DESIGNING NANOMATERIALS by SINTERING & CRYSTALLIZATION of VITREOUS MATERIALS

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Vitreous materials are known in every class of chemical bonding (molecular, ionic, covalent, metallic, mixed, etc.). However, they are metastable and only exist because the thermodynamically favorable path (crystallization) can be kinetically arrested in some circumstances. In addition, spontaneous (partial) crystallization of glassy articles during fabrication or use produces defects that often impart their use or commercialization. But, if one is able to control the crystal nucleation and growth of desirable crystalline phases in the volume or on the glass surface, a new generation of nano-materials having superior properties can be obtained. Finally, due to their high viscosity and slow kinetics, glasses are good model materials to experimentally test theories and simulations of sintering, crystal nucleation, growth and other types of phase transformations. Thus, the understanding and control of glass crystallization has both practical and scientific components and thus has been an issue of long-standing international interest.

Numerous studies of glass sintering were carried out in the late forties, fifties and sixties, but then almost stopped. However, this field reawakened due to the possibility to produce sol-gel derived materials, thin and thick films and micro and nano *glass-ceramics* via this route. While the kinetics of viscous sintering of monodisperse, spherical, glass particles are well described by the classical models (*Frenkel & Mackenzie-Shuttleworth*) the behavior of real glasses, having wide size distributions of irregular particles that show concurrent crystallization, is much more complex and is not fully understood so far.

In this article we present an algorithm based on the *Cluster model*, which includes all these complicating factors, and test it with different glasses: silica, soda-lime-silica and alumino borosilicate. The algorithm describes well the experimental results for a series of sintering temperatures and heating rates. Computer simulations demonstrate that the algorithm is extremely useful to avoid empirical experimentation and is a valuable tool for the design of new materials. Finally, to illustrate the technological importance of controlled glass crystallization and sintering, some examples of both monolithic and sintered, micro and nanostrutured *glass-ceramics* are presented.