Optical Properties of $Nd_{1-x}TiO_3$

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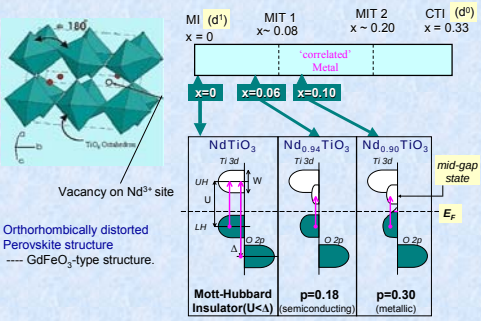
Abstract

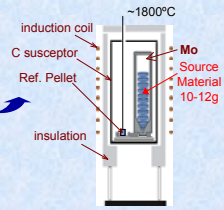
Temperature dependent optical spectra have been investigated in a well-characterized titanate system, $Nd_{1-x}TiO_3$, between 50 and 40 000 cm^{-1} at three different doping levels, x=0.0, 0.06, and 0.10, which are Mott-Hubbard insulator, semiconductor and correlated metal, respectively. Mid-gap states develop inside the Hubbard gap with hole doping. Based on the room temperature spectra of optical conductivity, the evolution rate of the inner-gap excitations below 1.2 eV with doping is related to the electron correlation strength of the parent insulator, which was observed in other titanates as well. In the metallic sample (x=0.10), an anomalous enhancement of spectral weight below 1eV grows with decreasing temperature. Meanwhile, the metallic sample displays a Fermi-liquid behavior.

Structure and Metal-Insulator Transitions of $Nd_{1-x}TiO_3$ system



Sample preparation of single crystals

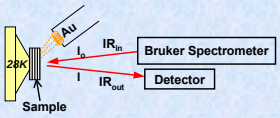
- Parent compound - $NdTiO_3$:
  Floating-zone method
- Doped $Nd_{1-x}TiO_3$:
  Modified-Bridgeman Method
- Doping characterization :
  Neutron activation analysis (NAA)



Modified-Bridgeman method

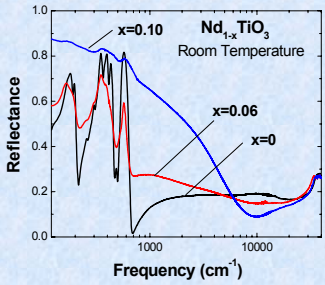
Measurement techniques --- Reflectance

- **Spectrometer**: Bruker IFT 66v/S –*FTIR*
- **Automated** temperature dependent measurement
  (^{4}He cryostat: Room Temperature → 28K)
- ***In-situ* Gold evaporation** on the sample as reference
  -- correction for geometrical effects of an irregular surface.
  (The absolute accuracy of the reflectance is <0.5%)

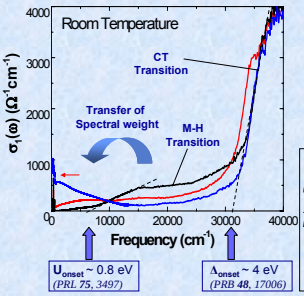


Sketch of experimental instruments

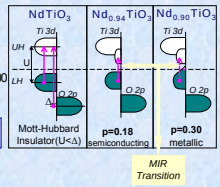
Room temperature Reflectance of Different hole dopings



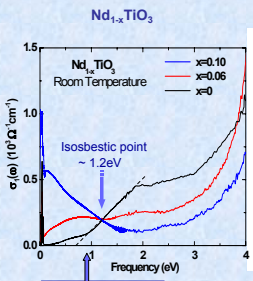
Transfer of Spectral weight with hole doping

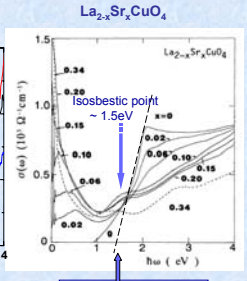


- Similar behavior has been found in the $R_{1-x}Ca_xTiO_3$ system. *(T.Katsufuji et al, PRL 75, 3497)*
- A transfer of spectral weight--a general feature of strongly correlated systems. *(PRL 67, 1035).*

