



JOURNAL OF
APPLIED
CRYSTALLOGRAPHY

Volume 49 (2016)

Supporting information for article:

**Compression deformation behavior of Zicaloy-4 alloy changing
with the activated twinning type at ambient temperature:
Experiment and modelling**

**Hongjia Li, Wupeng Cai, Zhijian Fan, Xuefei Huang, Yandong Wang, Jian Gong,
Bo Chen, Guangai Sun, Hong Wang, Jian Li and Shuming Peng**

Supplementary Information

Compression deformation behavior of Zircaloy-4 alloy changing with the activated twinning type at ambient temperature: Experiment and modelling

Hongjia Li, ^{a,*} Wupeng Cai, ^a Zhijian Fan, ^{a,b} Xuefei Huang, ^c Yandong Wang, ^d Jian Gong, ^{a,*} Bo Chen, ^a Guangai Sun, ^a Hong Wang, ^a Jian Li, ^a and Shuming Peng ^a

^a Institute of Nuclear Physics and Chemistry, China Academy of Engineering Physics, Mianyang 621999, People's Republic of China

^b Department of Materials Physics, Eötvös University Budapest, PO Box 32, H-1518 Budapest, Hungary

^c College of Materials Science and Engineering, Sichuan University, Chengdu 610065, People's Republic of China

^d Department of Materials Science and Engineering, University of Science and Technology Beijing, Beijing 100083, People's Republic of China

1. Determination of $2\theta_0$ in neutron diffraction for the calculation of lattice strain

Diffraction angle $2\theta_0$ for the initial state of a specimen was measured *in situ* under a pre-tightening force of -50N in this study. However, the $\{0002\}$ reflection for RD case was very weak at the initial state due to its strong texture. Therefore, the determination of its $2\theta_0$ is different from other reflections. The theoretical value of $2\theta_0$ of $\{0002\}$ peak with a wavelength of 2.31 \AA is 53.334° . With an additional force of -50N , the change of the peak position can be calculated according to the following relationship:

$$\varepsilon_{hkl} = \frac{\sigma}{E} = \frac{\text{Force}}{A \cdot E} = -\cot \theta_0 \Delta \theta_0 \quad (\text{S1})$$

where E is the elastic modulus (90 GPa), and A is the cross sectional area of the specimen (19.63 mm^2). Therefore, we can obtain that $\Delta \theta_0 = 0.002^\circ$, and $2\theta_0$ of $\{0002\}$ peak is 53.338° .

2. Other types of deformation twinning observed by TEM

The specimens for transmission electron microscopy (TEM) were prepared by twin-jet electro-polishing in a solution containing 3 ml perchloric acid and 297 ml ethanol at -50°C . Characterizations of the microstructure and phase analysis were performed in a Tecnai G² F30 TEM equipped with energy-dispersive X-ray spectrometer (EDX). Two types of deformation twinning rather than the dominant ones are shown below. It is difficult to determine the index of the deformation twinning. There are mainly two reasons: first, the twin volume fraction is usually small, therefore, the diffraction pattern of the twin grain is covered by that of its parent grain; second, the twin boundary is twisted by the plastic deformation.

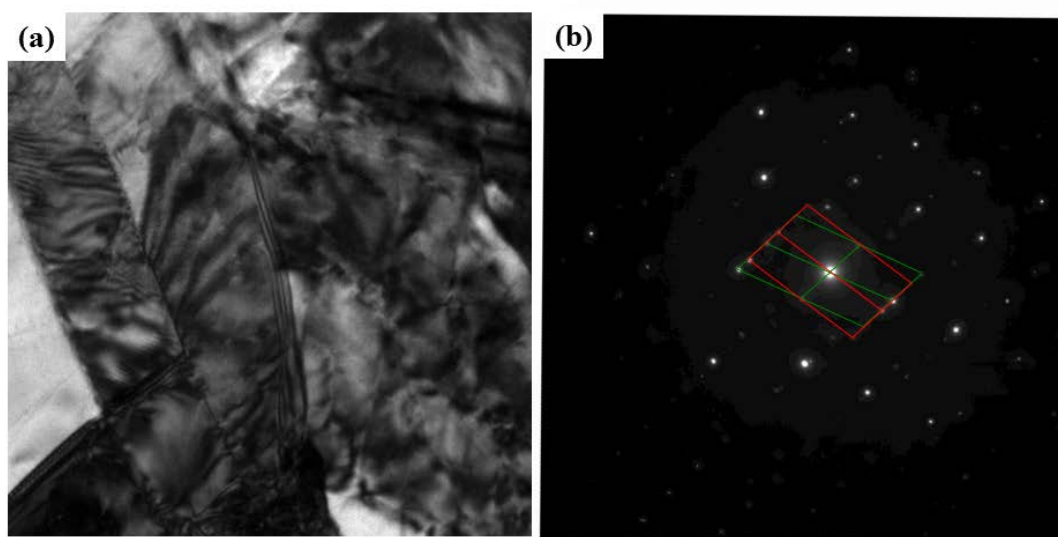


Figure S1 TEM image and the respective diffraction pattern of the rolled Zr-4 alloy after compression along TD at a strain of 5.8%. According to the inter-planar distance, the possible twinning type is $\{11\bar{2}\bar{4}\}$, which does not belong to the common twinning types observed in previous studies.

