Determination of polycrystal diffraction elastic constants of Ti-2.5Cu by using in situ tensile loading and synchrotron radiation

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Abstract

Residual stress determination in engineering components from diffraction strain measurements needs reliable diffraction elastic constants (DECs). From this sense, in situ uniaxial tensile loading experiment was performed on alpha titanium alloy Ti-2.5Cu at the HEMS beamline at DESY by means of a monochromatic synchrotron X-ray diffraction. A comparison between measured (polycrystal) and calculated (single crystal) DECs using for example Kröner model was presented and discussed. The results revealed that the measured DECs slightly differ from the calculated ones. Furthermore, changes in the lattice parameters a and c as well as c/a ratio during tensile loading were also investigated.

Keywords:

Residual stress; diffraction elastic constants; synchrotron X-ray diffraction; Ti-2.5Cu.

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1. Introduction

Ti-2.5Cu or IMI 230 (ASM) combines the formability and weldability of unalloyed titanium with improved mechanical properties, particularly at elevated temperatures. This alloy is used in the annealed condition as sheets, forgings and extrusions for fabricating component such as bypass ducts of gas turbine engines [1]. In order to enhance the fatigue performance of this alloy, mechanical surface treatments such as shot peening, laser shock peening or ball-burnishing can be applied [2]. This beneficial influence is often explained by two main contributions, namely surface strengthening by the process-induced high dislocation densities hindering crack nucleation at the surface and compressive residual stresses which retard microcracks growth from the surface. Since residual stress evaluation is one of the important stages to interpret the fatigue behavior, it is necessary to accurately measure compressive and balancing tensile residual strains generated after applying mechanical surface treatments by means of synchrotron X-ray and neutron diffraction as reported in Ref. [3]. In order to determine residual stresses from diffraction strains, it is essential to use reliable elastic diffraction constants (DECs) in polycrystalline materials. These constants can be obtained by calculations using elastic stiffness matrix of single crystals based on some models such as Reuss [4], Voigt [5] and Kröner [6] models. Nevertheless, the influence of crystallographic texture [7] and alloying elements [8] has to be considered when calculating DECs. In addition, DECs can be experimentally determined by using in situ diffraction methods as reported elsewhere [9,10].

Some earlier works [2-3,11] dealt with residual stress evaluation in Ti-2.5Cu alloy by using single crystal elastic constants for pure α -titanium obtained from literature values [12] which could be different from the realistic ones. Moreover, there is poor information about the elastic properties of the lattice planes (hk.l) in Ti-2.5Cu. Therefore, the present study mainly aimed at determining experimentally the DECs by using in situ uniaxial tensile loading and synchrotron X-ray diffraction. A comparison between measured (polycrystal) and

calculated (single crystal) DEC's using for example Kröner model was presented and discussed. Furthermore, a change in the lattice parameters a and c and c/a ratio during tensile loading in the elastic regime was also studied.

2. Material and Experiments

2.1. Material

Ti-2.5Cu was received as a 10 mm thick rolled plate. Solution heat treatment (SHT) was carried out at 805°C for 1 hour followed by water-quenching. The microstructures of Ti-2.5Cu (SHT) in the rolling plane and in the plane perpendicular to the rolling direction are shown in Fig. 1a and b, respectively. Obviously, the microstructure of Ti-2.5Cu consists of α grains and stringers of the eutectoid component $\alpha + \text{Ti}_2\text{Cu}$ (dark phase). Tensile samples were prepared from this plate with a diameter of 5.04 mm and a gauge length of 25.90 mm. The macroscopic tensile properties are listed in Table 1.

Due to relatively coarse grains in the rolling plane (Fig. 1a), the detector image shows discontinuous Debye-Scherrer rings (Fig. 2a) which could produce poor results due to insufficient grain statistics, in particular when analyzing cakes with small azimuth angles. Therefore, the tensile sample was plastically loaded up to 10.75 kN (just above the yield point at 10 kN) for grain refinement (see the detector image in Fig. 2b) followed by slowly unloading to 0 kN. This resulted in changes in the grain and sample size. Accordingly, the new diameter and gauge length of the tensile sample are 5.00 mm and 26.20 mm, respectively.

