XIX SBQT
Simpósio Brasileiro de Química Teórica 2017
12 a 17/Nov, 2017, Águas de Lindóia/SP, Brasil

A structural study of Ni/NiO interface materials by Rietveld Refinement and DFT calculations

Authors: Ericson H. N. S. Thaines[1],Carlos S. Ferreira[2],Raimundo R. Passos[2], Leandro A. Pocrifka[2], Renato G. Freitas[1]

Address: [1]LCM, DepartmentofChemistry, Federal Universityof Mato Grosso, 78060-900 Cuiabá, MT, Brazil.
[2]GEMATA - LEEN, Department of Chemistry, Federal University of Amazonas - UFAM - CEP 69077-000, Manaus-AM, Brazil
[3]Program of Natural Sciences, Federal University of Pará West - UFOPA - CEP 68035-110, Santarém-PA, Brazil

Abstract: Electrochemical capacitors (ECs) are devices that combine both the specific energy of the batteries and the specific power of the conventional capacitors characteristics [1]. This feature allows electrochemical capacitors to be present in the industries of renewable energy, digital cameras, mobile phones and electric vehicles [2]. The mixedtransition-metaloxides are emerging as promisingelectrodematerials for ECs, due their high electrochemical activities owing to the complex chemical compositions and their synergetic effects contribute to the exceptionally high specific capacity/capacitance [3].

The interface materials were obtained by calcination of a polymeric resin prepared by Pechini method. The X-ray diffraction (XRD) patterns were obtained using a SHIMATZU XRD-6000 model which provides Cu K_α radiation (λ=1.544Å). To obtain the microstructural data of the Ni, NiO and Ni/NiO materials, a Rietveld refinement (see figure 1) [4] was performed using the General Structure Analysis System (GSAS) program [5] suite with the EXPGUI interface [6].

All theoretical calculations were performed using the Ni and NiO crystallographic information file (CIF – ICSD 260169 and 9866, respectively). Calculations were performed using density function theory (DFT) [7,8] with the plane wave-pseudopotential framework, as implemented in the Quantum-ESPRESSO (QE) [9] package, with in the generalized gradient approximation (GGA). Electronic interactions were described by Perdew-Burke-Ernzerhof (PBE) exchange-correlation functional [10] with ultrasoft pseudopotential. We performed the electronic energy minimization with a tolerance of 10^{-6}Ry estimated scf accuracy, using a plane wave kinetic energy cutoff of 175 Ry and 700 for the charge densities. The Brillouin-zone (BZ) sampling is carried out with a 8 x 8 x 8Monkhorst - Pack k-points grid.The strain effects were calculated applying a strain compressive and tensile, consequently varying the volume of unit cell. The equilibrium volume parameters and bulk modulus were obtained by fitting energy vs volume curve to the Murnaghan, Birch-Murnaghan, Poirier-Tarantola and Vinet equation of state – EOS (see figure 2). The stress tensor

were obtained after full relaxations of allinternal atomic coordinates by means of the conjugate gradient (CG) technique.

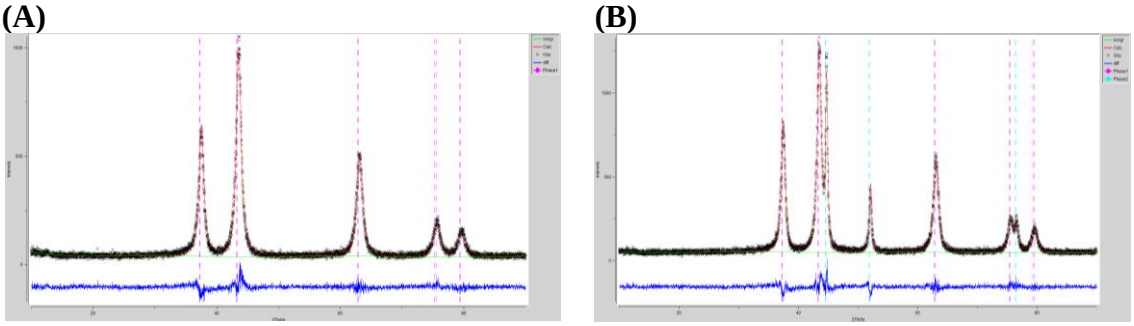

Figure 1 – Adjust by Rietveld method between the experimental and calculated X-ray diffraction patterns for the (A) NiOand (B) NiO/Ni.

The Fig.1 show that the results obtained by the Rietveld refinement method were in good agrément with the observed XRD patterns. The Fig. 2 show relation between energy versus volume curve with fitting of EOS. The value of the bulk modulus obtained from of EOS were in good agrément with the eq. Murnaghan for Ni of 253.52 GPa with experimental value of 229 GPa and for NiO of 278.77 GPa with experimental value of 205 GPa.

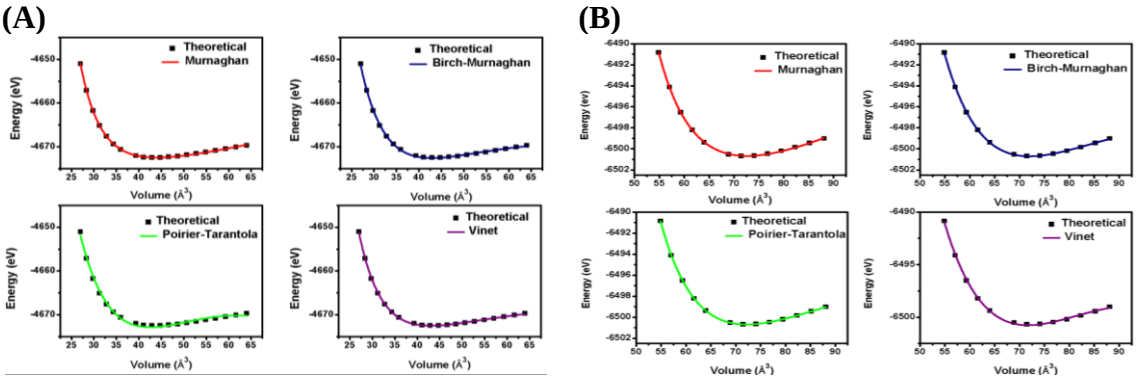

Figure 2- The energy as a functionofthe volume withfittingof EOS for the (A) Niand (B) NiO

Key-words: Ni/NiO interface, Rietveld refinement, DFT.
Support: This work has been supported FAPEMAT (214599/2015)for financial support and CENAPAD/SP for providing computational time.

References:

[1] S. K. Chang et al, Curr. Appl. Phys., 2012, 12, 1421-1428.
[2] B. E.Conway Electrochemical Supercapacitors. Kluwer-Plenum Pub. Co, 1 Ed. New York, 1999
[3] C. Yuan et al, Angew.Chem.Int.Ed.2014,53,1488–1504.
[4] H.M. Rietveld, J. Appl. Crystallogr., 1969, 2,65.
[5] A.C. Larson, R.B. von Dreele, Lab. Rep. LAUR., 2004, 86, 1.
[6] B.H. Toby, J. Appl. Crystallogr., 2001 34, 210.
[7] P. Hohenbergand W. Kohn, Phys. Rev., 1964, 136, B864–B871.
[8] W.KohnandL.J.Sham, Phys. Rev., 1965,140,A1133–A1138.
[9] G. Paolo et al,J. Phys.:Condens. Matter, 2009, 21, 395-502.
[10] J. P. Perdew, K. Burke and M. Ernzerhof, Phys. Rev. Lett., 1996, 77, 3865.