内殻素励起によるX線ラマン散乱を用いた電子構造の研究

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Collaborator

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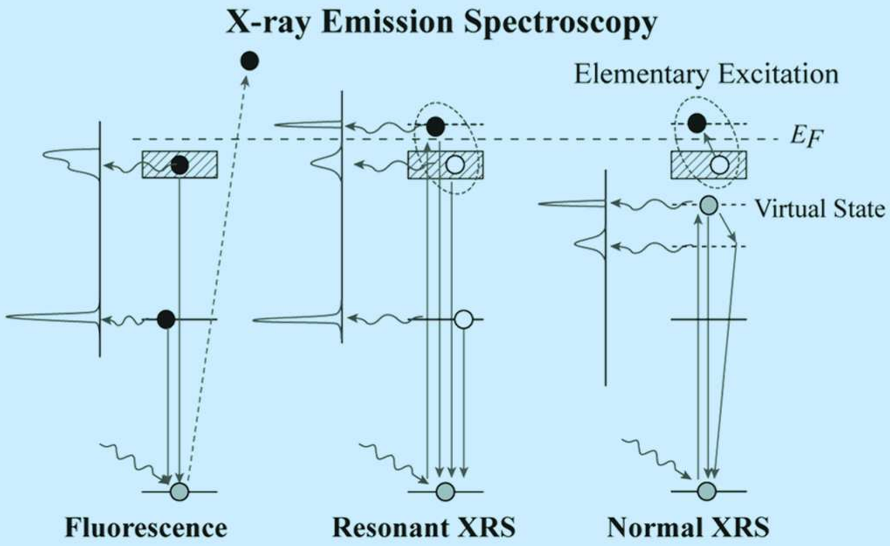
H. Sakama (*Sophia Univ.*)

Background / Experimental



Interaction between electron and radiation

$$H_{int} = \frac{e^2}{2mc^2}A^2 - \frac{e}{mc}(\mathbf{pA})$$

p: momentum of electron

A: vector potential

Kramers-Heisenberg formula (~pA) << **RIXS (RXRS)** >>

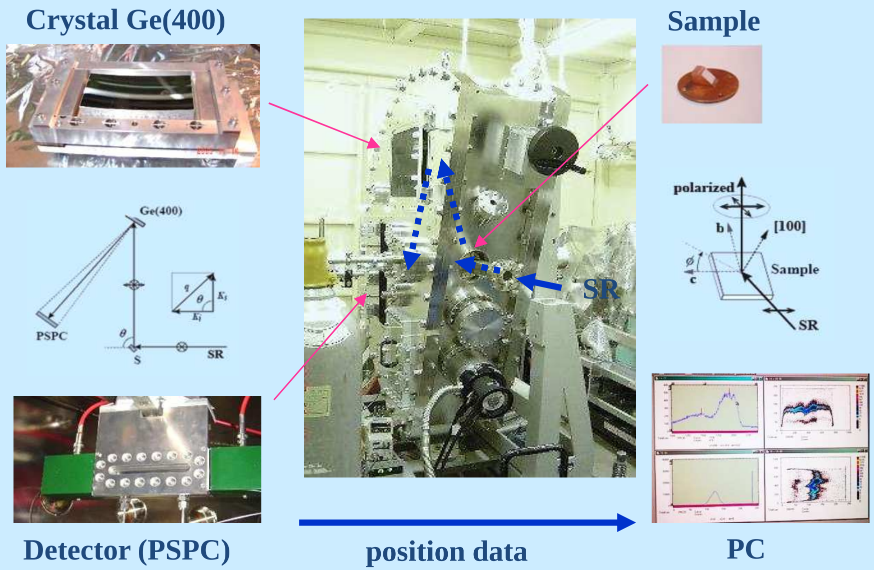
$$\frac{d^2\sigma}{d\Omega_{k_2} d(\hbar\omega)} \sim \sum_j \left| \sum_i \frac{\langle j|T_2|i\rangle\langle i|T_1|g\rangle}{E_g + \hbar\Omega - E_i + i\Gamma_i} \right|^2 \delta(E_g + \hbar\Omega - E_j - \hbar\omega)$$

Dynamical structure factor (~ A^2) << XRS >>

$$\frac{d^2\sigma}{d\Omega_{\mathbf{k}_2} d(\hbar\omega)} \sim \frac{\omega}{\Omega}\left(\frac{e^2}{mc^2}\right)^2 (\mathbf{e}_1 \cdot \mathbf{e}_2) S(\mathbf{k}_1 - \mathbf{k}_2, \Omega - \omega)$$

