Advanced Research Center for Beam Science
- Electron Microscopy and Crystal Chemistry -

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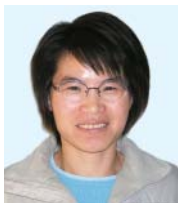

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Visitors

Dr MAGONOV, Sergei	Digital Instruments/Veeco Metrology, USA, 15 July 2005
Prof WANG, Hao	Beijing University of Technology, China, 26 July 2005
Dr FRANCO, Olga	Universidad Complutense, Spain, 1 - 21 August 2005
Prof CHOU, Li-Jen	National Tsing-Hua University, Taiwan, 1 September 2005 - 31 March 2006

Scope of Research

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

Single-grain Organic Field-effect Transistors Based on Pentacene Thin Film Phase, Minari T, Nemoto T, Isoda S, The 5th International Conference on Electroluminescence of Organic Materials and Related Phenomena, 17 - 21 January, Phoenix USA.

Core-hole Effects on Oxygen K-ELNES of Transition Metal Oxides, Kurata H, Tsujimoto M, Nomoto T, Isoda S, International EELS Workshop EDGE 2005, 1 - 5 May, Grundlsee, Austria.

Organic Field-effect Transistors Based on Thienyl-Furan Oligomers, Minari T, Terayama M, Miyata Y, *et al*., 8th European Conference on Molecular Electronics, 29 June-3 July, Bologna, Italy.

STM and STS Studies on Platinum Chains in Bis(1,2-benzoquinonedioximato)platinum, Yaji T, Yoshida K, Tsujimoto M, Nemoto T, Kurata H, Isoda S, KJF 2005, 26 - 29 October, Daejeon, Korea.

Polymorphs of Ni(salen) Grown on Substrates, Yoshida K, Isoda S, The 2005 International Chemical Congress of Pacific Basin Societies, 15 - 20 December, Hawaii, USA.

Structural Analysis of Bis (1,2-benzoquinonedioximato)platinum(II) Polymorphs Formed Epitaxially on Alkali Halides

We analyzed the crystal structures of bis(1,2-benzoquinonedioximato)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 β-form; unit cell dimensions are a=2.57 nm, b=0.66 nm and c=0.37 nm. The β-polymorph transforms into the ordinary orthorhombic α-form by heating at different rates depending on the substrate. The instability of the β-form was influenced by lattice-matching between the β-form and substrate used. On KI, $Pt(bqd)_2$ grows as another polymorphic tetragonal form (γ-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).

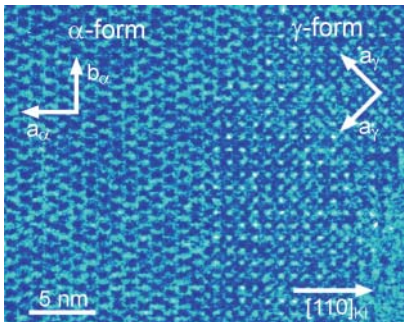

Figure 1. HRTEM image of the interface between the α- and γ-forms.

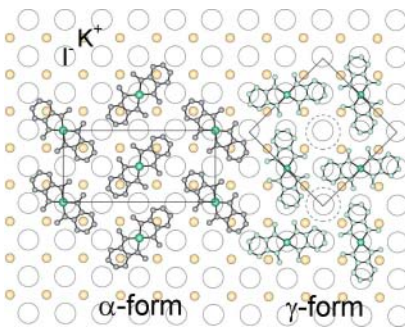

Figure 2. Model of interface between α-form and γ-form on KI substrate.

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 ~-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).

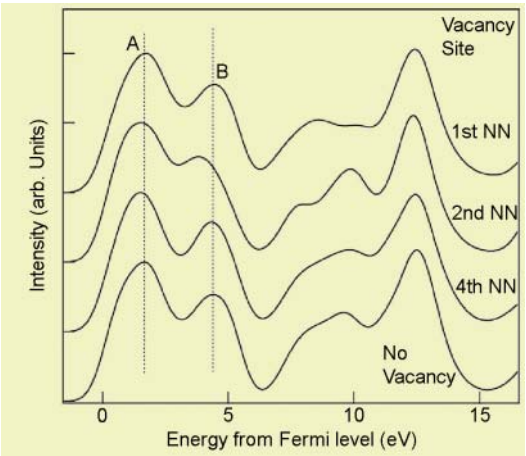

Figure 3. Site-resolved N K-ELNES for $TiN_{0.97}$ involving a vacancy at different distances from the excited atom.

Grants

Kurata H, Development of an EELS/XES Electron Microscope for Electronic Structure Analysis, Leading Project, The Ministry of Education, Science, Culture and Sports, Japan, 1 April 2004 - 31 March 2007.

Kurata H, Local State Analysis of Organic Materials by Spatially and Angular Resolved EELS, Grant-in-Aid for Scientific Research (B), 1 April 2003 - 31 March 2006.

Isoda S, Nanotechnology Support Project, The Ministry of Education, Science, Culture and Sports, Japan, 1 April 2005 - 31 March 2006.