

vantages attributed to titanium have been exploited in the aircraft industry, power industry, chemical industry, and medicine.

To improve the surface quality and increase the corrosion resistance of titanium and its alloys, anodic electrochemical treatment is usually applied. Electropolishing is a very effective method of removing the layer formed on the metal surface during mechanical treatment. This layer is the reason for the increased electrochemical activity of the metal because it is characterized by a deformed surface structure. Additionally, a thin protective passive layer is formed in course of the treatment. After electropolishing the metal surface roughness is decreased, the scratches are removed, and the surface is characterized by a significant gloss.

We present study of modified by ectropolishing and anodic passivation surface of Ti-15Mo alloy. The electropolishing process was carried out in solutions containing sulfuric acid, ethylene glycol, ammonium fluoride and oxalic acid. Whereas a voltage range from 20 to 100 V and a 1 M orthophosphoric acid solution were used during the anodic passivation. The influence of above mentioned processes parameters on the quality of the obtained oxide layer on Ti-15Mo alloy was investigated. The analysis of Ti-15Mo surface after modification was performed using scanning electron microscopy (SEM, X-ray photoelectron spectroscopy (XPS). It was found that electropolishing leads to an increase in the surface homogeneity and to the form of an oxide layer, which consisted of TiO_2 and MoO_3 . Whereas the oxide layers obtained during anodic passivation were characterized by different properties depending on the applied voltage. The anodic passivation at various voltages (20-100 V) increased the surface wettability (94.5° – 87.6°) in comparison to the electropolished sample (97.5°). Moreover, the obtained oxide layer after anodization exhibited a high hardness.

CALCULATION SCHEME BASED ON THE EXTENDED EQUATIONS OF DMFT

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Extended DMFT equations were calculated by means of exact diagonalization method. Metal-insulator transition was considered for squared cuprate-like lattice and triangular lattices of F and H on the Gr. Additional peaks were found in low-energy region of spin susceptibility caused non-local interactions of lattice sites.

Heisenberg-type part in lattice Hamiltonian for case of magnetic interactions was added. It gives an opportunity to describe these systems more fully. The impurity Hamiltonian was changed in the following way:

$$H_{imp} = \varepsilon_d \sum_{\sigma} c_{d\sigma}^{\dagger} c_{d\sigma} + U n_{d\uparrow} n_{d\downarrow} + \sum_k V_{dk} (c_{d\sigma}^{\dagger} c_{k\sigma} + c_{k\sigma}^{\dagger} c_{d\sigma}) + \sum_{k\sigma} \varepsilon_k c_{k\sigma}^{\dagger} c_{k\sigma} + \sum_p \Omega_p \vec{b}_p^{\dagger} \vec{b}_p + \sum_p W_p \vec{S}(\vec{b}_p^{\dagger} + \vec{b}_p)$$

where ε_d and ε_k are energies of the correlated impurity and fermionic bath states, $c_{d\sigma}^{\dagger}(c_{d\sigma})$ and $c_{k\sigma}^{\dagger}(c_{k\sigma})$ are the creation (annihilation) operators for impurity and bath electrons, V_{dk} is the hopping integral between impurity and fermionic bath states, μ is the chemical potential and U is one-site Coulomb interaction, $\vec{b}_p^{\dagger}(\vec{b}_p)$ - creation (annihilation) operator of p^{th} boson, Ω_p - boson frequency, W_p - fermion-boson interaction.

The proposed scheme gives us the opportunity to provide a complete description of the magnetic properties of a low-dimensional system, such as the momentum- and frequency-dependent magnetic susceptibility of the system.

In proposed scheme the self-consistency cycle is based on minimization of hybridization functions between reservoirs and impurity, as a result we obtain calculation where lattice model is in accordance with impurity model. The base of all calculations is the method of exact diagonalization and obtainment of spectral functions through Lehmann representation.

In this work two kinds of lattice (squared and triangular) and three compounds (cuprate-like lattice, C_2F and C_2H) have been studied, parameters of phase transition have been obtained also. Phase transition from insulator to metal state has been considered both DMFT way and EDMFT. In result one can see that accounting of the non-local magnetic calculations gives additional low-energy peak of the spin susceptibility.

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