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Supervisor report

of the thesis

Structure analysis of some transition metal silicides using X-ray diffraction and dynamical refinement against electron diffraction data

by **Cinthia Antunes Corrêa**

Cinthia Correa came to the Department of Physics of Material (DPM) in summer 2013 having been invited to the Czech Republic by the thesis co-supervisor dr. Lukas Palatinus from the Institute of Physics (IP) of the Academy of Sciences. After successful passing the entry exam she started her PhD studies at the Faculty of Mathematics and Physics (FMP) under the joint supervision of myself and dr. Palatinus. Very quickly she managed to balance the differences between the studies at the FMP and the Federal University of Goias, Goania, Brasil where she graduated. Unlike other students from abroad who usually need a certain time to adapt to the Czech system of education, Cinthia easily followed all lectures and passed all exams already in the first term of her PhD studies without any problems. This continued in fact during the whole course of PhD studies. She successfully passed the PhD state exam already in the second year of her PhD studies similarly as the best Czech students. Cinthia adapted very quickly to the Czech university environment and become familiar with students as well as colleagues at the DPM and IP also due to her enormous effort to learn the Czech language. Her progress in managing the Czech language was extremely fast and after one year she was able to understand Czech language including speaking.

Due to the easy handling of all her study duties Cinthia was able to start intensive scientific work soon after the beginning of her PhD program. Her research work was mostly performed at the

Institute of Physics AS CR. As a talented and hard working person Cinthia, guided by her co-supervisor dr. Palatinus, managed very quickly the enhanced techniques of precession electron diffraction and electron diffraction tomography both on the experimental and theoretical level. In her work she focused initially on the methodology of the inclusion of dynamical effects in the analysis of electron diffraction data. She implemented effectively the dynamical refinement procedures in the SW Jana2006 and showed unambiguously that inclusion of dynamic effects results in more precise structure parameters determination than if a kinematic or two beam approach is used only.

This theoretical approach was successfully verified on single crystals with known structure, namely silicide nanowires, by comparison of results obtained by dynamic refinement with those of standard XRD.

The most important result of the thesis is the application of dynamic refinement method to several specimens of unknown structure – copper silicides exhibiting different modulated structures which was a rather challenging task for a relatively short-term period of work within a PhD program. In her thesis Cinthia proved that she coped with this task in an excellent level.

In her work Cinthia showed outstanding abilities both in theoretical and experimental level. The quality of the literature overview including relatively high number of references demonstrates that she got a deep knowledge of the theory of electron diffraction including dynamic theory and was able to implement it into Jana2006 SW. In order to compare theoretical approach with experiment Cinthia needed to master several experimental techniques e.g. XRD, TEM etc. incl. specimen preparation for these techniques. Some of the results were obtained during her stays abroad (France).

During her PhD work Cinthia obtained a wide variety of novel and unique experimental results most of which she published in international highly reputed journals (5 papers in total thereof 3 times as the first author) and presented in many domestic and international conferences. The scientific value of her results was confirmed by several conference awards, e.g. Struktura 2015 in Luhačovice. Recently she presented an invited talk at the prestigious conference organized by the International Union of Crystallography in Hyderabad in India (24^{th} Congress of the International Union of Crystallography) in India. This is an outstanding achievement and something quite exceptional for a PhD student to get an invitation from an international conference committee to present an invited talk.

The scientific and competitive level of the subject of the thesis was also confirmed by the granting the project by the Grant Agency of Charles University (GAUK) in which Cinthia managed

a small team of PhD and undergraduate students in the years 2015-2017. Moreover, Cinthia was and continues to be a member of research teams of several projects of the Czech Science Foundation at IP and the project financed by the ERDF at the FMF.

In conclusion, it is my pleasure to state that during her PhD studies Cinthia Correa proved on a long-term basis that she has outstanding abilities for conducting the scientific and research work in the physics of condensed matter both independently and in a research team. In my opinion, her PhD thesis is of high international level and if successfully defended, it is without any doubt the background for granting Cinthia Correa the PhD degree.

Prague, 2 September 2017

prof. RNDr. Miloš Janeček, CSc.
supervisor of the thesis