heat and/or pressure is required to overcome surface impediments like roughness and contaminations for making a joint [6]. But in case of nano joining needs lower energy per unit surface area compared to micro- and/or macroscale joining as these above mentioned impediments on the surfaces are less at nanoscale. High temperature applications of nano material are huge [7-9]. Accordingly the study of creep behaviour of nano materials as well as nanoscale joining of nano material is highly necessary. Investigation of creep properties of nano materials through experiments is difficult, therefore few numbers of report based on experimental studies on creep deformation behaviour of nano materials is available in literature

[10-12]. Molecular dynamics (MD) simulation is well accepted approach for studying creep behavior of nano materials [13-16]. According to MD simulation based study performed by Keblinski et al. Coble creep mechanism is major role player for creep deformation of ultra-fine grained (d ≤ 10 nm) nano materials [14]. Creep behavior study of nano joint between two ultra-fine-grained nano crystalline material (d ≤ 10 nm) using atomistic simulation is not reported so far as per authors' knowledge. A detail study of creep properties of join between nano crystalline Stainless steel and nano-crystalline Nickel for different temperature is performed first time in this paper.

2.0 SIMULATION DETAIL

A three dimensional sample configuration having joining of nano-crystalline 304 SS stainless steel and pure Ni is presented highlighting particle type and grain structure in **Fig. 1 (a)** and **Fig. 1 (b)** respectively. The sample is developed in modified Voronoi method [17] using

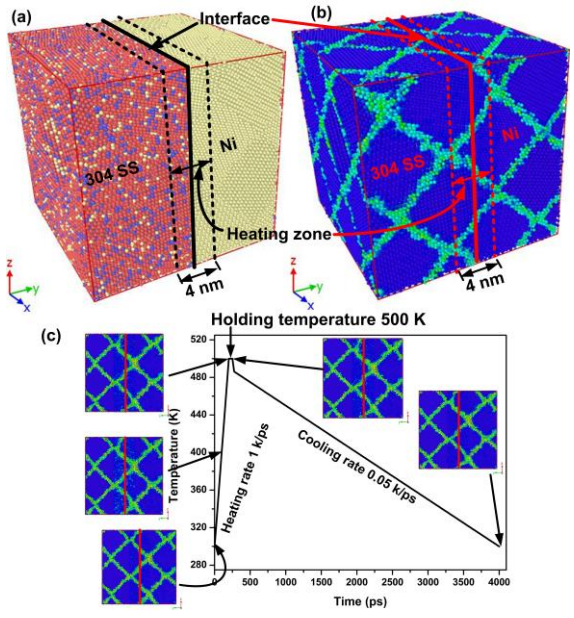

Fig.1: Sample preparation (a) highlighting particle type, (b) according to centro symmetric parameter (CSP) and (c) heating cycle with snap shots at different position.

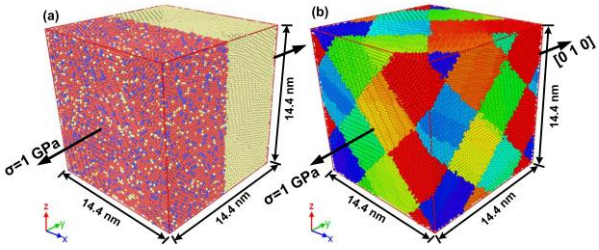

Fig.2: Prepared sample snap shots for creep and tensile (a) highlighting particle type and (b) grain color coding

Atomeye software [18]. The sample size is taken as 14.4 nm x 14.4 nm x 14.4 nm simulation box, which is contained total number of atoms is 254407. Nano scale joint is prepared in three stages : heating at 1K/ps rate from 300K to 500K, hold at 500K for 50 ps and then cooilng at 0.05K/ps to 300K as presented in **Fig. 1 (c).** The prepared sample is shown in **Fig. 2.** After that the specimen are subjected to uniaxial tensile loading along Y-direction [010] with a constant 1 GPa stress. Time step is taken as 0.002 ps for performing the creep deformation simulation.

