# Deformation Twinning in Bulk Aluminum with Coarse Grains

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Our traditional understanding that deformation twinning does not occur in aluminum has been largely revised in the past several years. Molecular dynamics simulations and transmission electron microscopy observations revealed that deformation twinning occurs in aluminum when it is nano-crystalline or thin foil. So far, no clear evidence has been provided on deformation twins in bulk aluminum with coarse grains. However, even if twinning does not occur, this issue may not be extraneous to coarse-grained bulk aluminum. It was found that pure fcc metals including aluminum neck down to be thin foil prior to failure under tensile stress, and the crack nucleation and propagation occur only in the thin foil portion, whose local thickness is a few tens nanometers, regardless of strain rate, temperature, and the initial specimen thickness. In this respect, deformation and fracture processes observed in thin foil specimens are certainly relevant to the final stage of plastic deformation leading to fracture of the bulk fcc metals. The next fundamental question is if twinning is a critical event dominating the fracture of those metals. The answer is yes for many fcc metals such as gold, copper and nickel, but no for aluminum. Although deformation twinning certainly occurred upon fracture in these fcc metals, this was an extremely rare case in aluminum.

## 1. Introduction

Until very recently, deformation twinning has been believed not to occur in pure aluminum. Due to its high stacking-fault energy, dissociation of a perfect dislocation into a pair of leading and trailing Shockley partial dislocations is unexpected in aluminum, whereas twinning is achieved via slips of multiple Shockley partials having the same Burgers vector on adjacent close-packed planes. Contrary to this traditional understanding, in the early 2000s a computer simulation using molecular dynamics (MD) codes suggested that nucleation of deformation twin bands could occur at grain boundaries in aluminum if the grain size is sufficiently small (<100nm) [1-2]. The output of MD simulations is sensitive to the inputs, i.e. inter-atomic potentials. Later, another MD simulation suggested that such nucleation was unachievable but grown-in twins could grow under stress in nano-crystalline aluminum [3-4]. Almost concurrently with these MD predictions, transmission electron microscopy (TEM) observations discovered deformation twin bands in nano-crystalline aluminum thin foils subjected to severe deformation (beneath of micro-indentation) [5] and in ball-milled aluminum powders (grain size: <100nm) [6]. Although the detail of nucleation process still remains unclear, based on the MD prediction and experimental validation, our traditional understanding about deformation twins was eventually revised at least for the case of aluminum having nano-crystalline structure.

Is being nano-crystalline a necessary condition for inducing deformation twinning in aluminum? In 2008 Han et al. claimed that they found deformation twins of one or two atomic-layer thickness

in a single crystal aluminum specimen subjected to equal-channel angular pressing (ECAP), by high-resolution TEM observation [7]. This is, however, most likely an artifact due to electron irradiation. They operated their microscope at 300 kV, whereas the critical voltage for Frenkel pair introduction into aluminum by electron irradiation is ~160-kV [8]. Agglomeration of point defects (self-interstitial atoms in thick specimens and vacancies in very thin specimens) in high purity aluminum at room temperature results in formation of Frank loops (i.e. single-layer stacking-fault) and double-layer faulted loops, which are visible exactly the same as the micro-twins claimed by Han et al in high-resolution TEM images. To eliminate such irradiation damage the accelerating voltage of microscopes is supposed to be well controlled in TEM observation of aluminum and its alloys.

MD simulations have also suggested that twinning occurs in aluminum at the tip of propagating cracks [9-10]. This phenomenon is essentially regardless of grain sizes. For this reason, it may have a large potential impact on aluminum research community, which focuses on both nano-grained and coarse-grained aluminum and its alloys. The MD result is a key input to multi-scale modeling for predicting mechanical properties and structural lifetime of materials under stress, specifically indispensable for describing the final stage of plastic deformation leading to fracture. In 1981 Pond et al. discovered a twin band at the tip of crack in aluminum thin foil specimen: they speculated that this was a deformation twin introduced during electro-polishing [11]. Moreover, in 2009 Li et al. detected a deformation twin band formed temporarily at the tip of a propagating crack in a pure aluminum thin foil specimen by in-situ high-resolution TEM [12]. These experimental results were obtained in thin foils, whose thickness is equivalent to the grain size of aforementioned nano-crystalline specimens. It is still unknown whether twinning occurs upon crack propagation in bulk aluminum. To shed a light on this issue, in the present study a systematic electron microscopy observation has been carried out on the fracture surface of bulk aluminum in comparison with the other face-centered cubic (fcc) metals.

## 2. Experimental Procedure

The specimens were polycrystalline pure fcc metals having various stacking-fault energies: aluminum (99.999%, 166 mJm$^{-2}$), gold (99.99%, 32 mJm$^{-2}$), copper (99.99%, 45 mJm$^{-2}$) and nickel (99.99%, 125 mJm$^{-2}$). The ingots were mechanically thinned down into ribbons of ~10-μm-thick by cold rolling, and subsequently homogenized by heat treatment: 870 K for 2 hr for aluminum and 1173 K for 2 hrs for gold, copper and nickel. The mean grain sizes were 337 μm for aluminum, 17 μm for gold, 19 μm for copper and 19 μm for nickel. With this ribbon thickness and grain sizes, those polycrystalline specimens were predominantly a single crystal in the thickness direction. Prior to the tensile straining and fracture experiment a half-way notch was introduced into the ribbon specimens by a razor blade. They were strained and fractured at 300 K and 77 K with a crosshead speed of 1 m s$^{-1}$ and 10$^{-7}$ m s$^{-1}$. Since deformation concentrates on the notch portion, the initial strain rate is given by the crosshead speed divided by the notch width, which was 1 mm or smaller.