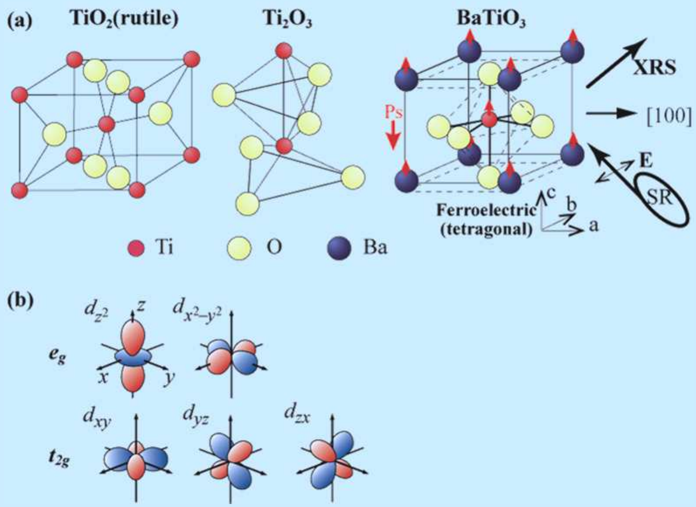
S: Dynamical structure factor

ESCARGOT (X-ray spectrometer) @KEK-PF BL7C, BL15B (bending)



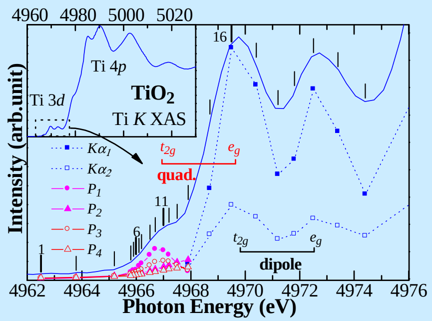
Sample

- TiO_2 (rutile) : powder, single crystal (100)
- Ti_2O_3: powder
- $BaTiO_3$ (BTO): powder, single crystal (100)

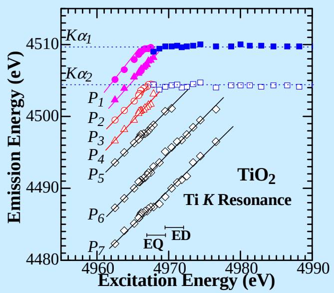


XRS Spectra of TiO_2

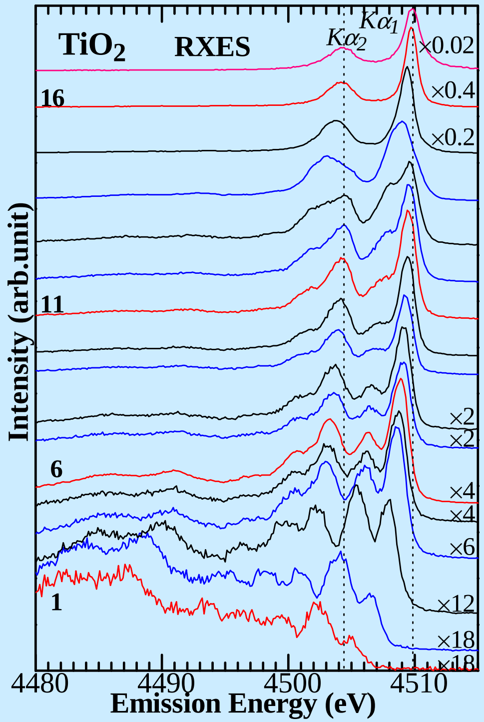
Y. Tezuka, et al., J. Phys. Soc. Jpn. **83**, 014707 (2014).