MSD calculations have been performed for all the temperatures (i.e. 1209K, 1309K and 1409K). The MSD provides information regarding atomic diffusion and it is defined mathematically by following expression [19-23];

$$MSD = \left\langle r^2(t) \right\rangle = \left\langle \frac{1}{N} \sum_{i=0}^{N} (r_i(t) - r_i(0))^2 \right\rangle \quad (1)$$

Where, N is the particle number, t is time duration, and $r_i(t) - r_i(0)$ is the vector distance travelled by a specific particle over the time duration.

All the MD calculations are carried out using **LAMMPS** [24] with an embedded atom method (EAM) potential [25]. Dislocations densities are extracted using OVITO software [26].

3. RESULTS AND DISCUSSION

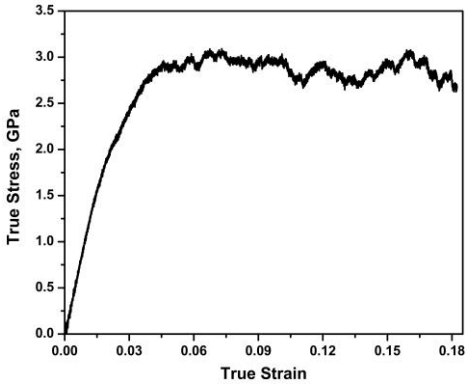

Fig.3: True stress- strain curve for tensile test.

Stress strain curve for the nano joint sample is presented in **Fig. 3**. It is observed that yield stress for this sample is around 2.9 GPa. The creep curves for join between NC stainless steel and NC Ni for different temperatures such as 1209K, 1309K and 1409K are presented in **Fig. 4(a)** and corresponding creep rate curves presented in **Fig. 4 (b)**.

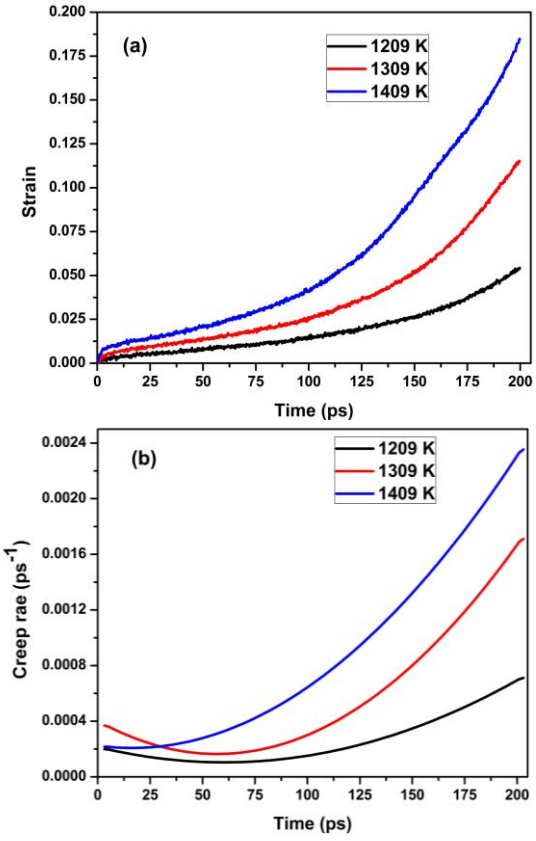

Fig.4: (a) Simulated creep curves and (b) Creep rate with respect to time

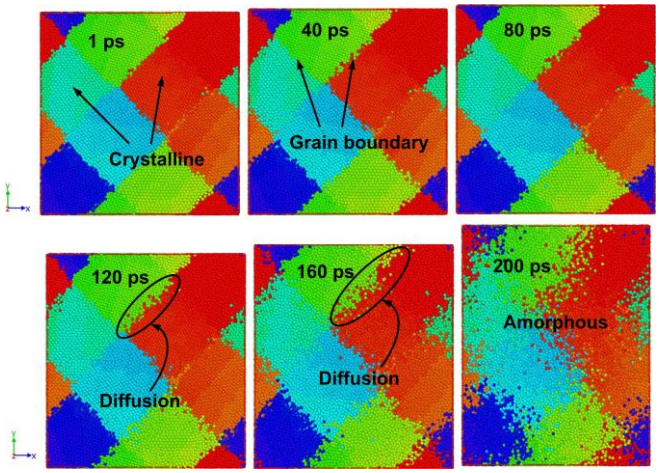

Fig.5: Snap shots during creep process at different time.

