Thermoelectric properties of ScN thin films

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Abstract:
Transition metal nitrides are promising for high temperature thermoelectric materials because of their high thermal stability, corrosion resistance, and their electrical properties which vary over a wide range from semiconducting to metallic depending on the transition metal elements. However, they are relatively unexplored to date for this purpose. Here, we have investigated the thermoelectric properties of ScN thin films grown by reactive dc magnetron sputtering in Ar/N_2 on a single crystal $Al_2O_3(0001)$. All films exhibit n-type behavior. High purity ScN films show high Seebeck coefficient ~90 μV/K and low electrical resistivity ~2.94 μΩ·m yielding a remarkably high thermoelectric power factor of ~2.5×10^{-3} W/(m·K^2), corresponding to an estimated thermoelectric figure of merit of ~0.2 at 800 K, using the thermal conductivity of ScN thin film material. We also demonstrate that the thermoelectric properties are highly sensitive to composition and impurities. Different Ar/N_2 flow rate ratios, gas pressure and target conditions were tested resulting in films with various crystal qualities, composition and impurities of for instance oxygen. All films contain trace amounts of F originating from the Sc target. It is found that the impurity level and crystal quality of the ScN tend to have very limited effect on the Seebeck coefficient while the electrical resistance is strongly affected. Generally, increased nitrogen flow in sputtering gas resulted in increased resistivity. However it was also found that the electrical resistance tends to increase with increased crystal imperfections related to defects and impurities.