

# GLOBAL CONFERENCE ON MATERIAL SCIENCES

13 - 15 November 2014

Mirage Park Resort & Hotel Convention Center  
Antalya, Kemer, Turkey

ABSTRACTS BOOK





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## **ABSTRACTS BOOK**

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# ABSTRACTS

## Synthesis of hydrocerussite hexagonal disk and its applications in battery anode

**Hengrui Zhou**, Department of Civil Engineering, The University of Hong Kong, Pokfulam Road, Hong Kong, Hong Kong SAR, China

**Kaimin Shih**, Department of Civil Engineering, The University of Hong Kong, Pokfulam Road, Hong Kong, Hong Kong SAR, China

### Abstract

A rapid, low temperature and additive-free hydrothermal process was firstly developed to synthesize hydrocerussite ( $\text{Pb}_3(\text{CO}_3)_2(\text{OH})_2$ ) hexagonal disk. The products were characterized by XRD, SEM and TEM. Single-phase  $\text{Pb}_3(\text{CO}_3)_2(\text{OH})_2$  hexagonal disk was obtained at 180 °C hydrothermal temperature with around 4  $\mu\text{m}$  in diameter. The precursor suspension pH was critical for the product particles composition and morphologies. The crystal growth direction in hexagonal disk was indexed as (102) plane from HRTEM, and the growth mechanism for hexagonal disk was proposed. Hydrocerussite ring, as a new member in hydrocerussite family, was also successfully prepared by controlling the pH value at 10. The obtained hydrocerussite product was applied for the lab-scale lead-acid battery anode and discharged a high capacity of 144  $\text{mAh}\cdot\text{g}^{-1}$  at constant current 50  $\text{mA}\cdot\text{g}^{-1}$ , which suggests that  $\text{Pb}_3(\text{CO}_3)_2(\text{OH})_2$  can be applied for energy storage devices.

Key words: hydrocerussite, hydrothermal, hexagonal disk, ring, lead-acid battery.

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\* ADDRESS FOR CORRESPONDENCE: **Hengrui Zhou**, Department of Civil Engineering, The University of Hong Kong, Pokfulam Road, Hong Kong, Hong Kong SAR, China. E-mail address: [kshih@hku.hk](mailto:kshih@hku.hk)

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## Optimization of CNC Turning for Aluminum alloy using Simulated Annealing Method

**Dr. Shukry H. Aghdeab**, Dep. of Production Engineering & Metallurgy, University of Technology, Baghdad, Iraq

**Dr. Laith A. Mohammed**, Dep. of Production Engineering & Metallurgy, University of Technology, Baghdad, Iraq

**Alaa M. Ubaid**, College of Engineering, University of Sharjah, UAE

### Abstract

Surface roughness is a main parameter in computer numerical control (CNC) turning technology. The aim of this paper is to obtain an optimal parameters of turning process (cutting speed, spindle speed, feed rate and depth of cut) which results in an optimal of surface roughness for machining aluminum alloy ENAC43400 shaft (46×150mm).

The developed objective model is modeled using regression method then optimized by simulated annealing method in order to determine the best set of turning parameter values. This work conclude that simulated annealing method can be used for high precision modeling and estimation of turning parameters.

Key words: CNC turning, regression analysis, optimization, simulated annealing method.

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\* ADDRESS FOR CORRESPONDENCE: **Dr. Shukry H. Aghdeab**, Dep. of Production Engineering & Metallurgy, University of Technology, Baghdad, Iraq. E-mail address: [shukry\\_hammed@yahoo.com](mailto:shukry_hammed@yahoo.com)

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# Effects of High Potential Cathodic Protection on Fusion Bond Epoxy Coated Steel

**Fawzi ElHamshri**, Chemical Engineering Department, Faculty of Engineering, Al-Margeb University, Garabolli, Libya,

**Hamza A. Khalfalla**, Chemical Engineering Department, Faculty of Engineering, Al-Margeb University, Garabolli, Libya,

**Mohamed M. Aboabboud**, Chemical Engineering Department, Faculty of Engineering, Al-Margeb University, Garabolli, Libya,

## Abstract

This paper describes experimental work investigating the effects of cathodic protection (CP) potentials on the disbondment of fusion bonded epoxy (FBE) coated steel samples. The objective of the work was to study the performance of FBE coated specimens with good and poor surface preparation and exposed to various applied CP potentials at 25 °C and 60 °C in aerated 3.5% NaCl solution.

