PostDoc Journal
Vol. 1, No. 10, Oct. 2013

Journal of PostDoctoral Research
www.postdocjournal.com

# Methodology for estimating the critical resolved shear stress ratios of α-phase Ti using EBSD-based trace analysis

Yiyi Yang
*School of Engineering, Brown University, Providence, RI 02912*

In a recent paper published by a group from Michigan State University (H. Li, *et al.* http://dx.doi.org/10.1016/j.actamat.2013.08.042), the authors proposed a novel method to calculate the critical resolved shear stress (CRSS) ***ratio*** of different deformation systems in titanium and its alloys, and examined its reliability using the statistical resampling technique of bootstrapping. The results indicate that the activity of these deformation systems varies as a function of alloying composition and deformation temperature. This intrinsic change of CRSS ratios in these alloys is especially important to increasing the accuracy of the crystal plasticity simulations.

The determination of CRSS values for different deformation systems in non-cubic metals and alloys, *i.e.* prismatic slip, basal slip, and pyramidal slip, has been a hot topic in metallurgy and computational simulation areas in past few decades. Either the experimentally measured or the computationally deducted values of the CRSS vary in a quite wide range, as pointed out in the introduction part of this highlighted paper. There are several reasons for this: (1) the difficulty in directly measuring the CRSS using traditional single-crystal approaches; (2) the variation of the textures of polycrystalline specimens used in other experimental approaches; (3) the variation of the stress tensors in some grains from a global stress tensor in polycrystalline environment.

In this paper, the authors calculated the relative CRSS ratios by an optimization methodology, using commercial purity (CP) titanium (α-titanium) and Ti-5Al-2.5Sn (near-α titanium alloy) as model materials. The advantage of this method is overcoming the fact that the local stress tensor in some grains can differ from a global stress tensor. The EBSD (electron backscattered diffraction) based trace analysis was used to identify the activated deformation systems in about 200 grains for each deformed specimens (at 22°C and 455°C). The experimental results indicate, not surprisingly, that some deformation systems can be oversampled in the deformation system-Schmid factor distribution due to a certain texture. The main goal of the methodology that the authors developed is to remove this inherent bias to deduce the underlying relative CRSS for different systems.

In this proposed methodology, the squared difference $d$ between the number of experimental observations of each deformation system-Schmid factor distribution pair $N_{ij}$ and the corresponding modified predicted number of observation $P_{ij}$ is given by:

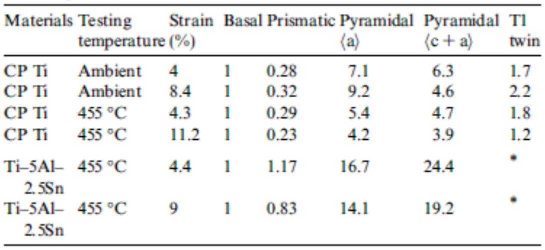
$$d\left(\tau_1,\tau_2,\tau_3,\tau_4,\tau_5,c\right)=\sqrt{\sum_{i,j=1}^{10,5}\left(P_{ij}-N_{ij}\right)^2} \tag{1}$$

where $\tau_1$ to $\tau_5$ represent the CRSS values for basal slip, prism slip, pyramidal <a> slip, pyramidal <c+a> slip, and T1 twin, respectively. The "optimal" values of the CRSS values ($\tau_1^*$ to $\tau_5^*$) are computed by solving the first-order derivative for $d$ with respect to $\tau_1$ to $\tau_5$, using the result to minimize $d$. Then, the CRSS ratio of basal : prism : pyramidal <a> : pyramidal <c+a> : T1 twin is given as:

$$\frac{\tau_1^*}{\tau_1^*}:\frac{\tau_2^*}{\tau_1^*}:\frac{\tau_3^*}{\tau_1^*}:\frac{\tau_4^*}{\tau_1^*}:\frac{\tau_5^*}{\tau_1^*} \tag{2}$$

Table 11 in the paper, shown as Table 1 in this highlight, summarizes the calculated CRSS ratios for different deformation systems for CP titanium and Ti-5Al-2.5Sn. The results are in good agreement with some of the literature data. Also, it is important to note that the relative activity of the ratio of different deformation systems does vary with respect to alloy composition and deformation temperature. With the increasing of the deformation strain level, the ratio of the CRSSs also varies, which is a good indication of hardening behavior in slip systems.

**Table 1.** Bootstrapped mean CRSS ratios of basal, prismatic, pyramidal **<a>**, pyramidal **<c+a>,** and T1 twin deformation systems for CP Ti at RT and 455 °C and Ti-5Al-2.5Sn at 455 °C with ~10% plastic deformation. Twinning was not observed for Ti-5Al-2.5Sn tested at 455 °C.



| Materials | Testing temperature | Strain (%) | Basal | Prismatic | Pyramidal ⟨a⟩ | Pyramidal ⟨c + a⟩ | T1 twin |
|---|---|---|---|---|---|---|---|
| CP Ti | Ambient | 4 | 1 | 0.28 | 7.1 | 6.3 | 1.7 |
| CP Ti | Ambient | 8.4 | 1 | 0.32 | 9.2 | 4.6 | 2.2 |
| CP Ti | 455 °C | 4.3 | 1 | 0.29 | 5.4 | 4.7 | 1.8 |
| CP Ti | 455 °C | 11.2 | 1 | 0.23 | 4.2 | 3.9 | 1.2 |
| Ti–5Al–2.5Sn | 455 °C | 4.4 | 1 | 1.17 | 16.7 | 24.4 | * |
| Ti–5Al–2.5Sn | 455 °C | 9 | 1 | 0.83 | 14.1 | 19.2 | * |

This methodology indeed provides a flexible means to assess the CRSS ratio for deformation systems in a variety of alloys and crystal systems, especially non-cubic crystals. If one of the absolute CRSS values of the deformation systems is known, or can be determined by experimental methods, then other absolute values of CRSS can be determined by using this method, which are important parameters for crystal plasticity simulations. In the future, more crystal plasticity simulations can be carried out using these calculated CRSS values to further assess the accuracy of the method. Still, this new method can miss certain activated deformation systems, which could influence the calculated CRSS ratios: (1) not well-defined or diffused slip bands; (2) the slip systems with Burgers vectors parallel to the specimen surface; (3) subsurface dislocation activity.