CERIC EXPERIMENTAL REPORT
Proposal number: 20217113
Title: Local structure in the bcc-based Ti-Nb-Zr-Ta-Hf based high entropy alloys

Proposer: Andrea FANTIN
Usages and assigned hours:
* LISA: LISA@ESRF (hours:96)
Achievements: ---

_____ do not change anything above this line _____

READ FIRST:

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Body text max. 3 pages including pictures and references (recommended 10-point Times New Roman, 1 cm indented, preferably left aligned, single spacing). Reports have to be self-contained. We cannot accept links to other documents.

Use this report to explain reviewers how productive your measurements were. In case some of your measurements did not produce the expected results, please mention the problems you encountered in this report. Mention all the instruments you used.

STRONGLY RECOMMENDED FLOW CHART:

Objectives (from proposal): The idea of producing a crystalline alloy with good properties based on a heavy mix of elements was completely new and pushed the boundaries of properties understanding beyond what was known so far from one- and two-element based alloys, leading to the discovery of High Entropy Alloys (HEA). A general lack of experimental data on the crystal structure and local distortions in HEA – all factors considered crucial for the understanding of mechanical properties – emerges from the latest reviews. This project plans to tackle directly some of these aspects: a bcc alloy, so-called Senkov alloy based on Ti-Nb-Zr-Ta-Hf elements, and its precursors, will be investigated by means of X-ray absorption spectroscopy (XAS). The Senkov alloy was chosen because it is the most studied in literature from the mechanical properties point of view, but detailed structural information at the atomic scale are still missing. The results will be then related to i) mechanical properties to be measured on the same compounds and integrated with the literature, and ii) on-going crystal structure investigation on similar hcp-based and fcc-based high entropy alloys.

1) Report

Five different edges Ti, Nb, Zr, Hf and Ta have been measured for reference foils, several reference compounds such as the ternary TiZrHf, TiNbHf, a quaternary MoNbTaW, an *hcp* based $Al_{15}Sc_{10}Ti_{25}Zr_{25}Hf_{25}$, and the main compound -also known as Senkov alloy -, TiZrHfNbTa. Some of the Fourier-transformed spectra are depicted in Figure 1. The evident features arising from this experiment is the low signal amplitude especially for the TiZrHfNbTa alloy, indicating a high degree of disorder, which is in line with the available literature [1,2].