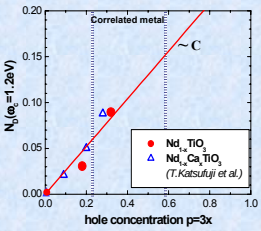


❖ Compared with Cuprates





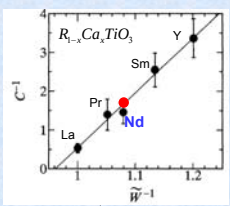
The transfer rate of effective electron numbers with hole concentration



$$N_D(\omega_c) = N_{eff}(\omega_c)_\delta - N_{eff}(\omega_c)_{\delta=0}$$

$$N_{eff}(\omega_c) = \frac{2 m_0 V}{\pi e^2}\int_0^{\omega_c} \sigma(\omega) d\omega$$

T.Katsufuji et al. (PRL 75,3497):

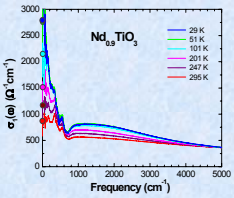


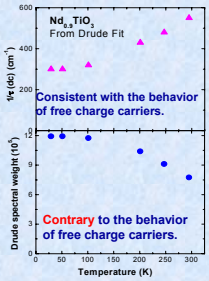
$$C = N_D/(N_{D0}p)$$

$$\tilde{W}^{-1} = W_{Le}/W_R \sim U/W_R$$

Strength of electron correlation of respective parent insulators.

Temperature dependent Optical conductivity of paramagnetic metallic $Nd_{0.9}TiO_3$





Anomalous enhancement of spectral weight with decreasing temperature below 1eV.

❖ How can we explain the anomalous enhancement of the spectral weight as temperature is decreased?

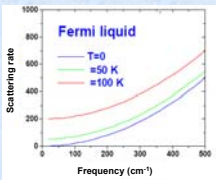
Possible solution:

Dynamics mean field theory of the Hubbard model, predicts an anomalous enhancement of spectral weight as a function of temperature in the correlated metallic phase of V_2O_3.
M.J.Rozenberg et al., PRL 75, 105 (1995)

Fermi Liquid behavior of $Nd_{0.9}TiO_3$

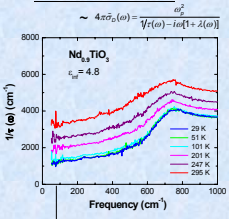
Fermi Liquid Theory: $\hbar/\tau = \hbar/\tau_0 + \alpha(k_B T)^2 + \beta(\hbar\omega)^2$, and $\alpha/\beta = \pi^2 \sim 10$

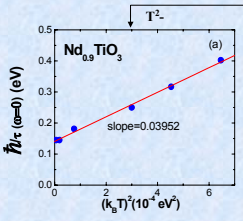
Theoretical Plot

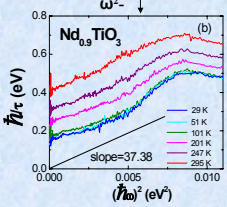


Extended Drude Model

$$\sim 4\pi\tilde{\sigma}_D(\omega) = \frac{\omega_p^2}{\sqrt{\varepsilon_\infty}[\tau(\omega) - i\omega(1+\lambda(\omega))]}$$







For $Nd_{0.9}TiO_3$, T< 300K and ω< 800 cm^{-1}~ 0.1 eV,

α=395.2 eV^{-1}, β=37.38 eV^{-1}. → $\alpha/\beta = 10.6$

Summary

- Metal-insulator transitions in $Nd_{1-x}TiO_3$ system by optical measurements.
- Mid-gap states develop with hole doping. The rate of the evolution of the inner-gap excitations is dependent on the strength of electron correlation of the parent insulator.
- Optical conductivity anomalies and Fermi liquid behavior in the correlated metallic sample.