



Title	Structure Control of SnO ₂ Thin Film Surfaces and Water Molecule Adsorption
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Abstract of Thesis

Name (HOU, linfeng)	
Title	Structure Control of SnO ₂ Thin Film Surfaces and Water Molecule Adsorption (SnO ₂ 薄膜表面の構造制御と水分子吸着に関する研究)
Abstract of Thesis The surface structure of SnO₂ plays a crucial role in determining its gas-sensing performance, particularly for water vapor, which strongly affects surface charge states, band bending, and electrical conductivity. In metal-oxide-based gas sensors, water adsorption often induces significant changes in electrical resistance and frequently causes cross-sensitivity, making a detailed understanding of water-surface interactions essential for both sensing performance and device reliability. While surface reconstructions of bulk SnO₂ (110) single crystals have been extensively investigated within the framework of surface science, the manifestation, stability, and functional implications of such reconstructed structures in thin-film systems relevant to practical sensing devices remain insufficiently understood. In this dissertation, SnO₂(110) thin films grown on TiO₂(110) substrates were investigated as a model system to clarify the relationship between preparation conditions, surface reconstruction, and water adsorption behavior at the atomic scale. The use of rutile TiO₂(110) substrates enables the preparation of structurally well-defined SnO₂(110) thin films and provides a controlled platform for systematic surface-science investigations. The effects of annealing temperature and oxygen partial pressure on surface morphology and reconstruction were systematically examined using scanning tunneling microscopy (STM) and low-energy electron diffraction (LEED). These complementary techniques allow correlation between local surface morphology and long-range reconstruction symmetry. The results demonstrate that well-defined (1×1) and (4×1) reconstructed surfaces can be reproducibly prepared within specific thermodynamic windows. Moderate thermal treatment promotes surface planarization and vacancy ordering, leading to long-range reconstruction, whereas excessive reduction under oxygen-deficient conditions results in surface roughening, defect aggregation, and loss of long-range order. These observations establish a preparation map that links temperature, oxygen chemical potential, and reconstruction stability in SnO₂(110) thin films. Based on these structurally characterized surfaces, the atomic-scale adsorption behavior of water molecules was investigated through a combined experimental and theoretical approach. STM observations were used to identify adsorption-induced features and spatial heterogeneity, while first-principles density functional theory calculations were employed to evaluate adsorption energetics, preferred configurations, and possible dissociation pathways. The results reveal that reconstructed surfaces provide ordered defective motifs, such as oxygen-vacancy-related structures and undercoordinated Sn sites, which strongly stabilize specific adsorption configurations of water and hydroxyl species. These adsorption-induced surface states lead to enhanced modulation of surface potential and depletion-layer width. Overall, this study demonstrates that surface reconstruction constitutes an intrinsic and effective strategy for controlling water-related sensing behavior in SnO₂ thin films. By extending reconstruction-resolved surface science from bulk single crystals to thin-film systems directly relevant to sensing devices, this work provides a structure-based framework for understanding and optimizing metal-oxide gas sensors, particularly with respect to humidity effects and defect-controlled surface reactivity.	

論文審査の結果の要旨及び担当者

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論文審査の結果の要旨 本論文は、金属酸化物ガスセンサーに広く用いられるSnO₂の表面構造が水蒸気応答に与える影響に着目し、作製条件、表面再構成、水分子吸着挙動の相関を原子スケールで解明することを目的としている。水の吸着は表面電荷状態やバンドベンディング、電気伝導度に大きな変化をもたらし、センサーの感度や信頼性に直結するが、実用デバイスに近い薄膜系における再構成構造の安定性や機能的意義については十分に理解されていなかった。本研究では、TiO₂(110)基板上に成長させたSnO₂(110)薄膜をモデル系とし、走査トンネル顕微鏡および低速電子回折を用いて、局所形態と長距離秩序の対応関係を体系的に評価した。その結果、特定の熱力学条件下で(1×1)および(4×1)再構成表面を再現性よく形成できることを示し、適度な熱処理が表面平坦化と欠陥秩序化を促進する一方、過度な還元は表面粗化と長距離秩序の消失を招くことを明らかにした。さらに、第一原理計算とSTM観察を組み合わせることで、水分子および水酸基が酸素空孔や配位不飽和Snサイトに強く安定化されることを示し、これらの吸着状態が表面ポテンシャルや空乏層幅の変調を通じてセンシング特性に影響を及ぼす機構を解明した。以上より、本論文は再構成構造に基づく薄膜表面制御が水関連センシング特性の理解と最適化に有効であることを示し、金属酸化物ガスセンサーの設計指針となる重要な知見を提供するものである。よって、本論文は博士（工学）の学位論文として価値のあるものと認める。			