| O-05 | Session A, Tuesday, 14.06., $10^{40}$ - $11^{00}$ |
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## EXAFS and DAFS from particles of ω phase in β-Ti(Mo) single crystals

E. Piskorska-Hommel[1]*, D.Kriegner[2], J. Šmilauerová[2] and V. Holý[2]

[1]*Institute of Low Temperature and Structure Research, Polish Academy of Sciences, Wroclaw, Poland*
[2]*Faculty of Mathematics and Physics, Charles University in Prague, Czech Republic*

Keywords: Ti alloys, precipitates, martensitic transformation, x-ray absorption spectroscopy

*e-mail: e.piskorska@int.pan.wroc.pl

Metastable β titanium alloys are important materials for various construction purposes, as well as for biomedical applications. They contain enough β stabilizing elements to suppress martensitic transformation from body-centered cubic β phase to hexagonal close-packed α phase upon quenching to room temperature. However, due to the metastable nature of the β phase, various other phases can form during ageing at elevated temperatures. In a certain composition range, nm-sized particles of meta-stable hexagonal ω phase form upon quenching in the β matrix by a diffusionless displacive transformation [1]. When exposed to elevated temperatures, ω particles grow by a diffusion-assisted mechanism. The ω phase particles play a significant role in alloy hardening, as well as in subsequent phase transformations, i.e. ω-assisted nucleation of thermodynamically stable α phase [2].

The growth of the ω phase particles is accompanied by the diffusion of β-stabilizing elements from the volumes of the growing particles creating "clouds" of the impurity atoms around each particle. We have investigated the kinetics of the growth of the ω phase particles by high-energy small-angle x-ray scattering (SAXS) in situ during annealing of Ti(Mo) single crystals [3]. The results indicated indeed the presence of local areas with increased Mo content.

Recently we perform an ex situ anomalous X-ray diffraction and fluorescence measurements around the MoK absorption edge at ESRF Grenoble (beamline BM02) in samples after various annealing steps. As an example, we show in Fig. 1(a) the reciprocal-space distribution of the diffracted intensity around the ω-reciprocal lattice point $44\overline{8}2$ of a Ti(Mo) sample after annealing at 370°C at 64h taken at 19.995 keV, just below the MoK absorption edge. Fig. 1(b) shows the energy dependence of the diffraction signal (XRD) integrated over the region denoted by a rectangle in Fig. 1(a), as well as the fluorescence signal collected far away from any reciprocal-lattice point. Both dependences clearly exhibit the EXAFS-like oscillations; however the fluorescence signal stems from the Mo atoms both in the ω particles and in the β matrix, whereas XRD originates exclusively from the ω particles.

The Athena program was used to subtract the pre-edge background, normalize to the experimental edge step and absorption data from the EXAFS data [4]. The DAFS spectrum χ(E) depends on the real (χ') and imaginary (χ") parts of the anomalous form-factor of the Mo atoms. The numerical Kramers-Kronig transformation was used to extract the imaginary part χ"(E) of the DAFS spectrum [5]. The Artemis program was used to analyse both EXAFS and DAFS data in order to obtain the structure parameters such as bond lengths (R), Debye-Waller factors ($\sigma^2$) and coordination numbers (N) [4]. The scattering amplitudes Mo-Ti were generated using the FEFF6 code implemented in Artemis program [6]. The magnitude of the Fourier transform (FT) of the EXAFS and DAFS oscillations is presented in Fig. 2. Although FTs for both cases look very similar some structural changes between EXAFS nad DAFS data are observed. In the presented paper the EXAFS and DAFS results for samples annealing in 300, 335 and 370°C in different time will be discussed in details.
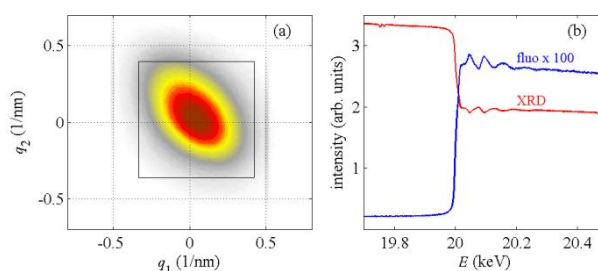


*Figure 1.* The reciprocal space intensity distribution around the maximum of the ω-phase (a) and the energy dependences of the diffraction and fluorescence signals (b).



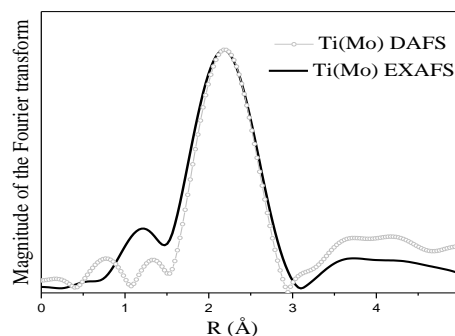*Figure 2.* Magnitude of the Fourier transforms of the EXAFS and DAFS oscillation.

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