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Abstract

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Electrochemical properties of composite films of some metal oxides and carboxylic acid-doped polyanilines

Hošić E., Šehovac S., Jukić M., Gutić S., Korać F.

Univerzitet u Sarajevu, Prirodno-matematički fakultet, Zmaja od Bosne 33-35, 71000 Sarajevo, Bosna i Hercegovina

Keywords:
Composite films
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Corresponding author:
Hošić Enida

E-mail:
enniiidddda@hotmail.co.uk

Abstract: The electrochemical synthesis of composite films of some metal oxides and carboxylic acid-doped polyanilines was done on carbon electrode. The obtained composite film was electrochemically characterized by cyclic voltammetry and impedance spectroscopy at different pH values. After characterization, electrochemical properties of composite films was compared with electrochemical properties of corresponding copolymer in order to study changes in capacitive behaviour.

Sažetak

Sinteza kompozitnog filma odabranih metalnih oksida i karboksilnom grupom dopiranih polianilina vršena je elektrohemijskim putem na grafitnoj elektrodi. Nastali kompozitni film elektrohemijski je okarakterisan metodama ciklične voltametrije i impedancijske spektroskopije pri različitim pH vrijednostima. Nakon karakterizacije je izvršeno poređenje elektrohemijskih svojstava nastalog kompozita sa odgovarajućim kopolimerom, s ciljem ispitivanja promjena u kapacitivnom ponašanju.

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Abstract

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Kinetics of the Conversion of $SrSO_4$ (celestite ore) to $SrCO_3$ in Solutions Containing Low CO_3^{2-} Ion Concentrations

Zoraga M., Kahruman C., Yusufoglu I.

Istanbul University, Engineering Faculty, Department of Metallurgical and Materials Engineering, 34320 Avcilar, Istanbul, Turkey

Keywords:
Celestite,
strontium carbonate,
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Corresponding author:
Ibrahim YUSUFOGLU

E-mail:
yusufogl@istanbul.edu.tr

Tel: +902124737070/17638
Fax: +902124737180

Abstract: Celestite ore which includes $SrSO_4$ as a main compound is the most important raw material used for the production of Sr compounds. In this study, concentrated celestite mineral was converted to $SrCO_3$ using solutions obtained by hydrolyzing mixture of 1:1 mole ratio of ammonium carbamate and ammonium bicarbonate (Merck) in a mechanically stirred reactor under isothermal conditions and constant stirring speed. Reactant solutions were prepared by dissolving 0.1, 0.15, 0.2, 0.3 and 0.4 moles of the mixture in 1 L distilled water. CO_3^{2-}, HCO_3^- and NH_4^+ ions and molecularly dissolved NH_3 are in equilibrium and the sum of the mole amounts of CO_3^{2-} and NH_3 was equal to the mole amount of dissolved mixture. The effects of stirring speed (300, 400 and 500 rpm), CO_3^{2-} ion concentration and temperature (293, 303, 313 and 323 K) on the conversion rate of $SrSO_4$ were investigated. The quantitative analyses of SO_4^{2-} ions in the solutions taken during certain time intervals were performed by ICP-OES. XRD was used for characterization of solid reactant and products. The effect of stirring speed on the reaction rate was negligible at 500 rpm. Concentration of CO_3^{2-} ions in the solutions has no effect on the reaction rate (zero order reaction). It is determined that reaction rate was increased by increasing temperature.