Creep deformation process of the sample is found to be very fast as grain boundary diffusion process is rapid in case of nano-materials. It is known that nano-materials have faster diffusibility of the atoms at the grain boundaries than the poly-crystal bulk materials [7]. Extended and prominent tertiary regime is observed for all the simulated creep curves. Primary creep and steady state creep deformation are very short. The creep rate at tertiary regime of creep curves is observed to be increased sharply as true stress increases. The effect of 100K temperatures variation (1209 K to 1409K) is prominent. The creep curves of sample having nano join are observed to be shifted towards higher creep strain during tertiary part of creep with increase of temperature from 1209 K to 1409K.

Representative initial microstructure and atomic arrangements snapshots of Nano joint sample during creep process along with corresponding time 1ps, 40ps, 80ps, 120ps, 160ps and 200ps are presented in **Fig. 5**. The nano joint interface is found to behave not so differently compared to matrix during creep deformation, which is evident from atomic snap shots presented in **Fig. 5**. The joined sample becomes amorphous at the end stage of tertiary regime of creep deformation. Each grain is homogenously deformed even near the interface. On the other hand, localized plastic deformation is occurred at the grain boundaries. These two events actually indicate that quasi-uniform deformation mechanism is playing major during the

creep deformation, which is one of the properties of Coble creep process [27]. So in sum up, it can be said that Coble creep is major contributing mechanism for creep deformation nano scale joint between ultra-fine grained NC Ni and NC stainless steel.

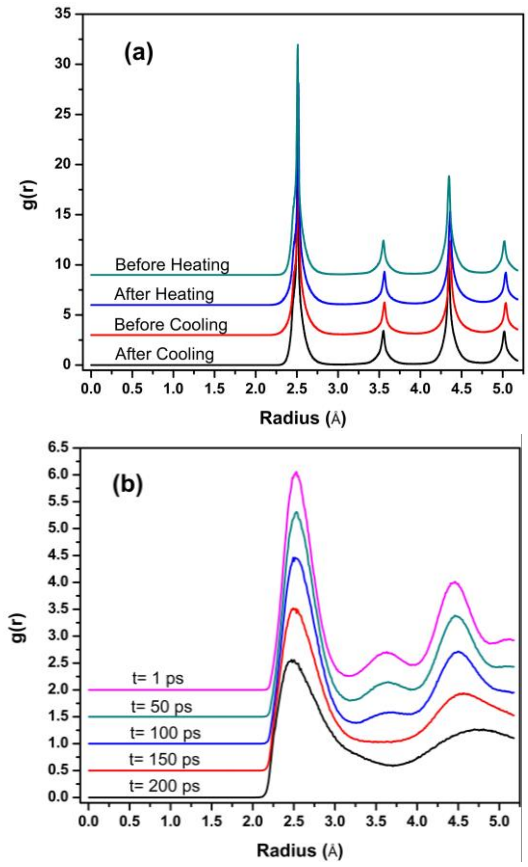

Fig.6: RDF plot (a) during sample preparation and (b) during creep process at 1409K temperature of Ni, Fe and Cr.

