

Referee's report on doctoral thesis

Title: Investigation of Vacancies in Fe-Al Alloys

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The submitted doctoral thesis is devoted to the study of the vacancy hardening phenomenon in iron aluminides. At the present time the Fe-Al alloys are intensively investigated due to their potential as structural materials for high temperature applications. The mechanical strength and corrosion resistance of iron aluminides are, besides the chemical composition of the respective alloy, strongly influenced by the vacancy concentration and the characterization of vacancies after various thermal treatments is therefore crucial for the understanding of physical properties of these alloys. In view of this fact, the thesis has a high scientific relevance.

The thesis is of a predominantly experimental character but a considerable part of the text is dedicated to the *ab initio* calculations of positron lifetimes and Doppler broadened annihilation peaks in relaxed lattice defects. All used experimental methods are up-to-date standard methods in respective field of solid state physics. Arc melting minimizes contamination of the prepared samples, X-ray diffraction is a standard technique for characterization of phase composition of alloys, Vickers microhardness $HV_{0.1}$ is a standard technique for the evaluation of mechanical properties of the samples and their homogeneity and positron lifetime spectrometry (LT) is a standard method for identification of lattice defects and their concentration. A relatively novel method of variable energy positron annihilation spectroscopy (VEPAS) has been used in cases where saturated positron trapping occurred.

All experimental methods related to the sample preparation a characterization and data acquisition were used in proper way and in accordance with common practice. The data evaluation meets all usual standards, the obtained results are discussed in detail and systematically compared with the already published results, and corresponds thus to the requirements for scientific publication.

From the formal point of view the thesis is well structured into chapters and contains all usual items like the lists of references, tables, figures and abbreviations used in the text. The first three chapters contain the "State of the art", description of experimental methods and basic equations for *ab initio* calculations. The "State of the art" is well written and contains generally accepted basic principles as well as the latest results. The experimental results are presented in the fourth chapter, the fifth chapter is dedicated to the *ab initio* calculations and the last two chapters bring discussion and conclusions. The figures, tables, references and the text itself are processed according to standards. The bibliography of the work contains 90 references in standard format. SI units are systematically used throughout the text. The quality of the thesis from the formal viewpoint is on a very good level.

Main results of the thesis, which are summarized in the seventh chapter, represent an original contribution of the author to the investigation of vacancy induced hardening in Fe-Al alloys. The VEPAS method was successfully applied to determine high concentrations of vacancies in bulk samples. In case of alloys with the Al content above 27 at.% the concentration of vacancies is very high which results in significant hardening. The decrease in vacancy concentration after annealing was found to be correlated with the decrease of microhardness. The hardness increment is proportional to the square root of vacancy concentration which is in accordance with the Fleischer theory. Probably the most important result is the explanation of the dependence of positron lifetimes on the composition of Fe-Al alloys in terms of varying number of Al atoms surrounding the vacancies and significant changes of the open volume of vacancies due to ionic relaxations.

The results of the thesis have been already published in six papers, mostly in reputable journals with high impact factor. Besides these six papers, František Luká is a co-author of further 26 papers, most of them again in journals with impact factor, which is an evidence of the quality of his research.

To conclude, František Luká has clearly proven his ability to solve complicated scientific problems and in his thesis he has presented valuable data. There is no doubt about his potential both to perform an independent creative scientific work and to co-operate effectively in large scientific teams.

I recommend this thesis to be accepted by the committee and I do believe that after successful defense František Luká will be awarded the PhD scientific degree.

Comments and remarks on the thesis:

- 1) In Figure 19, the values of Vickers hardness after annealing at temperatures above 800 °C seem to be in some cases higher than those after initial quenching from 1000 °C. This effect is probably most profound in the Fe₆₀Al₄₀ alloy. Can you make some comment regarding this fact?
- 2) In Figure 15, where a comparison of vacancy concentrations reported in literature is presented, the differences between the values from individual authors are substantially higher than the estimated errors. According to your opinion, can this fact be ascribed to the real difference in the structure of the samples or more likely to an underestimation of experimental errors by individual authors?