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Ductile-to-brittle fracture transition in polycrystalline nickel under tensile hydrostatic stress

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ABSTRACT

Large-scale molecular dynamics (MD) simulation was used to study the tensile deformation and failure of defective polycrystalline Ni at various external tensile hydrostatic stresses. A ductile-to-brittle fracture transition occurred. This fracture transition was attributed to the active void and crack propagations, and the suppressed activities of grain boundary (GB) and dislocation from the extra tensile hydrostatic stress applied. Moreover, this interplay between dislocation and GB can occur as dislocation emissions, trapping, absorption, and reflection and transmission, but these forms depend mainly on the local stress states and local geometric structures.

1. Introduction

The dislocation and/or grain boundary (GB) process is thought to dominate plastic deformation in materials. This characteristic has been proved to depend on the grain size. When the grain size was reduced to the submicrometer or nanometer scale, the mechanical property of this sample was completely different from a conventionally coarse-grained sample [1–4] because at micrometer or larger grain sizes plastic deformation occurs mainly by the abundant dislocation motions, including dislocation nucleation and dislocation migration, or by some point-defect-controlled diffusion processes [5]; but as the grain size decreases, the internal dislocation activities become small to mediate the plastic deformation [6,7]. As the grain size decreases to an ultrafine-grained regime below a critical value, GB associated plasticity such as GB sliding, GB diffusion, and GB rotation governs plastic deformation over the dislocation activity. Moreover, in the twinned nanocrystal at a similar grain size, the dislocation-nucleation-controlled plasticity associated with twin boundary (TB) migration dominated the deformation behaviour [8].

Materials have structural defects that are unavoidably introduced during production processes [9], which means that complex deformation arises from the interplay between dislocation, GB, pre-existing TB, defects, and free surfaces [10–13], etc. GBs that make contact with the free surface slide easier than those within the inner GB structures due to smaller geometric constraints. GB/surface triple junctions or voids, or the sites where the coherence of pre-existing TB are being lost, serve as effective sources for dislocation nucleation. In addition, the detwinning of a pre-existing TB and its role in blocking dislocation migration also influences plastic deformation, all of which may change the mechanical properties such as strength, yield stress, ductility, hardness and toughness. Further, the pre-existing voids/cracks may grow, coalesce, and form into intragranular or intergranular fracture as the imposed strain increases, which mean that deformation is controlled by the crossover processes of dislocation/twin, GB, and the propagation of voids and cracks. It is difficult to identify the complicated deformation process directly in nanoscale materials by experiments due to their intrinsically limited length and timescales, but computational techniques such as MD simulations provide a method of analysing plastic deformation and failure in nanocrystalline materials [14–17].

Many researchers have tried to understand the brittle versus ductile fracture transition using MD simulations by focusing on the controlling factors such as the model size [18,19], pre-existing twinning [11,12,20,21], and grain size [22], to study brittle versus ductile fracture transition. Only a few studies could reveal the mechanism of initial void (or crack propagation), or observe the ductile-to-brittle fracture transition in polycrystalline Face Centred Cubic (fcc) materials; most were limited to defect-free samples and used the uniaxial tensile force method. In reality, samples usually co-exist with defects (e.g. void, crack) and are subjected to extreme environments such as biaxial and triaxial tensile forces or other complex working conditions such as indentation, fatigue, and impact.

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The effect of pressure on plastic deformation is still not clear, although investigations revealed that nanocrystalline copper exhibited an unexpected ultrahigh strength behind the shock front [23] because as the shock loading increased, the softening mechanism was limited and the flow stresses were doubled compared to those at low pressure due to the GB sliding movement being suppressed. Similar results regarding an ultra-high strength behind the shock front due to increased dislocation activities were proved by Yuan and Wu [24]. Luo et al. [25–28] studied the spall damage and void growth/collapse induced by a shock wave loading in Cu where the shock waves also induced local and bulk melting associated with anisotropy, premelting, superheating, supercooling and re-crystallisation [29]. Other researches focused on the effect of hydrostatic pressure on deformation. Uniaxial compression experiments under a high hydrostatic pressure were carried out [30,31] and revealed that dislocation activity still occurred in a few nm-length scale at high hydrostatic pressure in polycrystalline Ni [31]. An MD simulation of the effects of hydrostatic pressure (tensile/compressive) on the deformation mechanisms in Al [32] and Cu [33,34] was also carried out and revealed that hydrostatic pressure contributed to a different behaviour of dynamic GB de-cohesion in bicrystal [32]; above and below the critical hydrostatic pressure, dislocation increased or decreased as the hydrostatic pressure increase, but this feature was related to the grain sizes. GB thickening increased as the hydrostatic pressure increased for all gain sizes [33], whereas GB sliding was suppressed by the increasing hydrostatic pressure because of the increasing barriers for GB sliding [34]. However, no work has ever been carried out to study the influence of hydrostatic pressure (tensile or compressive) on the transition from ductile-to-brittle fracture in polycrystalline fcc structures. While previous studies have already shown that void nucleation is associated with the localised hydrostatic pressure [14,18,35], a consideration of the effect of hydrostatic stress on the transition of ductile-to-brittle fracture in polycrystal is very important, so in this paper we used an MD simulation to explore the transition from ductile to brittle fracture in polycrystalline Ni with a central pre-existing crack under tensile hydrostatic stress, and to reveal the mechanism of the onset of void and crack propagation.

