attachment of cells on orthodontic appliances was followed in the presence and in the absence of prophylactic products. Brass sheets and pure cultures were also used with the aim of comparison. Microcolonies of different shapes, formation of water channels between microbial aggregates, different exopolymers/cells densities within the colonies and projection of exopolymers towards the bulk solution could be visualised by direct observations in real time.

09:20-09:40 EFFECT OF ELECTRONIC STRUCTURE AND CONFORMATION OF CELLULOSE AND CELLULOSE ETHERS ON THE GROWTH OF CALCIUM PHOSPHATE. S. Recillas', V. Rodriguez,' an J. Ascencio,' and V.M.Castano2. 1Instituto Nacional de Investigaciones Nucleares, Apdo. Postal 18-1027, México, 11801, D.F; México. 2Instituto de Física de la Universidad Nacional Autónoma de México, Apdo. Postal 1-1010, Querétaro, Qro. 76001, México.

The influence of electronic structure and conformation of minimal energy of cellulose and cellulose ethers in the morphology and kinetics of calcium phosphate growth from saturated solutions at 60°C with each of them are discussed. We used the following characterization techniques; X-ray Diffractometry (XRD), Scanning Electron Microscopy (SEM), Energy Dispersive Spectrometry (EDS) and Dynamic Molecular Simulation calculation with Cerius-software specially Dmol3 was applied to obtain the electronic structure and conformations of the substracts.

10:00-10:20 FORMATION OF TITANIUM COATINGS ON STAINLESS STEEL USING A THERMOCHEMICAL METHOD BASED IN THE MOLTEN SALT SYSTEM NaCl-KCl-TiH2. M.A. De la Rosa, J. López, G. Vargas, J. Méndez y M. Méndez. CINVESTAV-IPN Unidad Saltillo, Apartado Postal 663, 25000 Saltillo, Coahuila, México, Tel. 52 (84) 88 10 19, Fax. 52 (84) 88 13 00.

In biomedical applications, Stainless Steel is the alloy preferred for the fabrication of devices employed for the temporary fixation of fractured bones. However, the use of Stainless Steel for the fabrication of permanent orthopedic implants presents some serious disadvantages when compared with titanium-based or Co-Cr-Mo alloys, which have better biocompatibility and corrosion resistance in the long term. The application of a titanium coating constitutes an attractive alternative to improve such properties in Stainless Steel. In this work, a thermochemical process based on the employment of a molten eutectic mixture of NaCl-KCl (with small additions of TiH2 and titanium powder) was used to obtain a titanium coating on the surface of 316L Stainless Steel. The experimental runs were carried out at 800 and 900°C, under an argon atmosphere, employing holding times up to two hours. The titanium coatings were characterized by x-ray diffraction, optic microscopy and scanning electron microscopy. The titanium coatings were several μm thick and the presence of multiple
diffusive layers with different chemical compositions were detected in the coatings.

**COFFEE BREAK**


Three different heat treatments were performed on Ti and Ti-6Al-4V samples before they were implanted with $10^{16}$ cm$^{-2}$, 9 MeV Au and Pt ions at room temperature, using the 3 MV Pelletron accelerator at the Instituto de Física. The final ion positions were calculated using the TRIM code and determined by 6 MeV $^4$He rutherford backscattering. Vickers microhardness test were performed before and after implantation, and increases of up to 45% were observed, depending on the heat treatment and file type of ion implanted. The surface microstructure of the treated and implanted samples were observed with SEM.


Applying photothermal techniques we realized the thermal characterization of hydroxyapatite samples deposited on titanium and stainless steel. The thermal diffusivity $\alpha$ values were obtained by the photoacoustic technique in a heat transmission configuration with rear incidence of the modulated light and the thermal effusivity $e$ values were realized in a diffusion configuration with front incidence. The thermal conductivity $k$ and the heat capacity by unit volume $\rho c$ were determinate from the measurement values of $\alpha$ and $e$ for each sample. These composed materials were made by the thermal plasma technique. The microstructure was made by optical and scanning electron microscopy.

11:20-11:40 QUANTUM MECHANIC SIMULATION OF A POSSIBLE CURE TO DENGUE. L. Gonzalez Tovany and J. A. Ascencio, Instituto Nacional de Investigaciones Nucleares, Km. 36.5 Carr. México-Toluca Salazar. Edo. México 52045 México. E-mail: ascencio@nuclear.inin.mx

One of the most important problem attacked by material science in the last years is the medical materials. This has been explored by several of the new powerful tools, there are a full set of possibilities still. Almost all the efforts have been focused to prosthesis as the hydroxiapatite based materials to reproduce the bone properties. However, more in this work, pharmaceutical oriented, we present a quantum mechanic analysis of a specific molecule identified in Panama and other centroamerican countries as a solution to attack the Dengue disease, the molecule is a natural drug from a plant usually found in centroamerica. This molecule has a specific configuration which can be the responsible of its curative properties. By considering a Density Functional approximation, the HOMO, LUMO are analyzed and the charge distribution is studied to identify the molecular characteristic that influence over its medical properties. The molecule characteristic were calculated by an atomistic by a local density approximation to identify significant elements to recognize the optimal conditions and characteristic to improve medical drugs. The calculus were done in a SGI workstation with processor R10000, and the Cerius$^2$ software.

11:40-12:00 QUANTUM ANALYSIS OF CALCITE AND HIDROXIAPATITE TO FOLLOW AN IRREGULAR REACTION. J. A. Ascencio (1), V. Rodríguez-Lugo (1), V. M. Castaño-Meneses (2), (1) Instituto Nacional de Investigaciones Nucleares, Apdo. Postal 18-1027, México DF 11801, México. FAX: 53 29 73 03 (2) Instituto de Fisica, UNAM. Depto. de FATA. Apdo. Postal 1-1010, Queretaro, Qro, 76001, México. e-mail: ascencio@nuclear.inin.mx.