2.2. In Situ Tensile Loading

The in situ tensile test was carried out at room temperature at high energy beamline HEMS (PETRA III@DESY) with a strain rate of $5 \times 10^{-4} \text{ s}^{-1}$. The loading axis was parallel to the rolling direction (RD). A universal testing machine (UTM) with a capacity of 20 kN

was installed at the HEMS side station (Beamline P07B) [13]. The sample was loaded up to 10 kN with a step of 0.5 kN. The beamline with the UTM setup is schematically shown in Fig. 3. The monochromatic incident beam has a size of 0.5 mm x 0.5 mm and a wavelength of 0.1422 Å. The diffracted beam, Debye–Scherrer cone, was registered on the MAR345 detector with a pixel size of 100 µm that was located perpendicular to the beam. The distance between the sample and the area detector was 1147 mm.

2.3. Texture Measurement

Texture was measured at the same beamline used for in situ tensile loading experiment at different beam time with different experimental set up. The experiment was conducted using X-rays with a wavelength of 0.1426 Å, a beam size of 0.6 mm x 0.6 mm, sample-to-detector distance of 1190 mm. The sample was rotated from 0° to 180° with a step size of 5°. The detector was Perkin Elmer 16222 with a pixel matrix of 2048 x 2048 at 200 µm pitch. Since this detector outstands for its shorter read-out time compared to MAR345 detector, the texture measurement took about 5 minutes only. The calibration was done using a powder sample of lanthanum hexaboride (LaB₆). The Orientation Distribution Function (ODF) was evaluated by means of the series expansion method [14] with a maximum degree of series ($L_{\max}$) of 22 using a set of six pole figures data, namely (10.0), (00.2), (10.1), (10.2), (11.0) and (10.3), with output resolution of 5°x5°.

3. Data Evaluation

In order to determine the lattice spacing $d_{(hk.l)}$ in both loading and transverse directions, the X-ray diffraction rings were segmented as illustrated in Fig. 2b. The intensity-2-theta diffraction profiles were obtained from a 10° region for grains in both straining directions using the software program FIT2D [15]. It should be pointed out that the loading

direction is parallel to rolling direction (RD) of the sample. The instrumental parameters were obtained using a LaB₆ powder standard.

Material Analysis Using Diffraction (MAUD) software [16], which is based on Rietveld refinement, was used to determine the lattice parameters a and c of Ti-2.5Cu (hexagonal crystal structure with space group: P6₃/mmc) using 12 Bragg reflections in the loading direction and 11 reflections in the transverse direction due to very weak intensity of (10.4) in that direction. as shown in Fig 4. The lattice spacing for each reflection ($d_{(hk.l)}$) was calculated by Eq.(1).

$$1/d_{(hk.l)}^2 = 4/3*[(h^2+hk+k^2)/a^2]+l^2/c^2 \quad (1)$$

The reference lattice spacing ($d_{0,(hk.l)}$) has to be defined as well to calculate the lattice strains. Attention should be paid this reference lattice spacing was used only to extract DEC's results; not for residual stress calculations indicated in Section 4.3, since it is not a stress-free value. Due to the unstable loading (non-linear relation) at the beginning of tension process as shown in Fig. 5 which could be a result of insufficient pre-load for sample holding, the $d_{0,(hk.l)}$ was defined at the stress level where a steady-state elastic deformation takes place. Consequently, the lattice strain due the peak shift for each reflection ($\epsilon_{(hk.l)}$) is given by Eq. (2).

$$\epsilon_{(hk.l)} = (d_{(hk.l)} - d_{0,(hk.l)})/ d_{0,(hk.l)} \quad (2)$$

The DEC's (S_1 and $1/2 S_2$) are needed to calculate residual stresses from strains and they are dependent on lattice plane-dependent Young's modulus ($E_{(hk.l)}$) and Poisson's ratio ($\gamma_{(hk.l)}$) for each reflection ($hk.l$) (see Eq. 3&4).

