

O31 | **High entropy HfNbTaTiZr alloys: structure stability, short range order and vacancies**J. Kuriplach<sup>1,\*</sup>, J. Čížek<sup>1</sup>, O. Melikhova<sup>1</sup>, F. Lukáč<sup>2</sup>, J. Zýka<sup>3</sup> and J. Málek<sup>3</sup><sup>1</sup>*Department of Low Temperature Physics, Faculty of Mathematics and Physics, Charles University, V Holešovičkách, CZ-18000 Prague 8, Czech Republic*<sup>2</sup>*Department of Materials Engineering, Institute of Plasma Physics of the Czech Academy of Sciences, Za Slovankou 1782/3, CZ-18200 Prague 8, Czech Republic*<sup>3</sup>*UJP PRAHA a.s., Nad Kamínkou 1345, CZ-15610 Prague - Zbraslav, Czech Republic*

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High entropy (HE) alloys (HEAs) consist of several – usually at least four or five – components with nearly equiatomic concentrations [1]. “High entropy” in their name comes from the fact that they show a very large configurational entropy, which contributes to their stability. Such alloys started to attract attention – both from the scientific and applicational viewpoints – just a few years ago because of their unique properties, mainly mechanical and electrochemical ones. The properties of HE alloys are nowadays intensively studied, but investigations of defects are seldom. Positron annihilation (PA) may thus reveal details about open volume defects, and thereby about HEA microstructure related to HEA properties. HE alloys are not dilute but rather concentrated alloys. This fact has also consequences for positron annihilation research: Even simple defects like vacancies exist in many different atomic configurations. In addition, the “bulk” lifetime is not represented by a discrete value but exhibits a distribution with a certain (nonzero) width.

The HfNbTaTiZr high entropy alloy was discovered/introduced in 2011 [2] in quest of suitable materials for high temperature applications in the aerospace industry. All constituting elements are refractory metals, and so is the resulting alloy. The HfNbTaTiZr alloy displays excellent mechanical properties, like yield strength, but its defect structure is unknown to a large extent. In the present study, we first examine the phase stability of the HfNbTaTiZr alloys which crystallize in the bcc structure. We also attempt to determine the short-range order in these alloys using *ab initio* modelling based on a Monte Carlo approach [3]. The basic properties of single vacancies in the bulk are also investigated, including the possibility of the existence of structural vacancies. Finally, the first experimental PA results for HfNbTaTiZr samples produced by arc melting are shown and discussed with the help of computed positron characteristics for the bulk and vacancies.

[1] High-Entropy Alloys: Fundamentals and Applications, edited by M.C. Gao, J.-W. Yeh, P.K. Liaw and Y. Zhang, Springer (2016)

[2] O.N. Senkov et al., *J. Alloys Comp.* **509**, 6043 (2011)

[3] N. Metropolis et al., *J. Chem. Phys.* **21**, 1087 (1953)