Title: U-based thin films: electronic structure and physical properties

Author: Oleksandra Koloskova

Department / Institute: Department of Condensed Matter Physics, Faculty of Mathematics and Physics, Charles University

Supervisor of the doctoral thesis: Doc. RNDr. Ladislav Havela, CSc., Department of Condensed Matter Physics, Faculty of Mathematics and Physics, Charles University, Prague, The Czech Republic

Abstract: This thesis presents studies of U-based thin films synthesized by means of the DC sputter deposition, which allows to vary the composition and microstructure and perform in photoelectron spectroscopy studies. The subjects are U-Mo and U-Zr alloys, Uranium hydrides (UH<sub>3</sub> and UH<sub>2</sub>), and U hydrides with Zr/Mo substitution.

*In-situ* analysis was followed by *ex-situ* studies of structure, magnetic and transport properties. Despite the superconducting ground state of the U-T alloys, only one film ( $U_{0.92}Mo_{0.08}$ ) exhibited superconductivity, with the transition at 0.55 K.

All hydrides are ferromagnetic, with Curie temperatures around 120 K for UH<sub>2</sub> and 170 K for both  $\alpha$ - and  $\beta$ -UH<sub>3</sub>. This ferromagnetism is robust and independent of structural details. By varying sputtering parameters, one can obtain UH<sub>2</sub> (nonexistent in bulk form),  $\beta$ -UH<sub>3</sub>, or a mix of UH<sub>2</sub> and  $\alpha$ -UH<sub>3</sub> (first observed in film form). Inclusion of hydrogen atoms drastically changes properties, shifting from paramagnetic alloys to ferromagnetic hydrides, with the U-H polar bond being crucial for magnetism. The nature of UH<sub>3</sub> as a band ferromagnet was clarified by comparing DMFT calculations with XPS and UPS spectra, revealing final-state 5*f*<sup>2</sup> multiplet and emphasizing electron-electron correlations in UH<sub>3</sub>.

Zr substitution in hydride films stabilized UH<sub>2</sub> instead of the expected  $\alpha$ -UH<sub>3</sub> phase. Series (UH<sub>3</sub>)<sub>1-x</sub>Mo<sub>x</sub>, (UH<sub>3</sub>)<sub>1-x</sub>Zr<sub>x</sub>, and (UH<sub>2</sub>)<sub>1-x</sub>Zr<sub>x</sub> have lower Curie temperatures than their bulk counterparts and pure UH<sub>2</sub> or UH<sub>3</sub> films. This decrease is attributed to a destabilization of hydrogen caused by the incorporation of transition metals and the excessive energy from the deposition process.

Keywords: Thin Films, Uranium, Superconductivity, Hydride, Electronic Structure, Magnetism