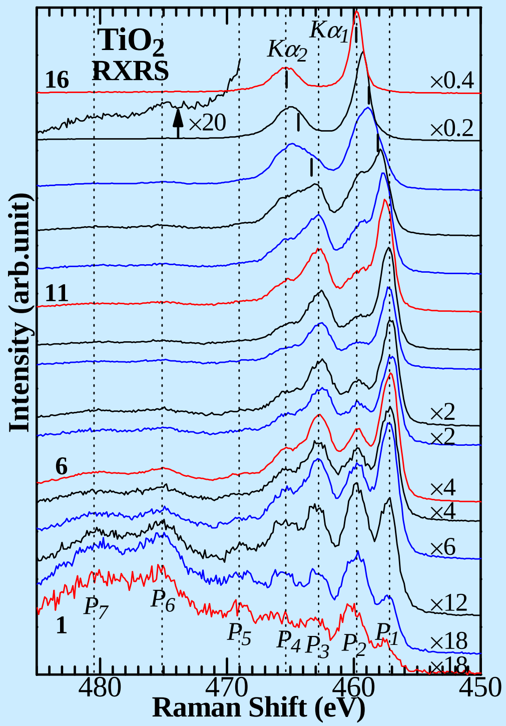
Ti *K* XAFS



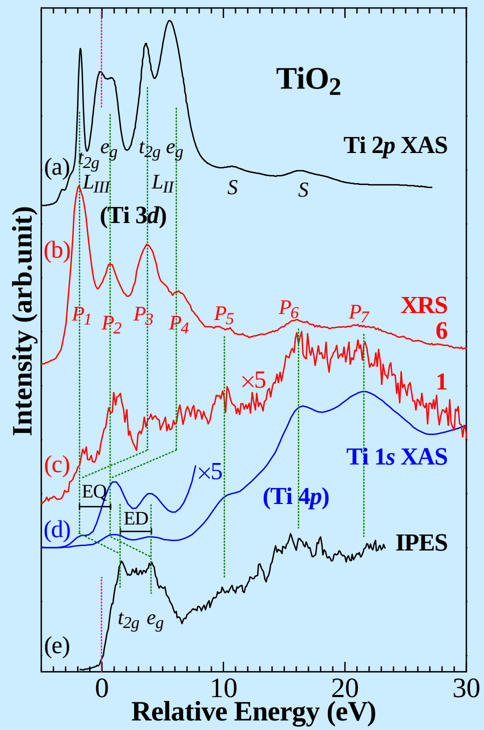
Energy of XRS peaks.



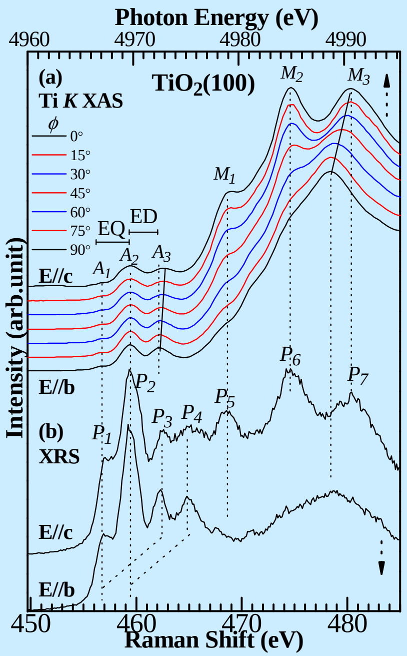
Ti *K* resonant XES.



Ti *K* resonant XRS spectra.

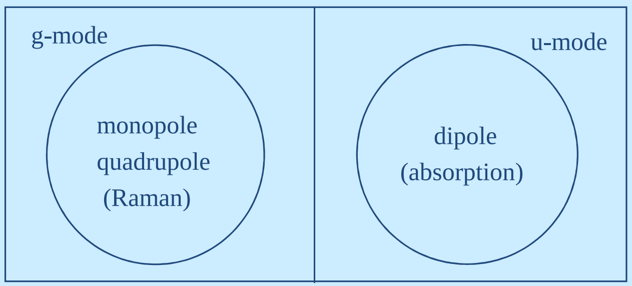


Comparison of misc. spectra.