$$S_1 = -\gamma_{(hk.l)}/ E_{(hk.l)} \quad (3)$$

$$1/2 S_2 = (1 + \gamma_{(hk.l)})/E_{(hk.l)} \quad (4)$$

The slope of linear fitting of macrostress vs. lattice strain for reflection ($hk.l$) gives $E_{(hk.l)}$ as shown in the next section. In addition, $\gamma_{(hk.l)}$ was calculated by dividing the slope in

the loading direction (or $\Delta\sigma/\Delta\varepsilon_{(hk.l),\text{loading}}$) to that in the transverse direction (or $-\Delta\sigma/\Delta\varepsilon_{(hk.l),\text{transverse}}$) which results in $(-\Delta\varepsilon_{(hk.l),\text{transverse}}/\Delta\varepsilon_{(hk.l),\text{loading}})$.

4. Results and Discussion

4.1. Change in lattice parameters during tensile loading

Lattice parameters a and c of the hexagonal unit cell as obtained from the Rietveld refinement of the diffractograms recorded at different tensile load in the elastic regime are presented in Fig. 6. It is clearly seen that both parameters increased linearly during loading in the loading direction, while they decreased linearly in the transverse direction. Obviously, the rate of change of a and c in the loading direction is greater than that in the transverse direction due to the Poisson effect.

As seen in Fig. 7, the c/a ratio at 0 kN was found to be about 1.5889 in the loading direction, while it is about 1.5870 in the transverse direction. This is attributed to the texture developed in the material by prior plastic deformation as explained later and probably due to pre-existing residual stresses. With increasing tensile loading the c/a ratio gradually decreased in the loading direction and increased in the transverse direction with similar rate. This can be explained by the crystallite orientation with respect to the loading axis (or texture). The ODF (Fig. 8) clearly shows that the texture is mainly composed of $\{00.1\} \langle 10.0 \rangle$ component. Accordingly, the basal poles (or c -axis) are mostly oriented perpendicular to the loading direction. Therefore, the decrease of c/a ratio in that direction is reasonable. This main texture component of Ti-2.5Cu differs from what was published in our research [17], since the tensile sample was plastically pre-strained as mentioned in Section 2.1.

4.2. Diffraction Elastic Constants

Macrostress-lattice strain diagrams for both loading and transverse directions are illustrated in Fig. 9a and Fig. 9b, respectively. It should be noted that the absolute values of

lateral strain are represented (Fig. 9b). As seen, the slopes were determined by linear fitting using Origin software for 8 reflections.

Obviously, the (10.0) plane was elastically deformed more than the (00.2) plane under the same loading condition, since the resistance to elastic deformation dramatically increases in the most closely packed crystallographic direction (i.e., perpendicular to {00.1} planes). Accordingly, the basal plane (00.2) has the greatest lattice plane-dependent Young's modulus $E_{(00.2)}$ or the smallest DEC's (S_1 & $\frac{1}{2} S_2$) as listed in Table 2. The relation between $E_{(hk.l)}$ and lattice plane angles with respect to the basal plane is represented in Fig. 10. The result indicates that the $E_{(hk.l)}$ gradually decreases with increasing the inclination angle of lattice planes with respect to the basal plane. Accordingly, the anisotropy factor ($E_{(00.2)}/E_{(10.0)}$) for that polycrystalline Ti-2.5Cu alloy is about 1.14, while this factor is about 1.40 for single crystal titanium [18] depending on the relation between c-axis and loading axis. Less pronounced variations in $E_{(hk.l)}$ values for Ti-2.5Cu is attributed to the grain orientation.

Since the aforementioned data analysis strategy results in exactly the same lattice strains for (10.0) and (11.0) reflections, a single peak fitting for (11.0) for different loading conditions was achieved using Pseudo-Voigt function [19] and then the lattice strains were calculated. Macrostress-lattice strain diagram for (11.0) reflection in the loading direction by means of either Rietveld refinement or a single peak fitting is also illustrated in Fig. 11. Obviously, a good agreement between the results was found not only in the loading direction (Fig. 11) but also in the transverse direction. Second order reflections, namely (20.0), (00.4) and (20.2), are not represented, since they have the same DEC's as with the first order ones.