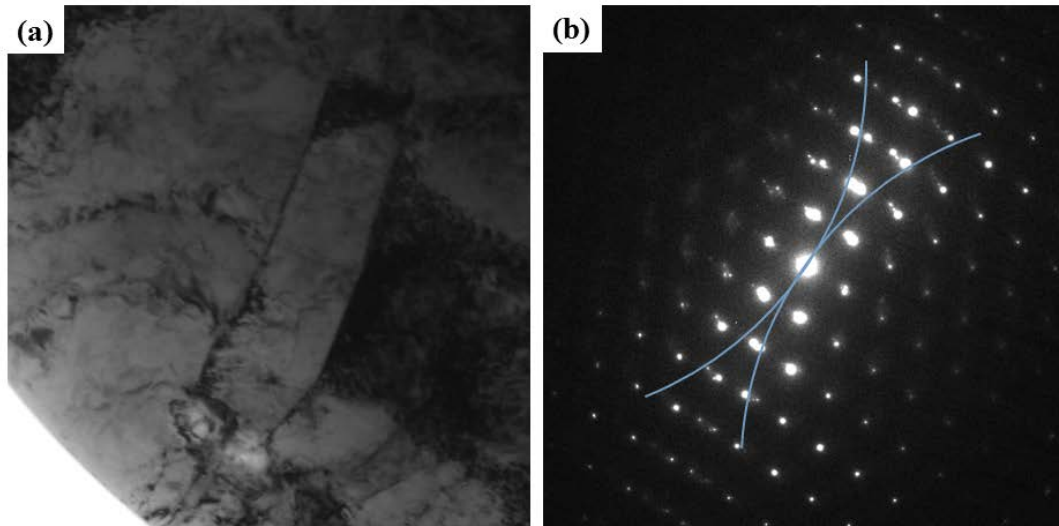


Figure S2 TEM image and the respective diffraction pattern of for the rolled Zr-4 alloy after compression along TD at a strain of 12.2%. The $\langle 1\ \bar{2}\ 1\ \bar{3} \rangle$ zone axes of the matrix and twin are symmetric, indicating the existence of twinning. However, the index of the deformation twinning is difficult to determine.

3. Schematics of twinning planes and orientation relationships between parent and child grains

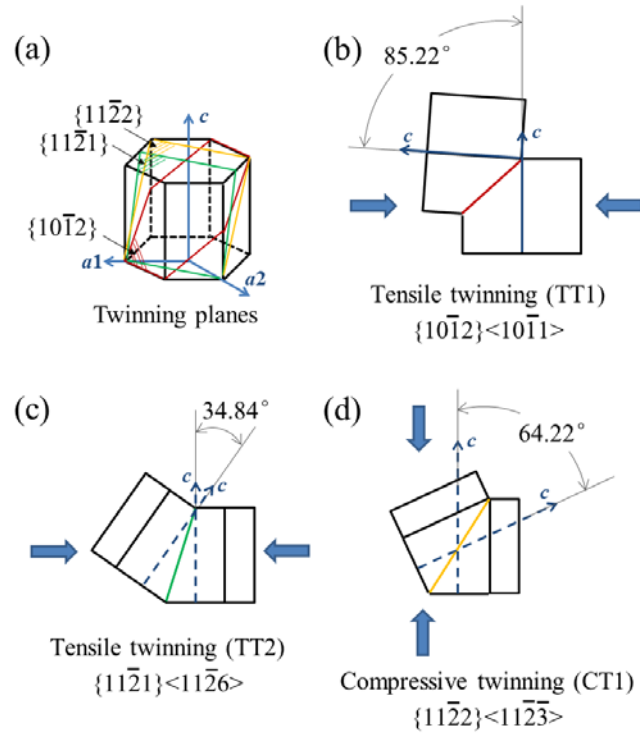


Figure S3 Schematics of (a) twinning planes and orientation relationships between parent and child grains of (b) tensile twinning $\{10\bar{1}2\} \langle 10\bar{1}1 \rangle$ (TT1), (c) tensile twinning $\{11\bar{2}1\} \langle 11\bar{2}6 \rangle$ (TT2) and (d) compressive twinning $\{11\bar{2}2\} \langle 11\bar{2}3 \rangle$ (CT1).