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STRAIN SENSITIVITY OF EPITAXIALLY STRAINED SrTiO3 and BaTiO3: FIRST-PRINCIPLE STUDY

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The effect of epitaxial strain on SrTiO3 (STO) and BaTiO3 (BTO) lattices has been studied by using density functional theory within the local-density approximation. The strain-induced sequence of phase transitions was determined to be c-p-aa for STO and c-r-aa for BTO in a wide range of misfit strain from -2% to +2%. All the transitions are second-order. It was strikingly found that the optical phonon of the strained BTO is characterized by overdamping and reorientation while that of the strained STO shows a perfect softening to zero frequency at the phase boundaries. Consequently, the dielectric constant of BTO shows a significantly low sensitivity to strain in comparison with that of STO. This behavior agrees with the experimentally observed dielectric behavior of Ba-based materials. The origin of this striking difference is attributed to the existence of the order-disorder component in the strain-induced transition mechanism in BTO.

Keywords: Dielectric, SrTiO3, phase transition

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Visible-Light Photocatalysis of Sr-Doped $TiO_{2-\delta}$ Nanobelts Synthesized by Chemical Vapor Deposition

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Titania (TiO_2) has been studied extensively as a photocatalytic material. High-efficient photocatalytic reactivity of TiO_2 can be very promising for electrodes of solar cells, the elimination of pollutants, and the photogeneration of hydrogen from water. However, the wide bandgap energy (~3.0-3.2 eV) of TiO_2 limits its photocatalytic reaction to ultraviolet light. Considerable efforts have been taken to extend the reactivity to visible light regime via doping of transition metals or nonmetals such as nitrogen and carbon. However, little information is available on visible-light photocatalysis of 1-D TiO_2 nanostructures (nanowires and nanotubes) because synthesis and doping of 1-D TiO_2 nanostructures still represents a challenging issue. So far, only ion implantation was introduced to dope nitrogen into TiO_2 nanotubes. Ion implantation is a straightforward approach, but it accompanies structural damages to degrade the photocatalytic reactivity significantly. In this study, we performed in-situ doping of strontium (Sr) in $TiO_{2-\delta}$ nanobelts during the synthesis by metallorganic chemicalvapor deposition (MOCVD). The Sr-doped $TiO_{2-\delta}$ nanobelts were self-catalytically grown without the use of any metal catalysts. Moreover, the $TiO_{2-\delta}$ anobelts also showed high-efficient visible-light photocatalytic activity, which were evaluated by the decomposition of methylene blue under visible light irradiation. We will further discuss growth mechanism and photocatalytic characteristics of Sr-doped $TiO_{2-\delta}$ nanobelts.

Keywords: Photocatalysis, TiO2, nanobelt