Results of this work showed that coating surface preparation, temperature, applied potential and exposure time all play an important role in the resistance of FBE coating to cathodic disbondment. Cathodic disbondment tests showed satisfactory performance of FBE coating protected under CP conditions to a potential of -1200 mV (w.r.t. SCE) at 25 °C. Potentials more negative than -1200 mV (w.r.t. SCE) at 25 °C and more negative than -1000 mV (w.r.t. SCE) at 60 °C resulted in coating failure. Poor surface preparation also caused premature coating failure.

**Key words:** **Cathodic disbondment** - The failure of adhesion between a coating and a metallic surface that is directly attributable to the effects of cathodic protection current and is often initiated at a coating holiday.

**Holiday** - A defect in a protective coating at which bare metal is exposed.

**Polarization** - Change in the potential of an electrode as a result of current flow.

**Current demand** – Current required for cathodic protection to define the minimum potential required to suppress corrosion.

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\* ADDRESS FOR CORRESPONDENCE: **Fawzi ElHamshri**, Chemical Engineering Department, Faculty of Engineering, Al-Margeb University, Garabolli, Libya, E-mail address: [fhamshri2003@yahoo.com](mailto:fhamshri2003@yahoo.com)

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## The Dielectric Properties of (PVA-PEG-PVP-MgO) and (PVA-PEG-PVP-CoO) Biomaterials

**Ibrahim R. Agool**, College of Science, Department of Physics, Al-Mustansiriyah University, Iraq

**Majeed Ali**, College of Education of Pure Science, Department of Physics, Babylon University, Iraq

**Ahmed Hashim\***, College of Education of Pure Science, Department of Physics, Babylon University, Iraq

## Abstract

In this paper, study of dielectric properties of two types of nanocomposites are (PVA-PEG-PVP-MgO) and (PVA-PEG-PVP-CoO) in frequency range (100 Hz- 5 MHz). The (PVA-PEG-PVP-MgO) and (PVA-PEG-PVP-CoO) nanocomposites have been prepared by casting technique. The dielectric parameters (dielectric constant, dielectric loss and A.C electrical conductivity) are increasing with the increase of concentrations of magnesium oxide and cobalt oxide nanoparticles. Also, the dielectric properties change with increasing of the frequency of applied electrical field.

**Key words:** nanocomposites, dielectric properties, electrical conductivity.

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\* ADDRESS FOR CORRESPONDENCE: **Ahmed Hashim\***, College of Education of Pure Science, Department of Physics, Babylon University, Iraq. E-mail address: [ahmed\\_taay@yahoo.com](mailto:ahmed_taay@yahoo.com)

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# Structural, Electronic and Optical Properties of Sodium Nitrate $\text{NaNO}_3$ : An ab initio Study

**S. Bourahla**, Physics Department, Faculty of Science, Laboratory for Theoretical Physics and Materials Physics, Hassiba Benbouali University of Chlef, Hai Es-Salem, B.P. 151, Route de Senjas, 02000 Ech Chlef, Algeria.

**S. Kouadri Moustefai**, Department of Process Engineering, Faculty of Technology, Laboratory of Water and Environment, Hassiba Benbouali University of Chlef, Hai Es-Salem, B.P. 151, Route de Senjas, 02000 Ech Chlef, Algeria.

## Abstract

The structural, electronic and optical properties of sodium nitrate are investigated using the pseudo-potential plane wave (PP-PW) scheme in the frame of generalized gradient approximation (GGA). The geometrical parameters of the unit cell have been fully optimized and are in good agreement with the experimental data. The electronic structure shows that sodium nitrate has a band gap of 2.917 eV. The dielectric functions, reflective index, extinction coefficient, reflectivity and energy-loss spectrum are calculated. The optical properties of sodium nitrate are discussed based on the band structure calculations. The 2p states of the nitrate moiety play the major role in optical transitions as initial and final states. The absorption spectrum is localized in the ultraviolet range between 60 and 380 nm.

