TECHNISCHE UNIVERSITÄT WIEN

VIENNA UNIVERSITY OF TECHNOLOGY

Institut für Festkörperphysik
Wiedner Hauptstraße 8-10
A-1040 Wien
http://www.ifp.tuwien.ac.at

Univ.Prof. Dipl.Ing. Dr.
Ernst Bauer
tel.: +43 1 58 801 131 60
fax: +43 1 58 801 131 99
bauer@ifp.tuwien.ac.at

To the Dean
Faculty of Mathematics and Physics
Charles University Prague

Prague
The Czech Republic

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Habilitations Thesis, Jiri Pospisil, Charles University Prague

The habilitation thesis submitted by J. Pospisil, Faculty of Mathematics and Physics, Charles University Prague, summarises extensive studies of the author, primarily with respect to uranium-based ternary compounds (one sub-chapter is devoted to Ti-alloys). These studies demonstrate that the author has great insight into the large variety of physical features and scenarios present in such materials and is able to involve theoretical concepts and ab-initio calculations to analyse and explain experimental findings. The results obtained prove that Jiri Pospisil has pervaded this specific field of solid state physics.

In about 10 years research, Jiri Pospisil has participated – in many cases as the leading researcher (as obvious from 6 publications as first author) – in many comprehensive studies on ternary U-based compounds. The majority of these studies were focused on 1:1:1 systems with a generic chemical formula UTX where T represents a transition metal element (either with a 3d, 4d or 5d electronic configuration) and X is in general a main group element. UTX compounds crystallise (in general) with two different types of crystal structures, the orthorhombic TiNiSi type or the hexagonal ZrNiAl type. Both of these types contain a number of members with exciting low temperature features, including magnetic order, quantum criticality or unconventional superconductivity. While the essential physical features of starting materials like UCoGe, URhGe or UCoAl, etc., have been already described previously in literature, the big issue in Jiri Pospisils research was to bridge such systems by systematically substitute (primarily) one *d*-element in UTX by another one in many small steps. This allows to obtain a deep understanding of the underlying parameters and interaction mechanisms present in these (pseudo-)ternary intermetallics.

The principal understanding of uranium intermetallics follows from the so-called Hill-criterion, which is based on the nearest neighbour distance of two uranium ions in the respective solid. A critical distance of 0.35 nm separates localised uranium systems (> 0.35 nm) from systems where the distance between uranium ions is below 0.35 nm. The later one experience strong hybridisation of the uranium 5f electrons with conductions electrons and thus the respective uranium magnetic moment becomes delocalised (itinerant). As a consequence, many magnetic features changes dramatically in their nature, e.g., an antiferromagnetic system may change to a ferromagnetic ground state, once Hills limit is crossed. In addition, in the proximity of such a dramatic modification, unexpected features such as unconventional superconductivity, superconductivity in presence of long range magnetic order or quantum critical behaviour may become obvious and can thus be studied in detail. The big upshot of Jiri Pospisils work is that these alterations can be intentionally driven by means of external parameters like the already mentioned substitution of *d*-elements (owing to changes of *d*-orbitals), but, additionally, also by externally applied pressure and magnetic fields.

Emplyoing bulk property studies like temperature, field and pressure-dependent electrical resistivity, specific heat, isothermal and field dependent magnetisation studies, as well as the usage of neutron diffraction experiments, Jiri Pospisil could resort to many diverse experimental results in order to develop on safe grounds a robust physical picture of the various U-intermetallics. The main outcome of Jiri Pospisils studies - in my view - is that not only Hills limit is the exclusive criterion, helping to judge about uranium compounds (particularly considering UTX intermetallics), but also changes of the electronic structure owing to *d*-element substitution is of eminent importance. It means that due to the alteration of the electronic configuration, triggered by the (partial) change of the *d*-element, a modification of the interaction with the uranium 5f electrons takes places - besides an increase or a decrease of the unit cell lattice parameters - which at the same time can drive an alteration of the uranium magnetic state in the compound.

The anisotropy of many physical properties of the present non-cubic uranium compounds requires the usage of single crystals as specimens. Jiri Pospisil managed to synthesize the pseudo-ternary uranium compounds by different, well known methods. The quality of these samples, which is an important puzzle-stone for the present successful studies, can be read-off e.g., from the large RRR values obtained experimentally.

The habilitation thesis of Jiri Pospisil is well organized and describes the various U-intermetallics, after an easy understandable introduction into the physics of uranium-systems, primarily on the basis of phase diagrams, either with respect to substitution, pressure or magnetic fields. Such phase diagrams condense the entire knowledge of a material into a single figure, which is almost always the target of any material dependent physical studies. Some drawback in the present thesis is the lack of original experimental data which would allow the reader to judge about changes, transitions or cross-over features, if a certain material is driven (e.g., by d-elements substitution) from x = 0 to x = 1. Such data and diagrams would help the reader to better understand and follow the discussions given in the experimental sections of the manuscript. In addition, in many sentences throughout the manuscript, single words are missing. The originality of this habilitation thesis has been checked by the system Turnitin; it turned out that there is just a negligible amount of coincidence, given the fact that the present review summarises publications with Jiri Pospisil as author or co-author.

The international visibility of Jiri Pospisils research can be exemplified from about 18 papers published in the previous 10 years (overall ~60); a good number of them appeared in one of the most acknowledged journals in solid state physics, namely in "Physical Review B".

To summarise, Jiri Pospisil has carried out high-quality research on (mostly) uranium compounds and has explained and analysed the experimental data obtained in these studies, utilizing most recent theoretical models as well as involving density functional theory ab-initio calculations. In addition, he managed being part of several international co-operations and using for his investigations large scale facilities, such as high field laboratories and neutron diffraction installations.

The outcome of the successful research of Jiri Pospisil allows me in firm conviction, to recommend the respective panel at the Charles University Prague, to positively consider his application for a habilitation at the Faculty of Mathematics and Physics, Charles University Prague.

[redacted]

(Univ.Prof. Dr. Ernst Bauer)

I declare herewith that I do not have any conflict of interest concerning the assessment of Jiri Pospisil's professional work. There are presently neither common publications, nor common research or other scientific projects.