Molecular dynamics simulation and crystal field calculations of the Eu2O3-PbO-SiO2 glassy system submitted to long annealing time

Titre	Molecular dynamics simulation and crystal field calculations of the Eu2O3-PbO-SiO2 glassy system submitted to long annealing time
Type de publication	Article de revue
Auteur	Lima, H. [1], de Oliveira, HCC [2], Bidault, Xavier [3], dos Santos, TS [4], Chaussedent, Stéphane [5], Couto dos Santos, M.A. [6]
Pays	Pays-Bas
Editeur	Elsevier
Ville	Amsterdam
Type	Article scientifique dans une revue à comité de lecture
Année	2016
Langue	Anglais
Date	15 Sept. 2016
Pagination	62-67
Volume	448
Titre de la revue	Journal of Non-Crystalline Solids
ISSN	1873-4812
Mots-clés	Crystal field parameters [7], Europium ion [8], Method of equivalent nearest neighbours [9], Molecular dynamics; Glasses [10], Simple overlap model [11]
Résumé en anglais	The Eu2O3-PbO-SiO2 glassy system submitted to a long annealing time (100 ps) has been obtained by molecular dynamics calculations. The average of 87/86 sites of the Eu3 + ion with six/seven nearest neighbours are used to discuss the number of lines and the local symmetry of the luminescent site through the crystal field parameters, using the simple overlap model in the frame of the method of equivalent nearest neighbours. The magnitude of the [View the MathML source] Bq2(q = 0, 1, 2) and the non-negligible [View the MathML source] B44 and [View the MathML source] B46([View the MathML source] B34, [View the MathML source] B36 and [View the MathML source] B66) lead to the indication of distorted C4h and C3i site symmetries of the six and seven nearest neighbours, respectively. We have then compared very satisfactorily our 7F1 sublevels calculations with those observed in the emission spectra of an Eu-borate glass annealed for 30 min and 17 h. This comparison is justified because the emission behaviour of europium ions in different glassy systems are honestly very similar. Further, the decrease observed in the 5D0→7F2/5D0→7F1 transition intensity ratio is a clear indication that the Eu3 + ion are nucleating a crystalline phase. Such satisfactory comparisons indicate that we have obtained a transparent glass-ceramics.
URL de la notice	http://okina.univ-angers.fr/publications/ua15615 [12]
DOI	10.1016/j.jnoncrysol.2016.06.031 [13]

Lien vers le document	http://www.sciencedirect.com/science/article/pii/S0022309316302472 [14]
Titre abrégé	Journal of Non-Crystalline Solids

Liens
[1] http://okina.univ-angers.fr/publications?f%5Bauthor%5D=26198
[2] http://okina.univ-angers.fr/publications?f%5Bauthor%5D=26199
[3] http://okina.univ-angers.fr/publications?f%5Bauthor%5D=11261
[4] http://okina.univ-angers.fr/publications?f%5Bauthor%5D=15433
[5] http://okina.univ-angers.fr/stephane.chaussedent/publications
[6] http://okina.univ-angers.fr/publications?f%5Bauthor%5D=26202
[7] http://okina.univ-angers.fr/publications?f%5Bkeyword%5D=22339
[8] http://okina.univ-angers.fr/publications?f%5Bkeyword%5D=22338
[9] http://okina.univ-angers.fr/publications?f%5Bkeyword%5D=22341
[10] http://okina.univ-angers.fr/publications?f%5Bkeyword%5D=22337
[11] http://okina.univ-angers.fr/publications?f%5Bkeyword%5D=22340
[12] http://okina.univ-angers.fr/publications/ua15615
[13] http://dx.doi.org/10.1016/j.jnoncrysol.2016.06.031
[14] http://www.sciencedirect.com/science/article/pii/S0022309316302472