Key words: Ab initio, sodium nitrate, electronic structure, optical properties.

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\* ADDRESS FOR CORRESPONDENCE: **S. Bourahla**, Physics Department, Faculty of Science, Laboratory for Theoretical Physics and Materials Physics, Hassiba Benbouali University of Chlef, Hai Es-Salem, B.P. 151, Route de Senjas, 02000 Ech Chlef, Algeria. E-mail address: [bourahlasaida2001@yahoo.fr](mailto:bourahlasaida2001@yahoo.fr)

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## Development of new Ti-Mo-Fe alloys as biomaterial

**Yasser M. Abd-elrhman**, Department of Materials Science and Engineering, Egypt-Japan University of Science and Technology, New Borg El-Arab City, Alexandria 21934, Egypt

**Mohamed A. Gepreel**, Department of Materials Science and Engineering, Egypt-Japan University of Science and Technology, New Borg El-Arab City, Alexandria 21934, Egypt

**Ahmed Abd El-Moneim**, Department of Materials Science and Engineering, Egypt-Japan University of Science and Technology, New Borg El-Arab City, Alexandria 21934, Egypt

**Sengo Kobayashi**, Department of Materials Science and Engineering, Ehime University, 3 Bunkyo-cho, Matsuyama 790-8577, Japan

## Abstract

Titanium and some of its alloys are known as being the most biocompatible metallic materials due to their high strength, low modulus, and high corrosion resistance in biological media. Besides other important material features, the corrosion parameters and corrosion products are responsible for limiting the biocompatibility of metallic materials, and can produce undesirable reactions in implant-adjacent and/or more distant tissues. Electrochemical corrosion behaviors of novel beta titanium alloys, Ti-4.7Mo-4.5Fe, Ti-3Mo-0.5Fe and Ti-2Mo-0.5Fe were characterized in naturally aerated Ringer's solution at room temperature compared with currently used biomedical titanium alloy, Ti-6Al-4V. The corrosion resistance of titanium alloys were investigated through open circuit potential (OCP), potentiodynamic polarization measurements and optical microscope (OM). A high corrosion resistance was obtained for all alloys due to the stable passive film formed on their surfaces. The new present alloys are promising metallic biomaterials for the future, owing to their very low elastic modulus and good corrosion resistance capabilities.

Key words: titanium alloys, passive film, corrosion resistance, electrochemical potentiodynamic.

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\* ADDRESS FOR CORRESPONDENCE: **Yasser M. Abd-elrhman**, Department of Materials Science and Engineering, Egypt-Japan University of Science and Technology, New Borg El-Arab City, Alexandria 21934, Egypt. E-mail address: [yasser\\_hmj@yahoo.com](mailto:yasser_hmj@yahoo.com)

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# Characterization of GaN nanostructures by electron beam techniques

**Lazhar Leghrib**, Department of Material Sciences, University of Oum El-Bouaghi, Algeria

**Redha Aouati**, Department of Physics, University of Constantine1, Algeria

**Abdelkader Nouiri**, Department of Material Sciences, University of Oum El-Bouaghi, Algeria

## Abstract

Cathodoluminescence (CL) is an important technique based on the light emitted from a specimen (semiconductor) in response to electron-beam irradiation. The light emitted is the results of radiative recombination of the electron-hole pairs. In the last few years the technology of group III nitride epitaxy has shown great progress on modern materials and electronic devices as well as on high electron mobility transistors (HEMTs), Light emitting diodes (LED) and photovoltaic solar cell, etc.

