Molecular scale origin of nuclear waste glass properties

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Assessing the long-term behavior of nuclear waste glasses implies predict their performance, and more precisely their evolution under irradiation and during interaction with water. Structure-property relationships depending on the local and medium-range structure of borosilicate glasses of nuclear interest [1] exemplify structural features rationalizing properties observed during glass elaboration or under forcing conditions (alteration, irradiation). Structural data are correlated with numerical simulations to determine the local structure of glasses, with a special attention to the interplay between glass components [2]. During alteration, some elements, such as Fe, change coordination, as other such as Zr only change coordination in under-saturated conditions. This may explain the chemical dependence of the initial alteration rate and the transition to the residual regime, illustrating the molecular-scale processes during glass-to-gel transformation [3]. Determining molecular scale processes helps in the exploration of new compositions of nuclear glasses [4].

Under irradiation, various structural effects are observed, including coordination change, ion migration or disorder effects. These studies show that glasses with a simplified composition do not show the same behavior as more realistic glasses. Molecular dynamics (MD) simulations provide complementary information on elastic effects [5]. Recent direct evidence for B-coordination change under external irradiation, together with structural models derived from MD, sheds light on the structural mechanisms at the origin of radiation-induced modifications of glass properties, emphasizing the importance of the thermal regime in the cascade core. Molecular scale view of nuclear glasses provides a unifying view of the processes that define the properties of this important class of materials.

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Occurrences of nickel in different host phases of a laterite deposit: An example from Berong, Philippines

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Despite being globally widespread and relatively easy to mine, nickel laterite ores prove to be difficult to process. Beneficiation of Ni and other economically extractable elements along with it, greatly depends on the mixture of the feed material (silicate phases and oxide phases) which, in turn, is dependent on the mineralogy of the raw ore. The type(s), concentration and consumption of acid to be used in dissolution are controlled by the percentages of both gangue and host minerals trapping the Ni, whether by sorption or isomorphous substitution. A modified selective sequential extraction was designed to recover Ni from from its various host phases to optimize the beneficiation process using samples from different zones in a nickel laterite deposit in Berong, Palawan. This deposit is defined by, from top to bottom, an iron oxide-hydroxide zone, a transition zone made up of serpentine and iron oxides, a nickel-enriched serpentine zone, and a nickel-depleted serpentine zone, based on mineralogy and geochemistry. The occurrence of Ni as adsorbed and exchangeable cations, in carbonates, in amorphous iron oxides, within the structure of crystalline iron oxides and hydroxides, and in residual silicate layers within each of the zones was determined. Qualitative analysis of nickel in iron oxides, serpentine and talc using electron-probe microanalyzer supports the results of the extraction experiment. In limonite zones, dominated by goethite and other secondary iron oxides, > 90% of the total nickel reside in the crystal structure of Fe oxides. In the iron oxide – magnesium silicate transition horizon and in the nickel-enriched saprolite zone, respectively, > 80% and an average of 77% of the nickel are distributed in Fe oxides and within the octahedral layers of serpentine. The remaining Ni ions not taken up by these crystalline minerals are mostly associated with amorphous Fe oxides. An EPMA image, depicting relative abundance of Ni, Mg, and Fe in a section of weathered bedrock, implies that Ni is more closely associated with Fe than with Mg. An industrially significant output of this research is the finding that residual silicates, which take an enormous amount of acid to dissolve, need not be dissolved in order to optimize the beneficiation of nickel.