doi:10.1017/S1431927610058885
Microsc. Microanal. 16 (Suppl 2), 2010

Electron-loss near-edge structure (ELNES) of $BaTiO_3$

V. Gallegos-Orozco[*], E. García-Sánchez[*], J.M Cervantes-V. [*], P. de Lira-Gómez[*], F. Espinosa-Magaña[**] , A. Santos-Beltrán[*]

[*]Unidad académica de Ingeniería I. Universidad Autónoma de Zacatecas, Av. López Velarde 801, C. P. 98000. Zacatecas, Zac. México.
[**]Centro de Investigación en Materiales Avanzados (CIMAV), Miguel de Cervantes No.120, C.P. 31109, Chihuahua, Chih., México.

Electron energy loss near edge structure (ELNES) commonly provides valuable information about electronic and atomic structure around an objective atom. The effect of changing the chemical environments in most of cases can clearly be detected by EELS. However, the energy resolution around 1.5 eV not sufficient to distinguish between structural modifications in the phase transition. An improvement of energy resolution can be achieved at expense of the sharply reduced beam intensity, but this leads to poor statistics en the collection of ELNES. A good theoretical tool is essential to utilize ELNES.

In this work were studied of Ti $L_{2,3}$ and O K edges of $BaTiO_3$. Electron energy loss spectra were obtained using a Gatan Parallel Electron Energy Loss Spectrometer (PEELS model 766). Spectra were acquired in diffraction mode with 0.1 eV/ch dispersion, an aperture of 3 mm and a collection semi-angle of about 2.7 mrad. The resolution of the spectra was determined by measuring the full width at half-maximum (FWHM) of the zero loss peak and this was typically close to 1.5 eV, when the TEM was operated at 200 kV. Also we performed within the generalized gradient approximation to density functional theory, using the FLAPW method. The *ab initio band-structure* calculations made with the Wien2k and TELNES packages.

ELNES Calculations different were perform for the Ti $L_{2,3}$ and O K edges as show in the Figures 1 and 2 respectively. The results obtained of the Figure 1 (d) shown the unit cell, (c) supercell without hole show a spectra where reveal an only big peak simulations $L_{3,}$ (b) in the supercell with hole we can observe L_3 and L_2 this reveals the important of the electronic excitation simulation from Inner-shell and in (a) show the experimental Ti $L_{2,3}$ edge. Results of calculations for O K (Figure 2) with (d) unit cell (c) super cell without core-hole effect (b) consideration of the core-hole effect. The experimental spectrum is plotted in (a).

It is found that the spectral features change by the introduction of the core-hole. A large supercell and introduction of core-hole are key for the accurate reproduction of the ELNES spectra through first principles calculations.

It has been shown that it is possible to us ab initio band-structure calculations to provide good simulations of the ELNES of Ti and O K. Although the interpretation of EELS can be more complicated, we have shown here that the aid of band-structure calculations that it is possible to interpret.

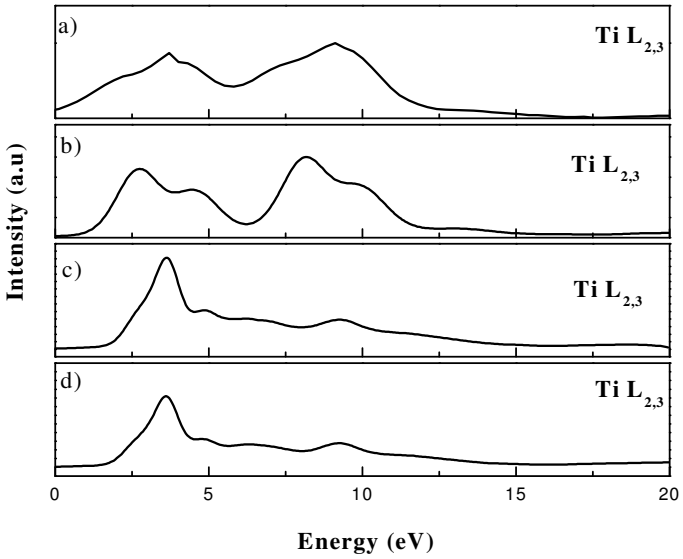

Figure 1. Results of calculations for Ti $L_{2,3}$ with (d) unit cell (c) super cell without core-hole effect (b) consideration of the core core-hole effect. The experimental spectrum is plotted in (a)

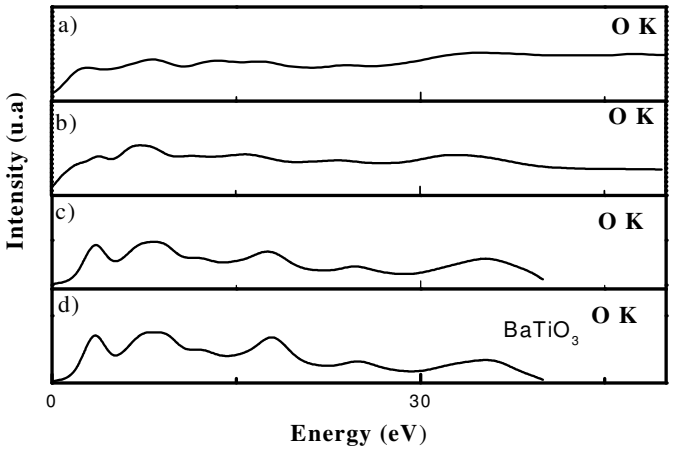

Figure 2 Results of calculations for O K with (d) unit cell (c) super cell without core-hole effect (b) consideration of the core-hole effect. The experimental spectrum is plotted in (a)

https://doi.org/10.1017/S1431927610058885 Published online by Cambridge University Press