The characterization of GaN nanostructures (e.g. quantum wells) by an electron beam technique (e.g. cathodoluminescence) needs a reliable simulation models because there are several phenomena associated with matter-electron beam interaction. In this paper, we present our hybrid model based on Monte Carlo and molecular dynamics methods. This model describes the electron beam interaction with the quantum wells of GaN and Al<sub>x</sub>Ga<sub>1-x</sub>N. According to results, the electron beam can modify the material properties at nano scales due to the electron beam heating, that depends on electron beam parameters (accelerating voltage, primary current and scanning duration). The influence of same material parameters also is studied.

Key words:

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\* ADDRESS FOR CORRESPONDENCE: **Lazhar Leghrib**, Department of Material Sciences, University of Oum El-Bouaghi, Algeria. E-mail address: [leghrib1982@gmail.com](mailto:leghrib1982@gmail.com)

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## Preparation of (PVA-PEG-PVP-MgO, CoO) Nanocomposites and Study their Optical Properties

**Ibrahim R. Agool**, College of Science, Department of Physics, Al- Mustansiriah University, Iraq

**Ahmed Hashim\***, College of Education of Pure Science, Department of Physics, Babylon University, Iraq

## Abstract

Nanocomposites have many applications such: optical integrated circuits, sensors, coatings, medical devices.. etc. So, this paper aims to preparation of new type (PVA-PEG-PVP- MgO, CoO) nanocomposites to production new nanocomposites use in many. applications. The nanocomposites were prepared by using casting technique. The polymers was mixed with different weight percentages are (PVA0.90-PEG0.05-PVP0.05). The nanomaterials (MgO and CoO) were added to polymers composites with concentrations are (0, 2, 4 and 6) wt.%. The results show that the absorbance (A) of nanocomposites is increased with increase of concentrations of magnesium oxide and cobalt oxide nanoparticles. The optical constants (absorption coefficient ( $\alpha$ ), extinction coefficient (k), refractive index (n), real and imaginary dielectric constants ( $\epsilon_1$  and  $\epsilon_2$ )) of nanocomposites are increasing with the increase of the weight percentages of magnesium oxide and cobalt oxide nanoparticles. The energy gap (E<sub>g</sub>) of (PVA-PEG-PVP) decreases with the increase of the weight percentages of magnesium oxide and cobalt oxide nanoparticles.

Key words: Nanocomposites, Optical Properties, Magnesium Oxide, Cobalt Oxide.

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\* ADDRESS FOR CORRESPONDENCE: **Ahmed Hashim\***, College of Education of Pure Science, Department of Physics, Babylon University, Iraq. E-mail address: [ahmed taay@yahoo.com](mailto:ahmed_taay@yahoo.com)

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# SURFACE FILM PROPERTIES AND THEIR ROLE IN THE STRESS CORROSION CRACKING OF STEELS

**Giuma A. Sasi\***, Chemical Engineering Department, Faculty of Engineering, El-Merghap University, Al-Khoms, Libya

## Abstract

Electrochemical techniques and scanning electron microscopy (SEM) were used to grow films on steel and study some of their properties. Polarization curve measurements were performed on Cr-Mo alloy steel specimens in carbonate/bicarbonate solutions at 25 C° 75 C°. It was found that stress corrosion cracking was most likely to occur between -660 and -750 mV (SCE). The films grown at -700, -725 and -750 mV (SCE) were completely passive, but the film grown at -800 mV was not. The films formed at 75 C° at different potentials had different morphologies according to the SEM analysis of air-dried samples.

Key words:

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\* ADDRESS FOR CORRESPONDENCE: **Giuma A. Sasi**, Chemical Engineering Department, Faculty of Engineering, El-Merghap University, Al-Khoms, Libya. E-mail address: [giumasasi@yahoo.com](mailto:giumasasi@yahoo.com)

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## A Nonlinear Material Model for Fibrous Composite Materials and Its Effect on In-Plane Lamina Stresses

**Ghazi A. F. R. Abu-Farsakh**, Professor at Civil Engineering Department, Jordan University of Science and Technology, Jordan

## Abstract

The composite material using a macro-scale approach is dealt with as a homogeneous continuum using averaged apparent properties. The corresponding mechanical properties of an orthotropic composite lamina are specified as:  $E_1$ ,  $E_2$ ,  $G_{12}$  and  $\nu_{12}$  where the subscripts 1 and 2 indicate the principal material directions. Direct investigation of these properties can be obtained experimentally from the various corresponding uniaxial tests.

