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Ab Initio Calculations and Measurements of Thermoelectric Properties of V_2O_5 Films

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Density functional theory and the Boltzmann transport equation were used to calculate the thermoelectric transport coefficients for bulk V_2O_5 and MV_2O_5 (M = Cr, Ti, Na, Li). The structural relaxation for the given compounds based on the ABINIT code was observed. The temperature dependences of the Seebeck coefficients as well as electrical and thermal electrical conductivities of all relaxed structures displayed anisotropic behavior. Electrooptical measurements of thermoelectric properties were carried out on V_2O_5 thin films obtained by thermal evaporation with different post-annealing treatments. A Seebeck coefficient of -148 μV/K at T = 300 K was obtained in the in-plane direction for V_2O_5 thin films with thickness less than 100 nm.

Key words: V_2O_5 thin films, density functional theory, Boltzmann transport equation, thermoelectric properties

INTRODUCTION

Interest in high-performance thermoelectric materials has increased in recent decades due to the development of new deposition methods for structural engineering with which one can tailor their properties at the atomic level. Vanadium oxides make up a fascinating class of materials with outstanding physical and chemical properties. Different oxidation states can be obtained depending on the preparation method and on the type of source material. The most studied are VO_2, V_2O_3, and V_2O_5, which are also used in many technological applications, such as electrical and optical switching devices,[1] light detectors,[2] temperature sensors,[3] and write–erase media.[4] Although scarcely explored, some works have revealed potential applications of V_2O_5 as thin-film thermoelectrics.[5,6] Theoretical calculations confirm a low thermal conductivity and reasonable electrical conductivity of V_2O_5 thin films.

EXPERIMENTAL PROCEDURES

In our investigations, amorphous samples of V_2O_5 were deposited without substrate heating and, after deposition, were subjected to annealing at different temperatures for 2 h. The post-annealing was performed under air atmospheric pressure conditions with ramp up of 10 K/min and holding time of 1 h. Increase of the annealing temperature led to the formation of V_2O_5 crystalline phases. It was observed that the measured room-temperature dark conductivity ($\sim 1 \times 10^{-5}$ S/cm) increases with increasing annealing temperature up to 600°C ($\sim 5 \times 10^{-2}$ S/cm), accompanied by a decrease in the activation energy from 0.34 eV to 0.17 eV and the appearance of crystalline grains. The measured Seebeck coeffi-

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