GLASS BIOACTIVITY STUDIES BY RAMAN ANALYSIS AND THE STEVELS PARAMETER

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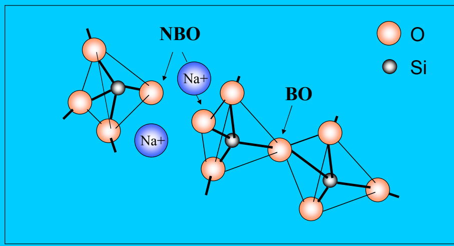
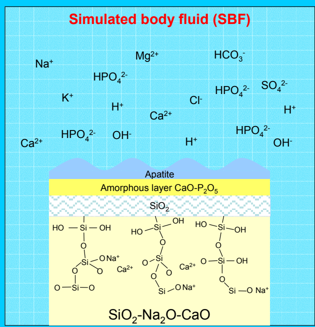
BIOACTIVE GLASS



Silica based glasses present:

- Open amorphous structure.
- Network modifiers: Na^+, K^+, Ca^{2+}.
- Disruption of the continuity of the glass network
- Formation of non-bridging oxygen ions (SiO-NBO).

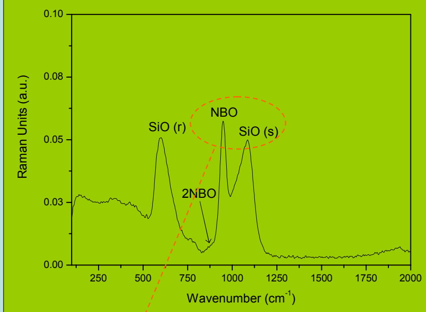


In contact with physiological fluids (SBF):

- Rapid exchange of ions (Na^+, Ca^{2+}) with the solution.
- Repolimerization of a SiO_2 rich layer.
- Formation of a CaO-P_2O_5 rich film on top of the silica.
- Crystallization of amorphous CaO-P_2O_5 film.

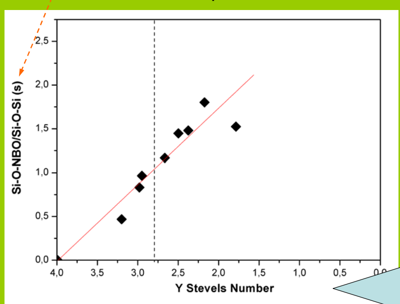
GLASS STRUCTURE STUDY: FT- Raman Analysis

FT-Raman spectroscopy is a sensitive technique to the local structural configurations of bioactive glasses.



The connectivity of the silica network in terms of non-bridging to bridging oxygen ratio (NBO/BO) can be evaluated.

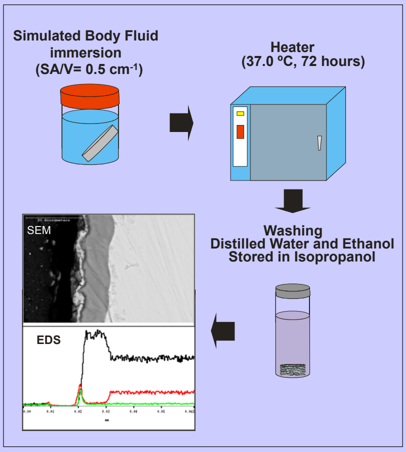
Si-O-NBO/Si-O-Si(s) ratio dependence with Stevels parameter.



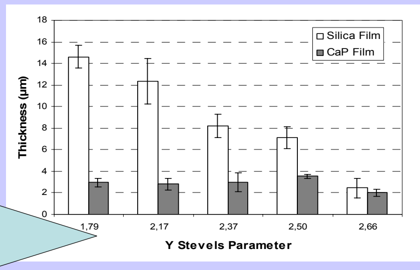
- A linear dependence of the Si-O-NBO/Si-O-Si(s) intensity ratio with the Stevels parameter was found.
- A decrease of the connectivity of the glass network (lower Y) led to a higher concentration of the NBO groups.

BIOACTIVITY STUDY: *In vitro* test

Test Protocol



Dependence of the bioactivity of the glasses in SBF with Y Stevels factor.



- The thickness of both silica-rich and CaP layers decreased for higher Stevels parameters.

THEORETICAL STUDY: Stevels model

According to Stevels model, the silica-based glasses can be seen as inorganic polymers where the degree of polymerisation is determined by the concentration of network modifiers.

The Stevels parameter Y, expressing the mean number of bridging oxygens (BO) per tetrahedron, is a very useful way to describe the cross-linking of the glassy network. This parameter is readily calculated from the molar composition of the glass,

Stevels Parameter

$$Y = 2Z - 2R$$

Z is the mean number of all types of O per tetrahedron.
R is the ratio of the total number of O to the total number of glass-forming cations

Glass	Y	SiO_2	P_2O_5	Na_2O	CaO	K_2O	MgO	B_2O_3
FS	3.99	99.1	0	0.3	-	0.1	0.1	-
CG	3.20	71.9	0.1	13.1	8.8	0.4	4.3	-
Y66	2.98	66	2	5	17	5	5	-
Y59	2.95	59	3	10	15	5	5	3
N58	2.66	58	4	14	24	-	-	-
N55	2.50	55	4	17	24	-	-	-
N53	2.37	53	4	19	24	-	-	-
N50	2.17	50	4	22	24	-	-	-
N45	1.78	45	4	27	24	-	-	-

CONCLUSIONS

- FT-Raman analysis and theoretical structure calculations have been joined to evaluate the bioactivity grade of silica-based glasses.
- Glasses exhibit a higher bioactivity grade for $Y \leq 2.78$ and Si-O-NBO/Si-O-Si(s) ≥ 1.

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