A group of failure envelopes were obtained for several fiber-orientation angles ( $\Theta=30, 45$  and  $60$ -degrees), in order to study the effect of shear stress ( $\tau_{xy}$ ) variation on failure behavior of a well-known type of a composite material namely; Boron-epoxy Narmco 5505. Representative figures were selected to show such effect accounting for material nonlinearity exerted on failure behavior of unidirectional fibrous composite laminates. An energy-based nonlinear material model was adopted to predict the mechanical properties of a unidirectional composite lamina. A compatible failure criterion for nonlinear composite materials was utilized which incorporates the material response into the failure model. The resulting failure envelopes were compared for all the cases.

Key words: Nonlinear model, composite material, shear stress, failure envelope, fiber-orientation

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\* ADDRESS FOR CORRESPONDENCE: **Ghazi A. F. R. Abu-Farsakh**, Professor at Civil Engineering Department, Jordan University of Science and Technology, Jordan. E-mail address: [ghazi@just.edu.jo](mailto:ghazi@just.edu.jo)

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# The effects of acid and thermal treatment on the characterizations of Iran natural diatomite

**Azimi Pirsaraei Seyed Reza**, Occupational Health Engineering Department, Faculty of Medical Sciences, Tarbiat Modares University, Tehran, IR Iran

**Asilian Hasan**, Occupational Health Engineering Department, Faculty of Medical Sciences, Tarbiat Modares University, Tehran, IR Iran

**Jonidi Jafari Ahmad**, Occupational Health Engineering Department, Faculty of Medical Sciences, Tarbiat Modares University, Tehran, IR Iran

## Abstract

The characterizations of natural diatomite from Birjand deposit (Iran) were studied such as chemical compositions, specific surface area, total pore volume, pore size distribution and XRD. The diatomite that was treated only with sulfuric acid displayed a larger surface area, expanded total pore volume and increased pore size in comparison with both washed natural diatomite with deionized water (D-H<sub>2</sub>O) and the diatomite treated with sulfuric acid then calcinated at 550°C (D-H<sub>2</sub>SO<sub>4</sub>+550). The specific surface area and total pore volume were increased 46.63% and 71.40%, respectively. The results showed that the diatomite samples were composed of cristobalite, quartz and feldspar phases. Acid treatment and then calcination at 550°C changed the Si/Al ratio and grew the crystallite size. BJH with DFT analysis showed that the diatomite samples had very disordered micro/mesoporous pore networks. The pore size distribution of the diatomite samples were from 1.4–100 nm. The isotherm of the samples were type IV and showed a long hysteresis loop that resembled the H3 type on the basis of the IUPAC classification. Therefore, the diatomite that was treated only with 3M H<sub>2</sub>SO<sub>4</sub> can be to serve as a catalyst support or an adsorbent.

Key words: Iran natural diatomite, acid treatment, X-ray diffraction, crystallite size determination, scanning electron microscopy

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\* ADDRESS FOR CORRESPONDENCE: **Azimi Pirsaraei Seyed Reza**, Occupational Health Engineering Department, Faculty of Medical Sciences, Tarbiat Modares University, Tehran, IR Iran.  
E-mail address: [seyedreza.azimi@modares.ac.ir](mailto:seyedreza.azimi@modares.ac.ir)

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# Synthesis, Crystal and Electronic Structures of CdAl<sub>4</sub>O<sub>7</sub>

**Minhua Sua**, Department of Civil Engineering, The University of Hong Kong, Pokfulam Road, Hong Kong  
**Kaimin Shiha**, Department of Civil Engineering, The University of Hong Kong, Pokfulam Road, Hong Kong  
**Qingyun Chena**, Department of Civil Engineering, The University of Hong Kong, Pokfulam Road, Hong Kong, Key Subject Laboratory of National Defense for Radioactive Waste and Environmental Security, Southwest University of Science and Technology, Mianyang 621010, China  
**Hengrui Zhoua**, Department of Civil Engineering, The University of Hong Kong, Pokfulam Road, Hong Kong  
**Chuanmin Meng**, Key Lab for Shock Wave and Detonation Physics Research, Institute of Fluid Physics, Chinese Academy of Engineering Physics, Mianyang 621900, China

