MOLECULAR DYNAMICS BASED STUDY ON DUCTILITY ENHANCEMENT EFFECT AND TEMPERATURE DEPENDENCE OF NANOCRYSTALLINE METALS WITH NANOSCALE VOID

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Summary Aiming at the ductility improvement of nanocrystalline metals, we investigate an influence of an intragranular nanovoid acting as a dislocation activity enhancement site. As reported in former studies, nanovoids act as the dislocation source and/or sink during plastic deformation. This could be a key issue to mitigate the grain boundary (GB) fracture, since smoother plastic deformation with higher dislocation activities is expected. MD simulation for Cu with grain size of 10 nm has been performed to study nanovoid function. The temperature dependence is also studied. As a result, an intragranular nanovoid can possess a positive influence on the ductility without the loss of yield strength. Furthermore, optimal balance between void growth and free volume preservation during the early stage of plastic deformation can cause the fracture mode transition from the GB fracture to the transgranular fracture. Significant ductility improvement is also observed at the low temperature region especially between 50 - 100 K.

INTRODUCTION

Ultra fine grain (UFG)/Nanocrystalline (NC) metals exhibit high yield stress but sometimes low ductility in comparison with coarse-grained (CG) metals[1]. Therefore, improving the ductility without the loss of yield strength is critically important. According to several MD simulations, the nanovoid acts as the dislocation source and/or sink during plastic deformation [2, 3]. However, an influence of introducing nanovoids on the ductility of NC metals has been hardly discussed quantitatively. Recent MD simulations have shown that plastic deformation becomes smooth due to intragranular nanovoids such as retardation of crack propagation [4, 5]. These suggest that intragranular nanovoids has a potential to transform the GB fracture into the transgranular fracture due to smooth plastic deformation in NC metals. Additionally, a MD simulation result that the critical resolved shear stress (CRSS) around nanovoids sensitively changes below 100 K in Cu [6]. These suggest that the ductility improvement significantly depends on temperature. In this study, introducing nanovoids for intragranular dislocation activity enhancement, a new method to mitigate the GB fracture has been proposed. Furthermore, intended for Cu, the temperature dependence of mechanical behavior changes due to intragranular nanovoids has been investigated.

SIMULATION METHOD

MD method has an advantage to discuss a function of the nanovoid such as the dislocation source and/or sink in comparison with others such as dislocation dynamics (DD) and finite element method (FEM) [7, 8]. The MD simulation has been performed on MPI based parallel computers. The Embedded Atom Method (EAM) potential has been employed to describe an interaction among constituent atoms of the system [9]. In order to visualize the fracture process based on atomic motions, four types of atoms are distinguished using the centro-symmetry (CS) and common neighbor analysis (CNA) parameter [10, 11].

SIMULATION MODEL

The MD simulation model consisting of Cu is shown in Fig. 1. A cubic NC grain perfectly surrounded by GBs is embedded in the perfect crystal. Each dimension of the MD simulation model is $\mathrm{H_x} = 21.3$ nm, $\mathrm{H_y} = 21.0$ nm, and $\mathrm{H_z} = 21.3$ nm, respectively. The crystal orientation in the NC grain is [1 1 $\overline{2}$]-[1 $\overline{1}$ 0]-[1 1 1]. The periodic boundary condition is applied for two boundaries perpendicular to the x and y-axis. Three structure types of GBs are embedded: two random GBs whose misorientation angle is 30.6° and 54.7° perpendicular to the x and y-axis, respectively, and the $\Sigma 3$ coincidence site lattice (CSL) GB perpendicular to the z-axis. An uniaxial tensile loading whose velocity is 1.0×10^9 s^{-1} is applied to the fixed region within 0.5 nm from both surfaces perpendicular to the z-axis. An intragranular nanovoid whose diameter is 1.0 nm and volume fraction is approximately 0.05 % is placed at the center of the NC grain. MD Simulations are performed for four different temperatures: $\mathrm{T} = 10$ K, 50 K, 100 K corresponding to the LT region, and 300 K corresponding to the RT region.

