

PhD dissertation's abstract

”Theoretical studies of electronic structure and selected physical properties of high entropy alloys”

High entropy alloys (HEA) are often referred as ”metallic glass on an ordered lattice” because of their unique physico-chemical properties. Despite high level of chemical disorder, those multi-atom systems usually crystallizes in simple crystal structures. PhD thesis presents results of modeling of physical properties of selected HEAs consisting transition metals. Theoretical studies have been carried out using electronic structure calculations, performed with the Korringa-Kohn-Rostoker method, where the chemical disorder have been taken into account with the coherent potential approximation (CPA). KKR-CPA is one of the well-established *ab initio* technique allowing to perform self-consistent electronic structure calculations of crystalline systems with high level of chemical disorder. From many known groups of HEAs, two families have been selected for investigations : (i) superconducting systems TaNbHfZrTi including predominantly *4d* and *5d* transition elements, and (ii) magnetic alloys CrCoFeNiAl, containing mainly *3d* transition elements and showing interesting structural phase transitions related to changes in constituent atoms concentrations.

Experimental data available for $(\text{TaNb})_{0.67}(\text{HfZrTi})_{0.33}$ HEA indicate conventional mechanism of superconductivity, where interactions between electrons and lattice vibrations are found to be the origin of attractive interactions between electrons. Electron-phonon coupling constant, one of the basic parameters characterizing classical superconductors, have been calculated by separating electron and phonon parts. In order to obtain electronic part, the Rigid Muffin Tin Approximation have been applied and McMillan-Hopfield parameters have been averaged over constituent atoms concentrations. Phonon part have been estimated with average atomic mass and experimental Debye temperature. The theoretical electron-phonon coupling constant remains in good agreement with the value extracted from experimental specific heat coefficient. Also, analysis of interplay between Coulomb pseudopotential and critical temperature have been carried out. Electronic dispersion relations have been determined with complex energy band technique, showing relatively small smearing due to chemical disorder, especially in the vicinity of the Fermi energy. Next, simulations of hydrostatic pressure impact on electronic band structure revealed subtle changes in Fermi surface topology interpreted as Lifshitz transition. Full analysis of relationship between pressure and electron-phonon coupling constant required

developing procedure allowing to calculate changes in Debye temperature when shrinking unit cell volume. The proposed scheme, partly based on parameters available from experiments (such as Grüneisen parameter γ_G at ambient pressure, bulk modulus B or volumetric thermal expansion coefficient α_V) have been successfully tested for elemental Ta and Nb. Assuming variations in Coulomb pseudopotential caused by pressure, satisfactory agreement between theoretical $T_c(P)$ function and experimental curve have been found. Since in real, multi-component HEAs lattice distortions are observed due to important differences in atom size, such effects have been simulated by relaxations of atomic positions carried out for representative $3 \times 3 \times 1$ supercells. Averaged electron-phonon coupling constants of distorted supercells allowed to reproduce experimental critical temperature using value of Coulomb pseudopotential much closer to standard value 0.13.

In second part of the PhD thesis concerning CrCoFeNiAl HEA family, results of theoretical studies of relative crystal stability, phase preference and magnetic properties have been described, what required spin-polarised KKR-CPA calculations. As a result, total (per unit cell) and atomic magnetic moments in function of constituent atom concentrations have been obtained. Computations revealed interesting tendency to antiparallel alignment of Cr magnetic moments with respect to magnetic moments of other $3d$ elements, being correlated with the phase preference. Calculated formation energy for the considered alloys allowed to determine energetically favorable crystal structures. Additionally, the concentration ranges where two phase may coexist have been estimated using common tangent line rule.