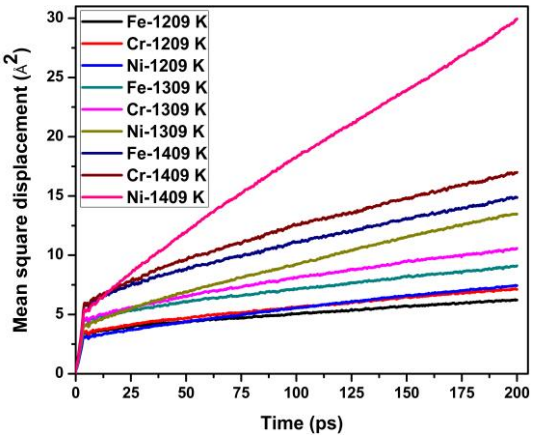

Fig.7: MSD Curve of Ni, Fe and Cr at different temperature

Grain boundaries are found to become wider as creep deformation progresses. Because of that the specimen becomes amorphous. This phenomenon is also justified by the obtained radial distribution function (RDF) plots, which is presented in **Fig. 6**. Mean square displacement (MSD) is also determined for different temperatures (e.g. 1209K, 1309K, and 1409 K) for estimating diffusivity and presented in **Fig. 7**. This MD simulation work shows that the creep deformation of the join of NC materials is significantly governed by atomic diffusion. Diffusivity of Nickel is observed to be more compared to iron and Chromium as per **Fig 8(b)**. The steep rise of self-diffusivity curve of Ni with increasing temperature is observed where as that of Fe and Cr is not steep.

Calculated activation energy of creep for nano join sample is equal 0.86 eV as per Fig. 8 (c). Calculated activation energy for diffusion of Ni, Cr and Fe is 1.22 eV 0.86 eV and 0.91 eV respectively. The evaluated dislocation density with the progress of deformation under creep process has been presented in **Fig.9**.

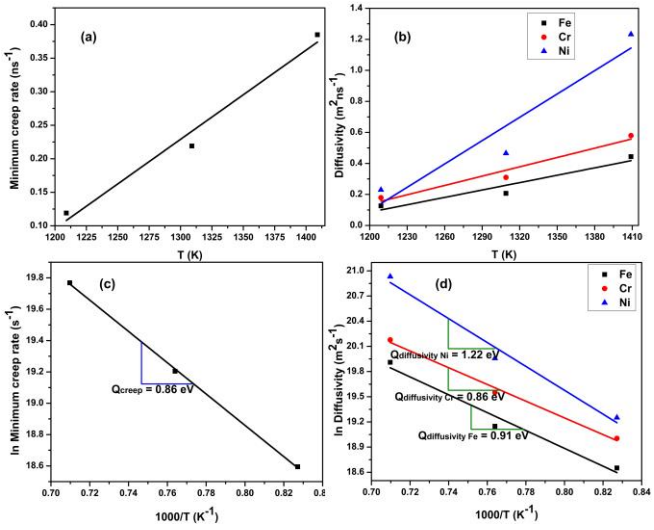

Fig.8: (a) Minimum creep rate vs T, (b) Diffusivity vs T, (c) ln Minimum creep rate vs 1000/T and (d) ln Diffusivity vs 1000/T.

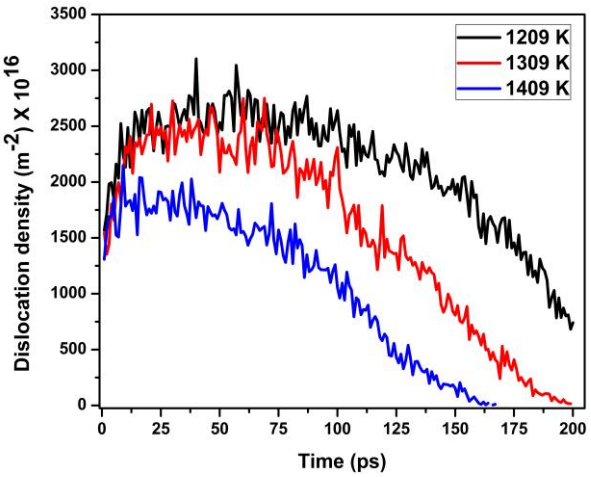

Fig.9: Evaluated dislocation density at three different temperatures vs. time.

Dislocation density is found to be increased during primary creep regime and then decrease sharply. At the end stage of tertiary creep no dislocation is observed as specimen loses crystallinity due to diffusion and accumulation of atoms in grain boundary.

4.0 CONCLUSIONS

Classical MD simulation is performed to investigate the creep behavior of nano joints of NC stainless steel and Nickel. Coble creep mechanism (i.e. grain boundary diffusion controlled mechanism) is observed to be strongly operative. The nano joint interface is found to behave not so differently compared to matrix during creep deformation. Rapid transformation from crystalline structure to amorphous structure is observed during creep process.

ACKNOWLEDGEMENT

The authors would like to thank the computer center of the institute for providing the high performance computing facility to perform the MD simulations on HPC cluster model no. HP DL360p

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