

Characterization of Mg-based nanoparticles in rare-earth-doped silicate optical fiber preforms: A modeling by Molecular Dynamics simulations

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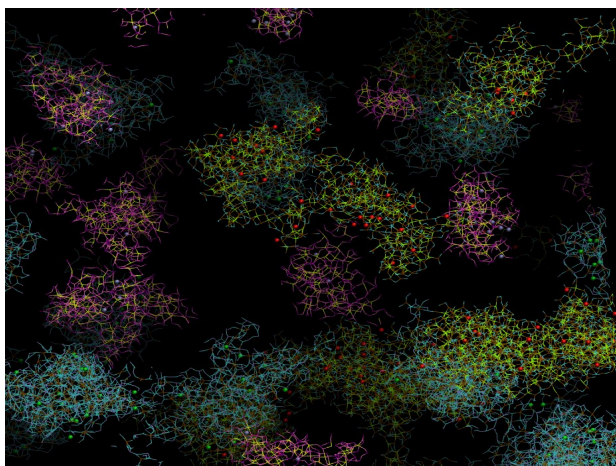


Fig1. A Molecular Dynamics modeling of rare-earth doped Mg-silicate nanoparticles

New rare-earth ion-doped optical fibres stand for potential applications in telecommunications, sensors, fibre lasers. Although silica-based optical fibres present attractive physical and economical properties as glass host, spectroscopic limitations appears when rare-earth ions are inserted in silica, such as clustering or inappropriate local environment.

It has been shown that improvement of Er^{3+} spectroscopy occurs when rare-earth ions are embedded in Mg-silicate nanoparticles.^[1] These latter are formed *in situ* in the MgO– SiO_2 binary system during melt/quench sequences through phase separation mechanism.^[2]

Bidault *et al.* succeeded in simulating by Molecular Dynamics phase separation in MgO– SiO_2 binary system through a new simple transferable adaptive model.^[3] It allows us to reproduce the formation of rare-earth-doped oxide nanoparticles and we present here an investigation of their structures and compositions as well as the local environment of the rare-earth ions Eu^{3+} and Er^{3+} .

In the aim of monitoring luminescence properties inside silica-based optical fibers containing rare-earth-doped nanoparticles, we show that Molecular Dynamics appears to be a powerful tool to understand the relationship between controlled local environments and their spectroscopic features.

[1] Francesco D'Acapito, Wilfried Blanc, Bernard Dussardier, *Journal of Non-Crystalline Solids*, Elsevier, 2014, 401, pp.50-53.

[2] Wilfried Blanc, Valérie Mauroy, Bernard Dussardier, *Int. J. of Nanotechnology*, 2012, 9 (3/4/5/6/7), pp.480-487.

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