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Pure $Ni_{0.5}TiOPO_4$ was prepared via a traditional solid–state reaction, and then $Ni_{0.5}TiOPO_4$/C composites with core–shell structure were synthesized by hydrothermally treating $Ni_{0.5}TiOPO_4$ in glucose solution. X–ray diffraction patterns confirmed that $Ni_{0.5}TiOPO_4$/C crystallized in the monoclinic $P2_1/c$ space group. The morphology and the microstructure were characterized by scanning electron microscopy and transmission electron microscopy. The small particles with irregular shapes were coated with uniform carbon film of ~ 3 nm in thickness. Raman spectroscopy also confirmed the presence of carbon in $Ni_{0.5}TiOPO_4$/C composites. The electrochemical performances of $Ni_{0.5}TiOPO_4$/C and $Ni_{0.5}TiOPO_4$ were compared through galvanostatic charge/discharge tests, cyclic voltammetry and electrochemical impedance spectroscopy. $Ni_{0.5}TiOPO_4$/C composites exhibited improved electrochemical performances due to the existence of carbon shell. During the first discharge, the NTP/C electrode delivered a capacity of 530mAh/g Fig 1. This high capacity corresponds the intercalation of more than 3 mol lithium ions per $Ni_{0.5}TiOPO_4$; however, not all lithium atoms could be extracted during the subsequent charge [1]. The redox couples of Ti^{4+}/Ti^{3+}, Ti^{3+}/Ti^{2+} and Ni^{2+}/Ni in NTP/C can involve the insertion of only 3 mol lithium atoms. Therefore, the excess capacity during the first discharge should attribute to the formation of SEI passivation layer

[1] R. Essehli, B.E. Bali, H. Ehrenberg, I. Svoboda, N. Bramnik, H. Fuess, Mater. Res. Bull. 44 (2009) 817.

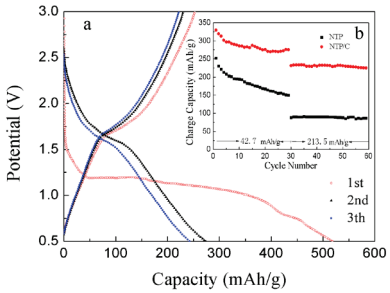

Fig. 1. The initial three galvanostatic charge/discharge curves of NTP (a) and the cycle performances of NTP and NTP/C measured at C/10 (42.7 mAh/g) and C/2 (213.5mAh/g) in the potential range of 0.5 to 3.0 V (b).

Keywords: $Ni_{0.5}TiOPO_4$/C, lithium–ion batteries, core–shell, anode materials

FA2-MS16-P25

X-ray diffraction study of σ-phase formation in super duplex stainless steel. Jorge Garin[a], Rodolfo Mannheim[a], Manuel Camus[b]. [a]*Metallurgical Engineering, Universidad de Santiago de Chile,Chile.* [b]*Mechanical Engineering, Universidad de Antofagasta, Chile.*
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Super duplex stainless steels (SDSS) are two-phase alloys based on the iron-chromium system, with minor contents of molybdenum, nitrogen, tungsten and copper. Their remarkable mechanical and chemical properties make them suitable for widespread industrial applications. The microstructure of these alloys is composed of approximately equal proportions of BCC ferrite and FCC austenite phases. However, exposure to elevated temperature processes causes embritlement and loss of mechanical properties due to precipitation of intermediate phases, principally sigma-phase, in the microstructure. This phase is a complex intermetallic compound of Fe and Cr, based upon an ideal stoichiometric composition AX_2, Pearson's code tP30 and space group $P4_2/mnm$, [1]. The formation of sigma-phase in cast ASTM A890 steel was investigated by means of quantitative X-ray diffraction. Three different temperatures (1023 K, 1073 K and 1123 K) and various annealing times (1 to 96 hours) were utilized in the experimental procedure. Owing to the usually complex powder diffraction pattern of the sigma compound, Rietveld refinements were performed based upon typical measurement and global parameters. The results obtained of the present study have assessed the application of the Rietveld method to quantify the formation of sigma-phase in SDSS subjected to annealing at relatively high temperatures. The refinement yielded the lowest R-values and much better represented the relative amount of phases in the samples. From the metallurgical standpoint, the results of XRD followed by Rietveld analysis indicated that the larger the annealing time of the alloy at a given temperature, the larger will be the volume fraction of the precipitated particles of sigma. Furthermore, sigma particles nucleates and grow reaching saturation levels depending on the specific type of the alloy.

[1] Yakel, H.L., *Acta Crystallogr,* 1983, B39, 20.

Keywords: σ-phase, X-ray diffraction, duplex steels

FA2-MS16-P26

Microstructure of coke deposited by a high temperature process. Sven Gerhardt[a], Reiner Staudt[b], Klaus Bente[a], Jörg Hofmann[b]. [a]*Institut für Mineralogie, Kristallographie und Materialwissenschaft, University of Leipzig.* [b]*Institut für Nichtklassische Chemie, University of Leipzig.*
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It is well known that metal dusting is an undesirable corrosion phenomenon that can be observed in a wide range of chemically and petrochemically working industries. Due to strongly carburizing atmospheres, it leads to a decomposition of materials into metal particles and carbon. The aim of this work is to clarify open questions by identifying and modeling fundamental correlations between vapour-solid reactions and their consequences for microstructure, surface morphology and catalytic behaviour of the metal. The high temperature grown coke coating and metal pipe were inspected by 3D X-ray tomography (volume properties), XRD (existing phases), XPS (chemical bonding), HRTEM (nanostructures), SEM (surface morphology), electron microprobe analysis and TEM-EDX (chemical composition).

Keywords: transmission electron microscopy, X-Ray tomography, coke

FA2-MS16-P27

Mullite-type $(Bi_{1-x}Sr_x)_2Al_4O_{9-x/2}$: HT-XRPD, TEM and XPS investigations. Thorsten M. Gesing[a], Marco Schowalter[b], Claudia Weidenthaler[c], Andreas