Electronic Structure and Superconductivity of the High Entropy Alloy Sc-Zr-Nb-Rh-Pd

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In 2014, the superconductivity was discovered in the new type of materials - High Entropy Alloys (HEA), the alloys that are formed by mixing relatively large proportions of five or more elements. Since then, the superconductivity was found experimentally in many HEAs. However, the theoretical research concerning the electronic structure and the mechanism behind forming of the superconducting state is scant. HEAs are of high interest from material science point of view due to their unique properties such as high fracture toughness, ductillity and yield strength in extreme temperatures as well as resistance to corrosion and oxidation.

The superconductivity of Sc-Zr-Nb-Rh-Pd alloy was experimentally confirmed in 2018 and reported in [1]. This research investigates electronic structure of the Sc-Zr-Nb-Rh-Pd HEA by employing the Korringa-Kohn-Rostoker Coherent Potential Approximation method (KKR-CPA) and Density Functional Theory. The main purpose of this work was to analyze how well the KKR-CPA method can describe the electronic properties of HEAs. Similar computations were carried out in [2] for Ta-Nb-Hf-Zr-Ti HEA superconductor.

The results obtained in this work concern the McMillan-Hopfield coefficients, the density of electronic states around Fermi Energy and dispersion relations for different concentrations of the components in Sc-Zr-Nb-Rh-Pd HEA for which the formation of the superconducting state was observed. The computations also showed that the CsCl structure should be observed in this type of alloy, and the experimental data in [1] shows that this is indeed the case. Additionally, strong smearing of the electronic bands show the significance of the chemical disorder in the properties of the alloy.

[1] *Sc–Zr–Nb–Rh–Pd and Sc–Zr–Nb–Ta–Rh–Pd High-Entropy Alloy Superconductors on a CsCl-Type Lattice*, K. Stolze, J. Tao, F. O. von Rohr, T. Kong, and R. J. Cava, Chemistry of Materials 2018 30 (3), 906-914

[2] *Pressure effects on the electronic structure and superconductivity of* $(TaNb)_{0.67}(HfZrTi)_{0.33}$ *high entropy alloy*, Jasiewicz, K. and Wiendlocha, B. and Górnicka, K. and Gofryk, K. and Gazda, M. and Klimczuk, T. and Tobola, J., Phys. Rev. B, Vol. 100,iss. 18 (2019)