Sažetak

Celestitna ruda koja se sastoji od $SrSO_4$ kao glavne komponente, je najvažniji sirovi material korišten za proizvodnju Sr jedinjenja. U ovom radu, koncentrirana ruda celestita je prevedena do $SrCO_3$ preko rastvora dobivenih hidrolizom smjese koja se sastojala od amonij karbamata I amonij bikarbonata (Merck) u omjeru 1:1 u reaktoru sa mehaničkom mješalicom pod izotermalnim i uslovima mješanja konstantnom brzinom. Rastvori reaktanata su pripremljeni rastvaranjem 0,1; 0,15; 0,2; 0,3; i 0,4 mola smjese u 1 l destilirane vode. CO_3^{2-}, HCO_3^- i NH_4^+ ioni I and molekularno rastvoren NH_3 su bili u ekvilibrijumu, suma količinskih molova CO_3^{2-} i NH_3 je bila jednaka sumi molova rastvorene smjese. Uticaj miješanja (300, 400 and 500 rpm), CO_3^{2-} ionske koncentracije I temperature (293, 303, 313 and 323 K) na stepen konverzije $SrSO_4$ je ispitivan. Kvantitativna analiza SO_4^{2-} iona u rastvoru urađena u određenim vremenskim intervalima je izvedena metodom ICP-OES. XDR je korišten za karakterizaciju čvrstih rekatanata I produkata. Uticaj brzine mješanja na red reakcije je bio jako mali pri 500 rpm. Koncentracija CO_3^{2-} iona u rastvoru nema uticaja na red reakcije (reakcija nultog reda). Utvršeno je da se red reakcije povećava sa povećanjem temperature.

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Abstract

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Molecular Dynamics Simulation of Graphene-Like Boron Carbide Nanosheet Under Biaxial Strain

Yusuf Nur[a], Yusuf Şimşek[b]

[a]*Department of Chemistry, Mustafa Kemal University, Antakya, Turkey*

[b]*Vocational School of Health Services, Gazi University, Ankara, Turkey*

Keywords:
Molecular dynamics,
boron carbide,
biaxial strain

Corresponding author:
E-mail: yusufsimsek@gazi.edu.tr
Tel: +905356503576

Abstract: Structural properties of graphene-like monolayer boron carbide nanosheet under biaxial strain have been investigated by performing classical molecular dynamics simulations at various temperatures. For boron carbide systems, Stillinger-Weber potential energy function parameters have been modified and published in reference study [1]. Hence, we embedded these modified parameters to our molecular dynamics program. Simulations have been performed with a written FORTRAN code that uses Velocity Verlet Algorithm for solving equations of motion with a time step 10^{-17} second. Biaxial strain application has been realized with two different strain speeds (slow and fast) at 1 K, 300 K, 600 K and 900 K. Each strain steps have been simulated up to the system reached equilibrium. To obtain a relaxed structure, we applied about half a million time steps for each model. It has been found that after a few biaxial strain applications, the nanosheet structure showed segregation like deformation at 1 K. Simulations at 300 K and 600 K showed that biaxial strain mostly created ripping like deformation after merging of emerged holes on the structure. But at 900 K, structure showed folding from the ripped regions and lost hexagonal geometries.

Sažetak

Strukturne osobine nano bor karbidnog monosloja sličnog grafitu pod biaksijalnim istezanjem su ispitivane klasičnim simulacijama molekularnom dinamikom pod različitim temperaturama, Za sistem bor karbida, funkcije parametara potencijalne energije Stillinger-Webera su modificirani I objavljene u posebnoj studiji [1]. Mi smo ugradili ove modificirane parametre u naš program molekularne dinamike. Simultacije su urađene sa pisanim FORTRAN kodom koji koristi Velocity Verlet Algoritam za rješavanje jednačina kretanja u vremenskom koraku od 10^{-17} sekundi. Aplikacija biaksijalnog istezanja je realizirana sa dvije različite brzine istezanja (brza I spora aplikacija) na 1, 300, 600 I 900 K. Svako istezanje je simulirano do uspostavljanja stanja ravnoteže. Da bi dobili opuštenu strukturu, primjenili smo pola miliona koraka za svaki model. Utvrđeno je da nakon aplikacije istezanja, nanostruktura pokazuje segregaciju u obliku deformacije na 1 K. Simulacije na 300 K I 600 K pokazuju da biaksijalno istezanje dovodi do pucanja nanostruktura I do gubitka heksagonalnih geometrija.