RESULTS AND DISCUSSION

The change in the yield stress is imperceptible through the all temperature range due to the sufficiently low volume fraction (approximately 0.05 %) of an intragranular nanovoid. The ductility significantly improves at LT corresponding

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to $T = 50$ K and 100 K except 10 K. In order to explain the intragranular dislocation activity quantitatively, transitions of the stacking fault (SF) structure fraction in the NC grain are studied, as shown in Fig. 2. Remarkable difference of the dislocation activity is observed shortly after an yield point, which indicates the dislocation activity is maintained during plastic deformation due to the existence of intragranular nanovoid.

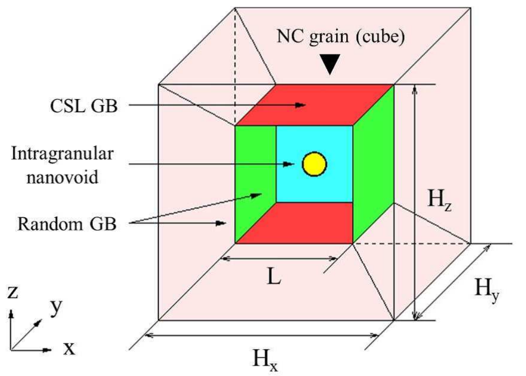

Fig. 1. Schematic of MD simulation model

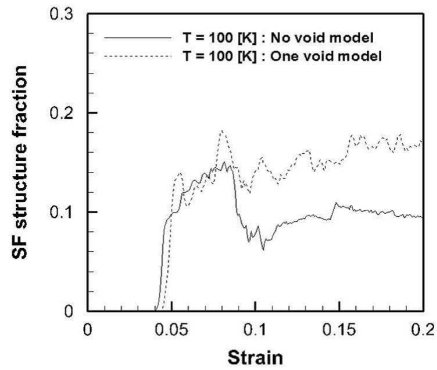

Fig. 2. Transitions of the SF structure fraction

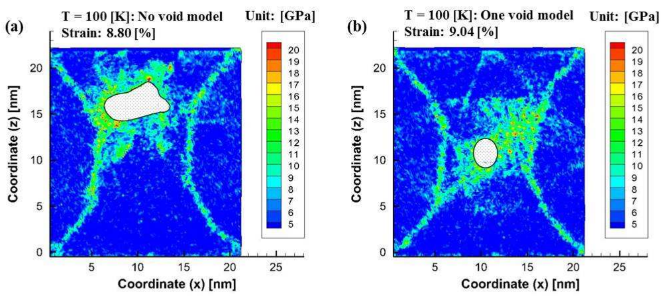

Fig. 3. Comparison of equivalent stress field

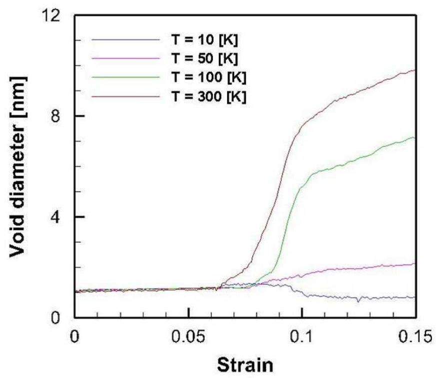

Fig. 4. Temperature dependence of void growth

CONCLUSION

An influence of dislocation activity enhancement due to intragranular nanovoid has been investigated. Acquired results are as follows: (1) An intragranular nanovoid whose volume fraction is approximately 0.05 % has an positive influence on the ductility without the loss of the predominant yield stress. (2) With an intragranular nanovoid, the fracture mode transition from the GB fracture to the transgranular fracture is observed. (3) The fracture mode transition is significantly observed shortly after an yield point. (4) The ductility improvement due to an intragranular nanovoid depends on a balance of void growth and free volume preservation. (5) In comparison with the LT and RT region, the significant ductility improvement is shown at the LT region especially between 50 - 100 K. According to these results, it has been revealed that introducing intragranular nanovoids has a potential to develop NC metals with both high yield strength and high ductility.

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