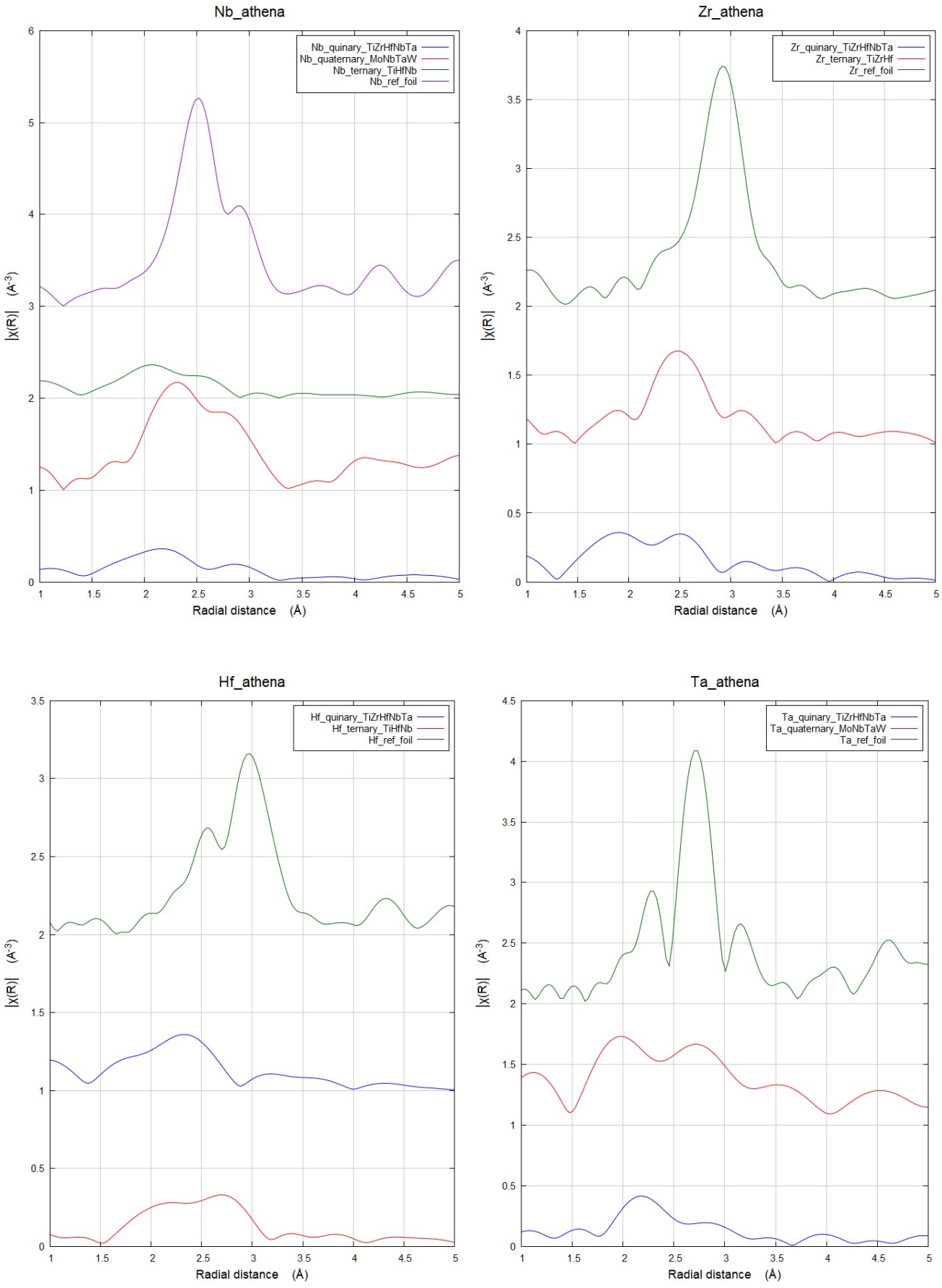

Figure 1: Normalized linear absorption coefficient χ, χ(R) as a function of the radial distance from the absorber. Data are stacked from bottom to top with decreasing alloy complexity (i.e. number of elements) for better visualization. The presented measurements were collected at room temperature (298 K), and in fluorescence mode.

All measurements went as planned. We did not encounter any relevant problems and we could maintain the expectations collecting data of very good quality. At present we are analyzing and comparing the data taken at LISA beamline with data on the similar specimens collected previously at LISA as well, PHOENIX (SLS), and at RGBL (BESSYII) for a more comprehensive understanding of the TiZrHf-based system, with special attention to the two opposite roles of Ti Nb and Ta (smaller elements), and Zr and Hf (larger elements) which tend to produce larger structural distortions in the unit cell [1,2,3].

At LISA beamline we employed the wide energy range attainable by the monochromator (Si 311 crystals for better resolution). We measured in both total electron yield and fluorescence mode simultaneously, finally determining that self-absorption was negligible (from TEY). Higher quality data was obtained in fluorescence mode using the 13-channels available HP Ge energy-selective detector. A cryostat was also used and selected specimens were measured at 80 K as well (not shown in Fig. 1).

2) References

[1] Tong et al. Acta Materialia Volume 183, 15 January 2020, Pages 172-181

[2] Senkov et al., Journal of Alloys and Compounds Volume 509, Issue 20, 19 May 2011, Pages 6043-6048

[3] Tong et al. Materialia, 2,(2018), 79