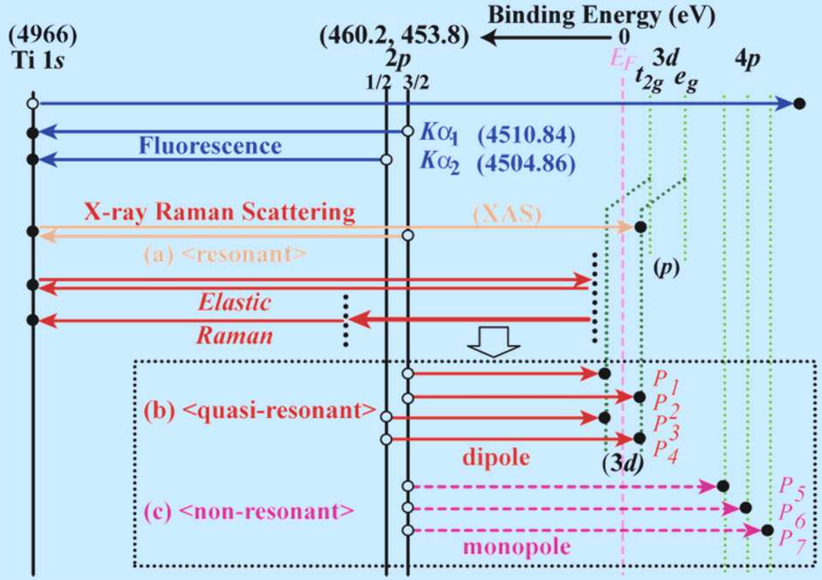
Azimuth dependence of Ti *K* XAS

Selection Rule (non-resonant) with inversion symmetry



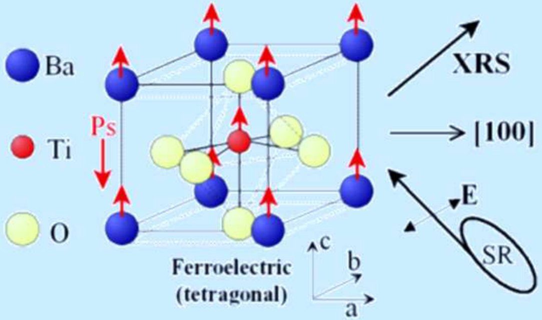
Ligand field splitting

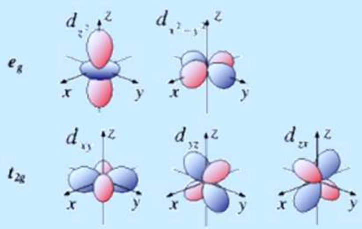
T. Uozumi, et al., Europhys. Lett. 18, 85 (1992).

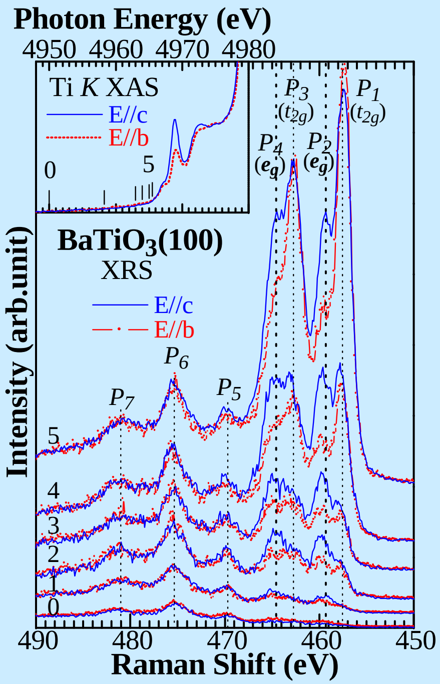


Energy diagram of X-ray emission.

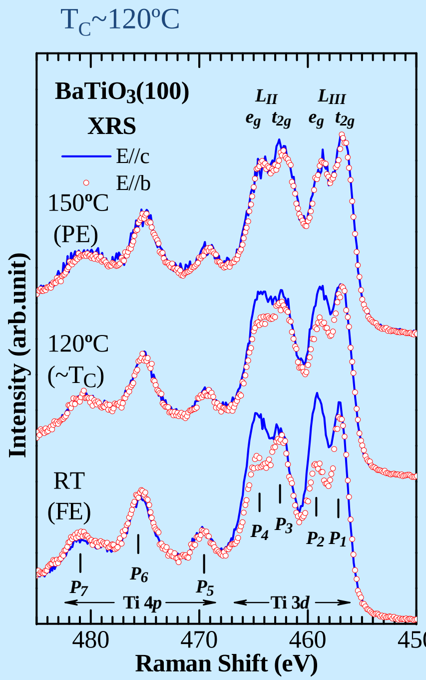
Ferroelectric $BaTiO_3$ (BTO) / Anatase (TiO_2)