## Abstract

Cadmium aluminate (CdAl<sub>4</sub>O<sub>7</sub>) is synthesized by solid state reaction in the presence of cadmium oxide (CdO) and gamma-alumina (γ-Al<sub>2</sub>O<sub>3</sub>) at temperatures ranged of 800-1000 °C. The preparation parameters, such as sintering temperature and molar ratios of Cd/Al, are thoroughly investigated. X-ray diffraction (XRD) technique is employed to monitor the phase transformations occurred in the sintered CdO + γ-Al<sub>2</sub>O<sub>3</sub> system. Experimental results show that the formation of cadmium aluminate(s) is highly influenced by the sintering temperature. A favored crystallographical temperature for the significant formation of CdAl<sub>4</sub>O<sub>7</sub> is found to be 950 °C. Single phase of CdAl<sub>4</sub>O<sub>7</sub> is obtained at 950 °C for 36 h and an identical sintering process is repeated to ensure the product quality. The crystalline degree and microstructural characteristic of the product is examined by HRTEM. CdAl<sub>4</sub>O<sub>7</sub> is identified to be a single phase with monoclinic structure (space group C2/m). The crystal structure of CdAl<sub>4</sub>O<sub>7</sub> is also solved and determined by Rietveld refinement analysis of collected XRD data. The obtained structural details may provide possibility and feasibility for the potential application of CdAl<sub>4</sub>O<sub>7</sub>. The electronic structures (band structure and density of states) are calculated by GGA-PBE based on density functional theory (DFT). The calculated electronic structures revealing semiconductor character of CdAl<sub>4</sub>O<sub>7</sub> with a direct band gap of 3.0 eV.

Key words: Aluminate, Monoclinic, CdAl<sub>4</sub>O<sub>7</sub>, Crystal Structure, DFT, Band Structure, DOS

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\* ADDRESS FOR CORRESPONDENCE: **Minhua Sua**, Department of Civil Engineering, The University of Hong Kong, Pokfulam Road, Hong Kong. E-mail address: [kshih@hku.hk](mailto:kshih@hku.hk)

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## Effect of saline environment on mechanical properties of adhesive joints

**Mustafa EL-MUSBAHI**, Faculty of Engineering, Al-Mergib University, Garaboulli, Libya  
**Ghassan S. EL-MASRY**, Faculty of Engineering, Al-Mergib University, Garaboulli, Libya  
**Hamza A Khalfalla**, Faculty of Engineering, Al-Mergib University Garaboulli, Libya  
**Ferhat Kadioglu**, Head of Mechanical Engineering, University of Turkish Aeronautical Association, Turkey.

## Abstract

Water diffusion into composite adhesive joints was experimentally studied by means of gravimetric measurements in bond specimens. The main parameters controlling the diffusion in the bond components were obtained from water uptake experiments carried out in bulk specimens of fiber-reinforced composite and epoxy adhesive. The diffusion of water in bonds is a complex mechanism due to the heterogeneous microstructure of the composite and its interface with the adhesive. This process was simulated through micro scale models which represent the microstructure of the composite and of the adhesive joint. Structural adhesive joints are adequate for joining aluminum with nearly constant. In terms of fatigue strength, for 10<sup>5</sup> cycles, a decrease about 25% and 39% occurred in specimens immersed during

Key words: Structural adhesives, degradation of adhesives, water, motor oil, flexion test.

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\* ADDRESS FOR CORRESPONDENCE: **Mustafa EL-MUSBAHI**, Faculty of Engineering, Al-Mergib University, Garaboulli, Libya. E-mail address: [ief.gha@gmail.com](mailto:ief.gha@gmail.com)

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