The experimental and calculated DEC's are compared and listed in Table 2. As seen, experimental DEC's are slightly greater than those calculated by Kröner model. This is mainly explained by the influence of the alloying element (Cu) addition on the elastic behaviors of the crystallographic planes, whereas single crystal elastic constants of pure α -titanium were used to calculate DEC's by means of Kröner model. This change in DEC's due to alloying with

a small amount of Cu (about 2.5 wt. % Cu) could be a result of a little change in the interatomic potential. On the other hand, the influence of crystallographic texture on DEC's could be less significant than the alloying element influence due to relatively weak texture (see Fig. 8) with maximum orientation density of 5.66 multiples of random distribution. DEC's may also exhibit variations by plastically deforming the material prior to the tensile testing [20].

The macroscopic Young's modulus (Table 1) is relatively smaller compared to the microscopic ones (Table 2). This could be explained by the contribution of the Ti_2Cu precipitates [21] which can influence on the bulk elastic properties. Presumably, there are pre-existing dislocations along the eutectoid component ($\alpha+\text{Ti}_2\text{Cu}$) due to the prior plastic deformation. This could result in relatively smaller value of the bulk Young's modulus compared to the microscopic ones obtained within a small gauge volume illuminated by X-ray beam through the tensile sample. This agrees with Koehler and DeWit classical theory [22,23] (Eq. 5) :

$$\Delta E/E = -K\rho L^2 \quad (5)$$

where E is Young's modulus, K is constant, ρ is dislocation density and L is average dislocation loop length, for the case of pinned dislocations in fcc crystals.

4.3. Residual Stress Depth-Profiles Corresponding to Calculated and Experimental DEC's

Residual stress depth-profiles in Ti-2.5Cu produced by a mechanical surface treatment, namely shot peening process with Almen intensity of 0.20 mmA, are shown in Fig. 12. As seen, compressive residual stresses were generated in the near-surface layer due to impacting a surface with shot with a sufficient kinetic energy to create plastic deformation. The surface of the material must yield in tension. Below the surface, the material tries to

restore its original shape, thereby producing below the dimple a hemisphere of cold-worked material highly stressed in compression. These stresses were determined by using energy-dispersive X-ray diffraction with an energy range of 10-120 keV based on $\sin^2\psi$ method as reported in Ref. [3]. By means of this method, the residual stress can be calculated without reference to a stress-free standard as explained in details in Ref. [24]. Attention should be paid that the reference lattice spacing ($d_{0,(hk.l)}$) mentioned in Section 3 was used only to extract DECs results; not for residual stress calculations, since it is not a stress-free value.

Obviously, the values of compressive residual stresses are greater (4 to 10%) when using the calculated DECs by Kröner-Model compared to the experimental ones. This difference should be taken into account when designing various engineering components.

Conclusion and Outlook

For accurate residual stress calculations, in particular in critical applications, it would be suggested to determine the diffraction elastic constants DECs experimentally in order to validate models, since texture and alloying elements influences have to be considered. The addition of alloying element Cu in α -titanium could play more significant role in the DECs evaluation for solution heat treated (SHT) Ti-2.5Cu than texture. Further investigation is still needed to study the influence of aging on DECs compared to SHT condition, since this alloy is being used in an annealed state.

It would be proposed to shift the detector perpendicular to the beam direction to analyze the higher order reflections such as (21.3) which mainly used for residual strain measurements by laboratory X-ray diffraction, since moving the detector close to the sample results in a strong peak-overlapping for that material. Furthermore, texture influence can be investigated by performing deformation process such as rolling to develop stronger texture and cut tensile samples from different directions with respect to the reference direction (e.g. rolling direction) for in situ experiments.

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Figures Captions

Figure 1: Microstructures of Ti-2.5Cu (SHT) in the rolling plane (a) and in the plane perpendicular to the rolling direction (b).