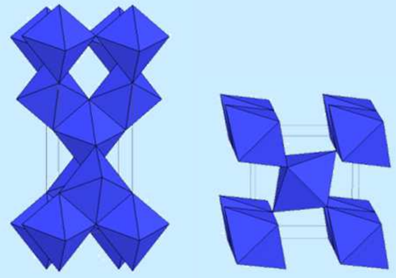




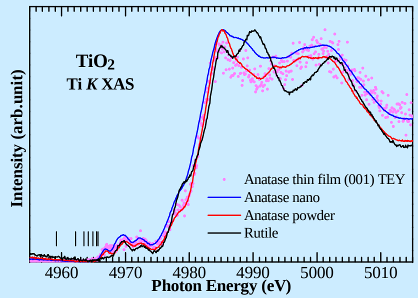
Ferroelectric Phase (RT)
Azimuth-dependence



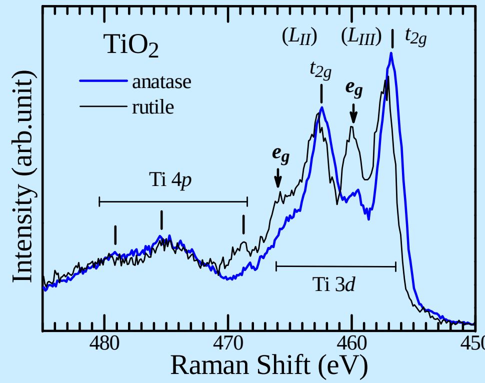
Ferroelectric Phase Transition



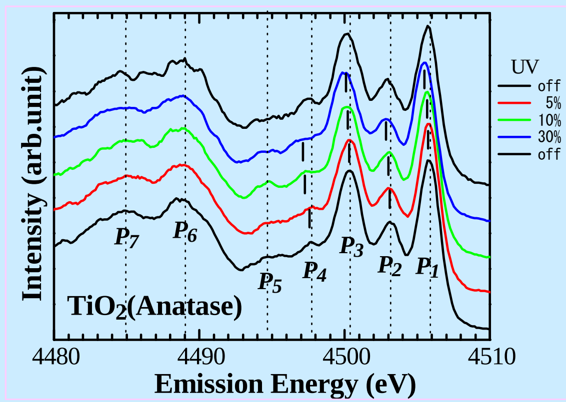
Anatase Rutile



Ti K XAFS

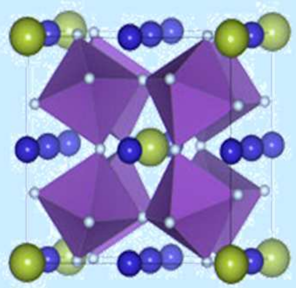


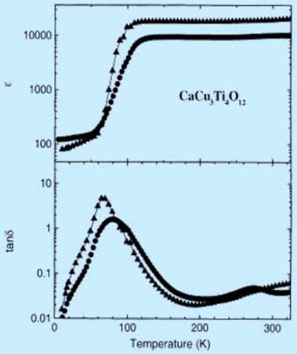
Ti K XRS spectra



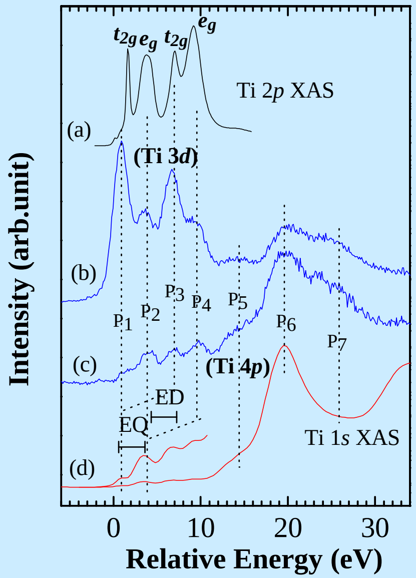
UV-irradiation effect

$CaCu_3Ti_4O_{12}$ (CCTO) / CuO

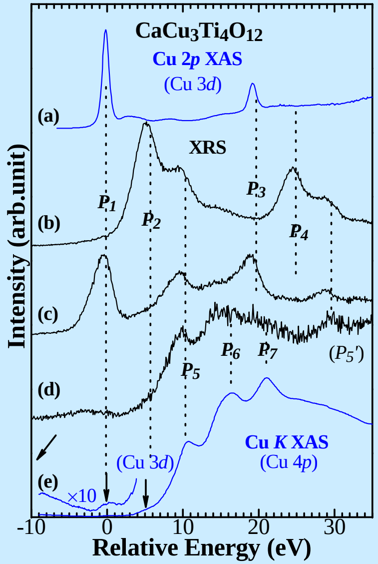




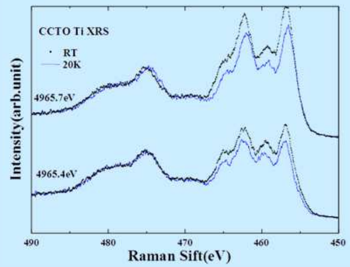
A.P. Ramirez, et al.,
Solid State Commun.,**115**, 217 (2000).