2. Model set up

Molecular Dynamics (MD) simulations were performed with the open-source code Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) [36] to investigate the influence of hydrostatic stress on the fracture behaviour of nano grained nickel. The Embedded Atom Method (EAM) interatomic potential [37] was employed in all the simulations. This potential was calibrated using experimental and *ab initio* data for Ni. It has been shown to precisely predict the lattice properties, point and extended defects, various structural energies and transformation paths. The geometric size of the simulation domain was 355.52 Å × 337.92 Å × 123.2 Å in the *X*, *Y* and *Z* directions, respectively, with 1302485 atoms in total as shown in Fig. 1. Grains were generated by virtue of the Voronoi polyhedral construction. Randomly selected crystallographic orientations were assigned to all the grains and most GBs were high-angle GBs. A through-*Z* crack with an elliptical shape was placed in the centre of the sample and its size was 50 Å × 20 Å × 123.2 Å in the *X*, *Y*, *Z* directions, respectively.

In the simulation the atoms were first subjected to energy minimisation by the conjugate gradient method, and relaxed at 1 K and zero pressure along three directions for 200 ps using the Nose–Hoover isobaric-isothermal ensemble (NPT) with a time step of 3 femtoseconds. Once the system reached the thermal and pressure equilibrium, a constant strain rate of 2×10^8 s^{-1} was applied along the *Y* axis with a time step of 5 femtoseconds until it stretched to a strain (ε) of 30% and the temperature was maintained at 1 K. During the deformation the tensile hydrostatic stress was applied to all the atoms. MD simulations with various tensile hydrostatic stresses (mean stress, σ_m) ranging from 0 GPa to 5 GPa were carried out in *X*, *Z* directions using NPT. The periodical boundary condition was imposed in all three directions. Ovito [38] software was used to visualise the deformation plasticity, while the common neighbour analysis (CNA) method was used to identify the perfect fcc lattices (grey atoms), stacking faults (red atoms), and GBs, dislocation cores and free surface structures (green atoms). The stress components were calculated using the expression taken from the Virial theorem, and the average atom volume was used in the stress calculations [39]. The von Mises equivalent stresses (σ_e) and derivative stress along the *y* direction ($\sigma'_y = \sigma_y - \sigma_m$) were then determined and discussed in the following context, where σ_y was the normal stress along the *y* direction.

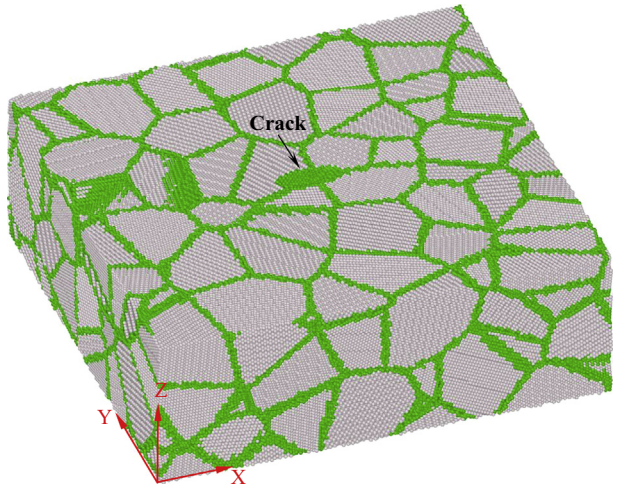

Fig. 1. MD simulation model.

3. Results and discussions

Fig. 2(a) shows the derivative stress along the y direction (σ'_y) as a function of the applied strain (ε) for various hydrostatic stresses (σ_m). σ'_y exhibits a nearly-linear relationship in the early stage of the deformation. The slopes of the curves gradually decrease after the strain exceeds about 4% until the maximum stress, followed by the decrease of the stress with increasing the strain. It can be seen that both the maximum σ'_y and its corresponding strain decreases with the hydrostatic stress. The toughness was calculated by the integration of each of the stress–strain curves and plotted in Fig. 2(b) as a function of the hydrostatic stress. When the hydrostatic stress is low ($\sigma_m \leqslant 1$ GPa), the toughness is high and it is independent of the hydrostatic stress. As the hydrostatic stress increases the toughness decreases. When the hydrostatic stress is equal to and great than 4.5 GPa, the toughness remains at a very low value. These results clearly imply that the fracture behaviour of the studied nano grained Ni strongly depends on the applied hydrostatic stress. Three failure modes can be identified: ductile failure for 0 GPa $\leqslant \sigma_m \leqslant$ 1 GPa, ductile-to-brittle transition for 1.5 GPa $\leqslant \sigma_m \leqslant$ 4 GPa and brittle failure for $\sigma_m \geqslant$ 4.5 GPa. Under the uniaxial tension condition, the increase of tensile hydrostatic stress could transfer the fracture from the ductile mode to the brittle mode.

Fig. 3 shows snapshots of simulation cell at four strains (4%, 6%, 8% and 12%) after fcc and hcp atoms are removed. Fig. 3(a)–(c)