Crystallographic and electronic structures of materials and their transformations are studied through direct imaging of atoms or molecules by high-resolution spectromicroscopy which realizes energy-filtered imaging and electron energy-loss spectroscopy as well as high resolution imaging. It aims to explore new methods for imaging and also obtaining chemical information in thin films, nano-clusters, interfaces, and even in solutions. By combining this with scanning probe microscopy, the following subjects are urging: direct structure analysis, electron crystallographic analysis, epitaxial growth of molecules, structure formation in solutions, fabrication of low-dimensional functional assemblies.

Research Activities (Year 2005)

Presentations


Organic Field-effect Transistors Based on Thiienyl-Fu-
Structural Analysis of Bis(1,2-benzoquinonodioximato)platinum(II) Polymorphs Formed Epitaxially on Alkali Halides

We analyzed the crystal structures of bis(1,2-benzoquinonodioximato)platinum(II), (Pt(bqd)$_2$), thin films fabricated by vacuum deposition on the (001) surfaces of NaCl, KCl, KBr and KI substrates at room temperature. Pt(bqd)$_2$ thin films exhibited some polymorphs. These structures and crystallographic orientations were studied by transmission electron microscopy (TEM). On NaCl, KCl and KBr, Pt(bqd)$_2$ grows in the $\beta$-form; unit cell dimensions are $a=2.57$ nm, $b=0.66$ nm and $c=0.37$ nm. The $\beta$-polymorph transforms into the ordinary orthorhombic $\alpha$-form by heating at different rates depending on the substrate. The instability of the $\beta$-form was influenced by lattice-matching between the $\beta$-form and substrate used. On KI, Pt(bqd)$_2$ grows as another polymorphic tetragonal form ($\gamma$-form: $a=1.42$ nm and $c=0.656$ nm). From the result of high-resolution TEM observations, many defects or domain boundaries in this film were observed, which are related to the structural change during the growth. Yoshida K et al., JJAP, 44(1B), 491-494 (2005).

Influence of Nitrogen Vacancies on the N K-ELNES Spectrum of Titanium Nitride

We have calculated the nitrogen K-ELNES of TiN$_x$ including N vacancies by the first-principles band calculations (WIEN2K). It has been demonstrated that the change of ELNES due to the vacancy depends on the atomic configuration between the vacancy site and the excited atom. The influence of vacancy appears to be strong when the vacancy occurs at the second nearest neighbor site from the excited atom. The vacancy levels, mainly consisting of Ti d states at first nearest neighbor site, are found to occur $\sim$2 eV and near the Fermi level. These levels reduce the intensity of the N p-DOS at the top of the conduction band on account of the hybridization between Ti d and N p states, which causes the decrease of energy separation between the relevant peaks observed in experimental ELNES spectra. The calculated spectra agree fairly well with the experimental ones, although a supercell of considerably larger size than that afforded by the computational powers available in this study is needed to simulate composition-induced changes in calculated ELNES spectra. Tsujimoto M et al., J. Electron Spectrosc. Relat. Phenom., 143, 159-165 (2005).

Grants

