

A Molecular Dynamics study of rare-earth doped Mg-silicate nanoparticles in vitreous silica: from the preform to the fiber.

Jérémy Turlier^{a*}, Xavier Bidault^a, N. Balu Gaumer^a, D. Guichaoua^a, P. Raso^a, S. Chaussedent^a, H. Fneich^b, A. Mehdi^b, D.R. Neuville^c, M. Vermillac^d, and W. Blanc^d

^aUniversité d'Angers, Laboratoire de Photonique d'Angers (LPhiA)–UPRES EA 4464, 2 Bd Lavoisier, 49045 Angers Cedex 01, France

^bUniversité de Montpellier, Institut Charles Gerhardt, CMOS, CC 1701 Place Eugène Bataillon, 34095 Montpellier Cedex 5, France

^cGéomatériaux, CNRS-IPGP, Sorbonne Paris-Cité, 1 Rue Jussieu, 75005 Paris, France

^dUniversité Côte d'Azur, INPHYNI–CNRS UMR 7010, Parc Valrose, 06108 Nice, France

New lasers and amplifiers still require an enhancement of the spectroscopic performance of rare-earth-doped silica optical fibers. In order to tailor their optical behavior, a route of interest consists in embedding rare-earth ions within dielectric nanoparticles in the core of optical fibers. Nanoparticles are formed through spontaneous phase separation phenomenon within a MgO–SiO₂ binary melt, during melt/quench sequences of MCVD fabrication process of the preform^{[1][2]}. Then, fibers are obtained by drawing at high temperature a preform containing nanoparticles. First report on the drawing process reveals an elongation of the nanoparticles in the drawing direction as well as a breakup of the larger ones^[3].

In this Molecular dynamics study, we use a new simple transferable model^[4] to show that phase separation occurring in the MgO–SiO₂ binary melt, leads to separation of liquid phases with mixed composition: Si-rich Mg-poor phases on one hand, Mg-rich Si-poor phases on the other hand. These latter phases, the so-called nanoparticles, are amorphous, non spherical and exhibit a wide range of sizes. Mg-O coordination and MgO content increase with the nanoparticle size. With rare-earth doping, the larger nanoparticles are over-concentrated in luminescent ions. Due to an oxygen-rich environment in the nanoparticles, we show that the rare-earth clustering effect is greatly prevented, compared with a pure silica matrix. Finally, at high temperature, we apply a uniaxial elongation to the nanostructured preform to mimic the experimental drawing step leading to the fiber. We report here results on the effects of this drawing process on the nanoparticles characteristics.

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[3] Vermillac M, Lupi JF, Peters F, et al, *J Am Ceram Soc.* 2017;00:1–6.

[4] Xavier Bidault, Stéphane Chaussedent, Wilfried Blanc, *J. Chem. Phys*, 2015, **143**, 154501.