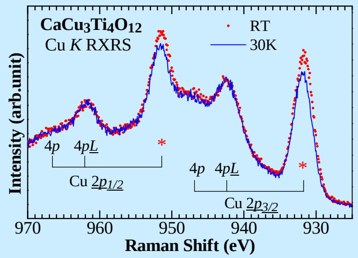
Comparison of misc. spectra.
Ti *K* resonance



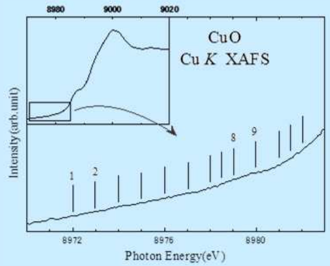
Comparison of misc. spectra.
Cu *K* resonance



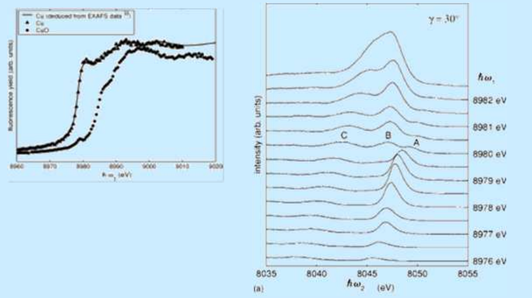
Temperature dependence of XRS
Ti *K* resonance



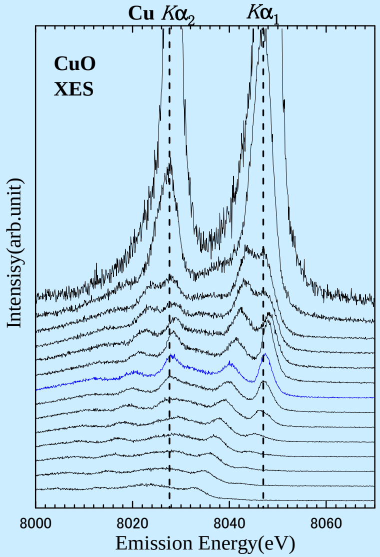
Temperature dependence of XRS
Cu *K* resonance



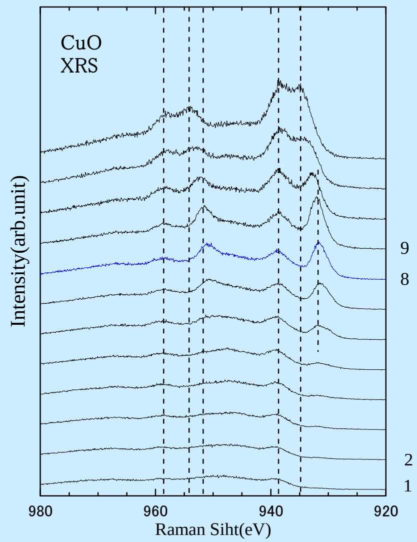
Cu *K* XAFS



G. Döring, et al., Phys. Rev. B**70**, 085115 (2004).



Cu *K* resonant XES.



Cu *K* resonant XRS spectra.

Summary

Other results

- Ti_2O_3
  - Much lifetime broadening

- Anatase TiO_2
  - Photocatalyst
  - More 3*d* electrons than rutile
  - Peak shift by UV-radiation

- Nano-particle Anatase TiO_2
  - Size dependence
    - Much 3*d*-electrons at large (loose → fasten)
  - Dope effect
    - Electron is doped in t_{2g} state

- Steel (Fe)
  - Electronic state change by heat and pressure.

Feature Plans of XRS / XES

X-ray Raman Scattering

- Photon-in/photon-out
  - Bulk sensitive
  - Unnecessary conductivity → Insulator
  - Stable in changed environment → Excited state
  - Time dependence
- Coherent Process
  - Selection rule ~ strict
  - Nonlinear Process
- Joint DOS (Elementary Excitation)
  - Core-excitation → Partial DOS of unoccupied state
  - Mapping (Elements, Excitations)
  - k-dependence

Need High Brilliance !!

X-ray Emission Spectroscopy

- Partial DOS of occupied state