

Referee's report of the Thesis
Investigation of Vacancies in Fe-Al Alloy
by František Lukáč

The Thesis deals with experimental and theoretical investigations of vacancy concentrations in Fe-Al alloys with Al content in the range from 18 to 49 at.%. The positron annihilation spectroscopy was employed as the main experimental method. These results were correlated with hardness measurements. Quantum mechanical ab initio calculations were carried out for the explanation of the measured positron annihilation characteristics.

The Thesis was accomplished at Charles University in Prague, Faculty of Mathematics and Physics, Department of Low Temperature Physics, under the supervisor by doc. Mgr. Jakub Čížek, Ph.D.

In the first chapter the author describes experimental methods:

- a) Positron annihilation spectroscopy principles mixed together with experimental arrangements (~12 pages),
- b) Vickers hardness (~0.4 page)
- c) X-ray diffraction (~0.4 page)

The first principle calculations are described in chapter 2 where density functional theory is introduced and discussed.

The third chapter is devoted to investigations of vacancies in Fe-Al alloys. At the beginning (in two pages only), published data on Fe-Al alloys are summarized. Information on preparation of the Fe-Al samples is also very short. The results obtained by positron spectroscopy dominate there.

The next chapter concerns with the thermal development of vacancy concentrations in the studied alloys. The changes in vacancy concentrations derived from positron spectroscopy data are compared with the results of microhardness measurements.

Theoretical calculations of positron annihilation characteristics and their comparison with the experimental data are given chapter 5.

In the chapters 6 and 7 are given short discussion (2 pages) and conclusions (1 page), respective. It documents a weakness in the organisation of the Thesis. There are mixed results and their discussion on many places without a clear separation, e.g., by a new subsection.

In the evaluation of the Thesis I would like to emphasize its merits:

- i/ high quality of experimental results obtained by various methods of positron annihilation spectroscopy;
- ii/ theoretical calculations of positron annihilation characteristics for vacancies in Fe-Al alloys.


Finally it must be mentioned that František Lukáč published the results with co-workers 6 papers in journals and conference proceedings.

Comments and questions.

1. Information of final chemical composition of Fe-Al samples is missing. The composition of these alloys may change by melting (even in protective atmospheres) and by additional heat treatments.
2. Information on conditions of additional heat treatments is missing.
3. XRD results (changes in lattice parameters) are explained as a result of changes in atomic ordering but very similar changes may be influenced by fine differences in Al contents, e.g., due to heat treatments.
4. A checking of the presence of oxides (Al_2O_3 , FeAlO_3 , ...) in the samples is not reported. These impurities may appear namely the case of mechanically milled powders, by sample handling in air, or heat treatments.
5. A progress a/o differences in comparison with the published results by Kuriplach, Melikhova, and co-workers should be discussed in more details.

To sum up, I can state that František Lukáč has shown his research abilities in the field of applications of positron annihilation spectroscopy and quantum mechanical calculations for explanations of the measured positron annihilation characteristics. He showed independence in the scientific work and collaboration in a research team. The Thesis demonstrates the innovation and high degree of creative thinking and skilful performance. I recommend the Thesis for the defence.

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