The initial strain rate is therefore estimated to be ~$10^3$ s$^{-1}$ for 1 m s$^{-1}$ and ~$10^{-4}$ s$^{-1}$ for $10^{-7}$ m s$^{-1}$, respectively. The microstructure of fracture surfaces was examined using transmission electron microscopes operated at 120-kV for aluminum and 200-kV for the other fcc metals. The dynamic process of fracture was examined by in-situ TEM using a straining stage at 300 K with a crosshead speed of $10^{-7}$ m s$^{-1}$. The time resolution of in-situ observation was 30 frames s$^{-1}$.

## 3. Results and Discussion

Although the fracture surface of ductile metals typically consists of dimples due to coalescence of microvoids, this feature did not appear in the case of pure fcc metals. These metal ribbons necked down to a sharp point before fracture and the ruptured edge consisted of electron-transparent thin foil ligaments aligned at the same height in the thickness direction. These metals failed in this manner regardless of strain rate, temperature and initial specimen thickness. To explore the effect of grain sizes on the fracture mode, the fracture surface of a thick specimen (gold, 0.5 mm) was also examined. Although this specimen contained ~30 grains in the thickness direction, it failed in the same manner as the 10-micron-thick ribbon specimens. These results indicate that in pure metals crack nucleation and propagation always occur in the electron-transparent thin foil portion even if the materials are originally 'bulk'. Accordingly, the fracture processes observed by in-situ TEM studies using thin foil specimens are directly relevant to the fracture of bulk pure metals.

The thin foil ligaments retained only a few dislocations, whereas their root portion retained dislocations at high density. TEM analysis using thickness fringes revealed that the local thickness of the thin foil portion was <30 nm for gold and <58 nm for aluminum and the local thickness drastically changed at the root portion retaining dislocations. This indicates that the applied tensile stress concentrated on the electron-transparent thin foil portion when fracture occurred. The size of thin foil portion was <1 μm, which is three orders of magnitude smaller than the initial notch width. The local strain rate at the moment of fracture is therefore estimated to be ~$10^6$ s$^{-1}$ for 1 m s$^{-1}$ and ~$10^{-1}$ s$^{-1}$ for $10^{-7}$ m s$^{-1}$, respectively.

The thin foil ligaments often form into crystallographically unique zigzag shapes, depending on cracking direction. The size of ligaments was primarily dependent on strain rate. The ligament size was ~1 μm at $10^{-1}$ s$^{-1}$, and the size decreased with increasing of strain rate. Strain rate and temperature did not cause any qualitative difference in the ligament shape and its microstructure. In the case of gold, copper and nickel, when the crack propagation direction was close to [1$\bar{1}$0], their ligaments had a twin band on one edge parallel to the [1$\bar{1}$2] direction and the other edge ruptured in the [001] direction. This cracking direction was one of the most favorable crystallographic conditions for twin band formation. The local thickness of ruptured edge was nearly zero, indicating that this edge failed via the Mode-III shear accompanied with thickness reduction. On the other hand, the deformation twin band formed on a slip plane corresponding to the Mode-II shear in the present crack geometry, whereas the dominant failure mode in thin foil specimens is typically the Mode-III. The number density of deformation twin bands increased with increasing of strain rate.

Note that in general deformation twins do not form even in fcc metals having low stacking-fault energy such as gold and copper when strained at room temperature with a strain rate of $10^{-1}$ $s^{-1}$. These results indicate that the crack tip is certainly a favorable location for deformation-twinning, which is in good agreement with preceding MD results.

In-situ TEM observation revealed that the thin foil portion first developed wide with tapering down without cracking. All dislocations glided during the thickness reduction were swept out from the thin foil portion most likely due to the image force from foil surfaces. After the dislocation starvation, multiple twin bands were produced in the dislocation-starved portion with an interval of ~1 μm. Eventually, crack nucleation occurred in between twin bands at the center of the thin foil portion several tens nanometers away from the thick portions retaining the tangled dislocations. The original crack introduced by a razor blade advanced with coalescing with those new cracks independently grown up to sub-micrometers. Hence, thin foil portion separated into two pieces due to cooperative effect of slips along twin bands and crack nucleation in between twin bands, resulting in zigzag-shaped ligaments. In other words, the zigzag shape originates from the formation of deformation twin bands.

In the case of aluminum such zigzag-shaped ligaments whose edges are parallel to the $[1\bar{1}2]$ and $[1\bar{1}0]$ directions were rarely observed: the shape of ligaments was rather irregular. Moreover, the majority of zigzag-shaped ligaments did not contain a twin band. These results indicate that twinning is not a critical event dominating the fracture morphology of aluminum.

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