Genetic Algorithm – Assisted Combinatorial Search for New Phosphors

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We developed an evolutionary optimization process involving a genetic algorithm and combinatorial chemistry (combi-chem), which was tailored exclusively for the development of LED phosphors with a high luminescent efficiency, when excited by soft ultra violet irradiation. The ultimate goal of our study was to develop oxide red phosphors, which are suitable for three-band white light emitting diodes (LED). To accomplish this, a computational evolutionary optimization process was adopted to screen a Eu^{3+} - doped alkali earth borosilicate system. The genetic algorithm is a well-known, very efficient heuristic optimization method and combi-chem is also a powerful tool for use in an actual experimental optimization process. Therefore the genetic algorithm – assisted combinatorial chemistry (GACC) would enhance the searching efficiency when applied to phosphor screening. We adopted a Eu^{3+} activated alkali earth borosilicate system, which contains 7 cations, including Eu, Mg, Ca, Sr, Ba, B and Si. 108 compositions randomly chosen from this system constitute the first generation.

The operation of GACC was described schematically in Fig. 1. Two parent members chosen by the roulette wheel selection method were represented as composition bands as can be seen in Fig. 1. One of them was shaded in order to make discrimination between them and hence to trace them out after the crossover. They were treated as chromosomes and the element sectors consisting of the composition band were regarded as genes that have some information affecting the luminance of the member. The crossover created two offspring by exchanging the genes of the parents and the subsequent mutational operation were executed on these offspring. The roulette wheel selection was adopted and the highest two compositions in the former generation were elicited and copied to the next generation. The single point crossover was adopted and the crossover point was determined randomly. The composition was normalized after the crossover. The mutation was achieved by adding and subtracting 0.01 mol for two arbitrary chosen components, respectively.

Fig. 2 shows the actual experimental results, in which both the maximum and average luminance values increase with increasing generation number and the maximum luminance is reached only after the sixth generation. Consequently, the composition of the highest luminance was fixed at $Eu_{0.14}Mg_{0.18}Ca_{0.07}Ba_{0.12}B_{0.17}Si_{0.32}O_{\delta}$ after that. Fig. 3 shows the first and tenth generation photographed under an excitation of 365 nm. It can be seen that the tenth generation contains much more promising compositions than the first.

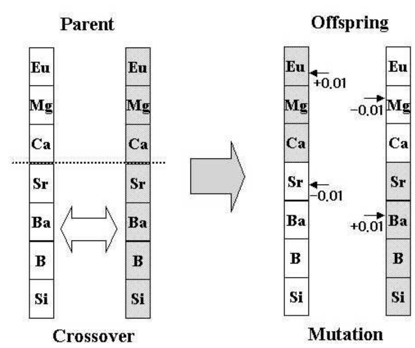

Fig.1 Schematic description of crossover and mutation in the genetic algorithm used for both simulation and experiment

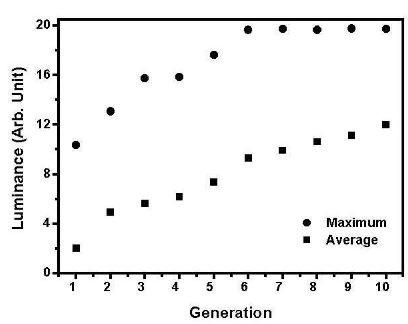

Fig. 2 Experimental maximum and average luminance as a function of generation number.

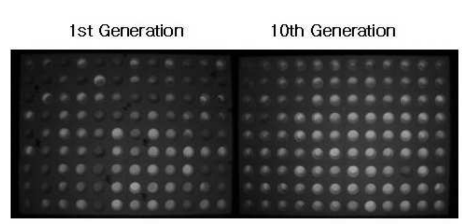

Fig. 3 Libraries of both the first and tenth generation at the 365 nm excitation.