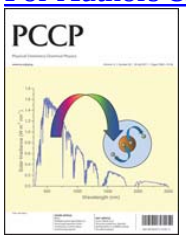

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Synthesis, surface morphology, and photoluminescence properties of anatase iron-doped titanium dioxide nano-crystalline films

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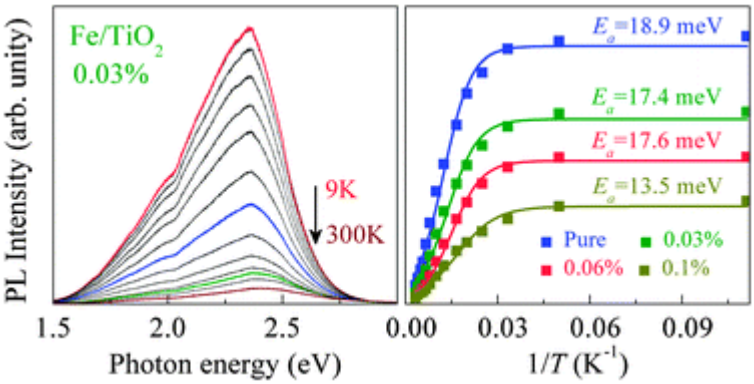
Iron (Fe)-doped (0 to 4%) TiO_2 nano-crystalline (*nc*) films with the grain size of about 25 nm have been deposited on n-type Si (100) substrates by a facile nonhydrolytic sol–gel processing. X-ray diffraction measurements prove that the films are polycrystalline and present the pure anatase phase. X-ray photoelectron spectroscopy spectra indicate that the chemical valent state of Fe element is +3 and the Fe^{3+} ions replace the Ti^{4+} sites. The Fe dopant effects on the surface morphology, microstructure, and dielectric functions of the *nc*-Fe/TiO_2 films have been studied by atomic force microscope, ultraviolet Raman scattering and spectroscopic ellipsometry. With increasing Fe composition, the intensity of Raman-active mode B_{1g} increases, while that of the A_{1g} phonon mode decreases. The dielectric functions have been uniquely extracted by fitting ellipsometric spectra with the Adachi's dielectric function model and a four-phase layered model. It is found that the real part of dielectric functions in the transparent region and the optical band gap slightly decrease with the Fe composition due to the introduction of acceptor level Fe t_{2g}. Finally, the composition and temperature dependence of the surface and lattice defects in the Fe/TiO_2 films have been investigated by photoluminescence spectra in detail. At room temperature, the emission intensities decrease with increasing Fe compositions since the Fe incorporation could prolong the radiative lifetime and/or shorten the non-radiative lifetime. By analyzing the low temperature photoluminescence spectra, the intensities and positions of five emission peaks and shoulder structure can be unambiguously assigned. The phenomena could be reasonably explained by the physical mechanisms such as oxygen vacancies, localized excitons, self-trapped excitons, and indirect transitions, which are strongly related to the electronic band structure perturbed by the Fe doping.



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