

Nano-mechanical Characterization for Multi-scale Modeling in **Mechanical Behavior of Metallic Materials**

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Background & Purpose

Muti-scale modeling of mechanical behavior especially in nano scale is crucial for understanding and controlling mechanical properties of metallic materials. This paper is aiming to present plastic deformation behavior focusing on plasticity initiation characterized through nano-mechanical testing in a small scale associated with microstructures including interphase and grain boundary. A statistical analysis is also shown to discuss physical models in an indentation-induced deformation behavior.

Plasticity initiation associated with a coherency of α - θ interface ⁽¹⁾

Message: Continuous/discontinues yielding on stress-strain behavior in

Experimental procedure

Every specimen surface was mechanically polished carefully and subsequently electropolished to remove the mechanically damaged layer. Nanoindentation tests were performed using a Hysitron Triboindenter (Bruker Nano Surface division, MN) with 60° or 115° (Berkovich) threesided pyramidal indenter. The position of the indent on the specimen surface was confirmed using scanning probe microscopy (SPM) before and after the indentation measurements.

Dislocation-grain boundary interaction through TEM in- situ straining⁽²⁾

Message: Grain interior dislocation could be absorbed at grain boundary

macro scale could be dominated by lower/higher critical stress in plasticity initiation at ferrite-cementite interface.



Fig. 1 Load-displacement curves obtained by nanoindentation in the vicinity of ferrite-cementite interface. (a)semi-coherent in the spheroidized sample, (b)incoherent in the recrystallized sample. The three curves with Arabic numbers correspond to the indent marks on the SPM image. The critical load (*Pc*) for plasticity initiation is indicated by the arrow on the loading segment. The #1 in the vicinity of the interface of the semi-coherent sample only shows significantly lower *Pc* than the others, suggesting an easy micro-yielding leading to the continuous macro-yielding on stress-strain curve.

resulting in a reduction of dislocation density leading to increasing the yield stress in ultra-fine grained IF steel.



Fig. 2 TEM in-situ straining for UFG IF steel. (a)BF image before straining including six grains. (b)Stress-strain curve obtained during straining. (c)Snap shots of dislocation motion in grain 1 in DF mode showing absorption of dislocation at GB. Image (a) to (e) corresponds to the symbols on the S-S curve in (b). (d)Dislocation density reduction in grain 1 with applied compressive stress. Since the series of the dislocation-GB reaction is the stress range significantly lower than macro yielding (solid arrow in (b)), the reduction in dislocation density could lead to the high yield stress in UFG materials.

Inhomogeneous plastic strain evolves dislocation interaction in Message: grain interior generating a reacted dislocations to form a new grain boundary as an elementally step of grain refinement.

Fig. 3 TEM in-situ straining demonstrating grain boundary formation induced by plastic strain in bcc Iron. Left: (a)-(f) snap shots of dislocation motion and interaction in TEM and schematics showing formation of three grain boundaries. Right: analysis in the activated slip system based on the TEM snap shots. Assuming the activated dislocation as <111> screw type, Burgers vector in each region of A to D can be specified. The reaction of the <111> dislocations generates <001> or <110> dislocations, and they are arrayed to

Message: Plasticity initiation and subsequent plastic deformation in crystalline materials could include different physical origins of stochastic and avalanche models.

(a)Typical Load-displacement curve showing pop-ins including first Fig. 4 one at lower load in high magnitude and subsequent ones at higher load in much smaller event size. (b)probability distribution density of the first (in blue) and the subsequent (in red) pop-in events. The blue plot shows a Gaussian-like distribution suggesting a thermallyactivated dominancy while red marks represent power-law functions indicating a catastrophic model presuming dislocation avalanche.

minimize the interaction elastic energy, forming a new grain boundary at the positions of 1,2 and 3. This is a direct observation of grain refinement induced by plastic strain.

This result messages that an elementally step of the plasticity initiation can be modeled in single dislocation motion but the subsequent behavior should be treated by a different model like collective motion of dislocations.

Applications of nano-mechanical characterization to various metallic materials are shown with the effectivity, and given results are discussed for the multi-scale physical modeling of a crystal plasticity. The characterization technique can probe a local mechanical behavior at a specific position in a microstructure, therefore a structure-property relation can be revealed more clearly. The probed behavior can be modeled based on dislocation theory on a closer scale with dislocation structures.

References

Summary

- Y. Wang, Y. Tomota, T. Ohmura, W. Gong, S. Harjo, M. Tanaka, Acta Mater., 196, (2020) 565-575. 1)
- H. Li, S. Gao, Y. Tomota, S. Ii, N. Tsuji, T. Ohmura, Acta Mater., 206, (2021) 116621. 2)
- H. Li, S. Ii, N. Tsuji, T. Ohmura, Scripta Mater., 207, (2022) 114275. 3)
- Y. Sato, S. Shinzato, T. Ohmura, T. Hatano, S. Ogata, Nature Comm., 11, (2020) 4177. 4)