Figure 2: Detector image taken for undeformed tensile sample (a) and plastically deformed tensile sample at 10.75 kN ((just above the yield point at 10 kN)) (b).

Figure 3: Schematic view of the beam line setup installed at PETRA III at DESY (Beamline P07B).

Figure 4: An example of diffraction intensity-2-theta profile. The solid line represents the best fit obtained by MAUD. A difference diffractogram is also marked.

Figure 5: Applied stress-strain curve of Ti-2.5Cu.

Figure 6: change of lattice parameters during loading in elastic regime.

Figure 7: change of c/a ratio during tensile loading in elastic regime.

Figure 8: ODF of Ti-2.5Cu sample calculated with pole figure output resolution of $5^\circ \times 5^\circ$ (maximum degree of series $L_{\max} = 22$).

Figure 9: Macrostress-lattice strain diagram of Ti-2.5Cu in the loading direction (a) and the transverse direction (absolute values of strains) (b). The solid lines represent the linear fitting using Origin software.

Figure 10: Relation between $E_{(hk.l)}$ and lattice plane angles (α) with respect to the basal plane.

Figure 11: Macrostress-lattice strain diagram of (11.0) plane in the loading by means of either Rietveld refinement or a single peak fitting. The solid lines represent the linear fitting using Origin software.

Figure 12: Residual stress-depth profiles in shot peened Ti-2.5Cu determined by energy-dispersive X-ray diffraction using diffraction elastic constants (DECs) by means of Kröner-Model or in situ experiment.

a)

b)

Figure 1: Microstructures of Ti-2.5Cu (SHT) in the rolling plane (a) and in the plane perpendicular to the rolling direction (b).

a)

Loading direction // Rolling direction

85° to 95°

b)

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Table 1. Tensile properties of solid solution heat treated Ti-2.5Cu

E [GPa]	σ_y [MPa]	UTS [MPa]	e_u [%]	$\varepsilon_f = \ln (A_o/A_f)$
105	520	610	14	0.62

E = Young's modulus, σ_y = yield stress, UTS = ultimate tensile stress, e_u = elongation, ε_f = true fracture strain

Table 2: Experimental $E_{(hk.l)}$, $\gamma_{(hk.l)}$ and DEC's of Ti-2.5Cu compared with calculated ones by Kröner Model.

Reflection [angle from basal plane]	$E_{(hk.l)}$ (GPa)		$\gamma_{(hk.l)}$ absolute value	DECs (Experimental) (10^{-6} MPa $^{-1}$)				DECs (Kröner Model) (10^{-6} MPa $^{-1}$)	
	Value	Error		S_1	Error	$\frac{1}{2} S_2$	Error	S_1	$\frac{1}{2} S_2$
(10.0) & (11.0) [90.00°]	107.6	1.0	0.41	-3.81	0.07	13.10	0.24	-2.98	12.03
(11.0) Single peak fitting	106.2	1.1	0.41	-3.87	0.07	13.29	0.24	-2.98	12.03
(00.2) [0.00°]	122.4	1.5	0.35	-2.89	0.07	11.06	0.27	-2.32	10.11
(10.1) [61.38°]	110.7	1.1	0.40	-3.59	0.07	12.63	0.25	-2.90	11.80
(10.2) [42.50°]	115.2	1.2	0.38	-3.29	0.07	11.98	0.25	-2.72	11.28
(10.3) [31.42°]	118.0	1.3	0.37	-3.13	0.07	11.61	0.26	-2.58	10.87
(11.2) [57.79°]	111.4	1.1	0.35	-3.13	0.07	12.11	0.24	-2.87	11.73
(20.1) [74.74°]	108.5	1.0	0.40	-3.74	0.07	12.96	0.24	-2.96	11.97

$E_{(hk.l)}$ =lattice plane-dependent Young's modulus, $\gamma_{(hk.l)}$ = lattice plane-dependent Poisson's ratio,
DECs= diffraction elastic constants (S_1 & $\frac{1}{2} S_2$).