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Understanding the Features of Crystal Structure, Electronic Structure and Electrical Conductivity of RuO_2-SiO_2 Binary Oxides

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Density functional theory calculations combined with experiments were performed to investigate the stability, crystal structure, electronic structure and conductivity of RuO_2-SiO_2 binary oxides. Our calculations indicate that $Ru_{1-x}Si_xO_2$ solid solutions are unstable, and both their total energies and lattice parameters deviate from Vegard's law, revealing a strong interaction between RuO_2 and SiO_2. With an increase in x (doping concentration of SiO_2), the conductivity of $Ru_{1-x}Si_xO_2$ underwent first-order exponential attenuation, but the compound remained metallic even when x was 0.875. $Ru_{0.5}Si_{0.5}O_2$/Ti electrodes were prepared using the thermal decomposition method, and at different annealing temperatures, varying degrees of phase separation were observed in all the samples, proving the instability of the $Ru_{1-x}Si_xO_2$ solid solutions. The impedance test of the $Ru_{0.5}Si_{0.5}O_2$/Ti samples showed that the total impedance of the samples and the degrees of phase separation conform to the first-order exponential relationship. The dual effects of Si doping attenuation and phase separation attenuation can explain the rapid decline in the conductivity of the RuO_2-SiO_2 electrode material.

Keywords: First-principles; RuO_2-SiO_2 binary oxide; crystal structure; phase separation; electronic structures; electrical conductivity

FULL TEXT