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On the impact of the nano-scale fluctuations of electronic structure in solid solutions on the scintillating properties

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Many mixed crystal scintillators have been investigated during last years. It appears that tuning the composition of a mixed crystal allows to increase the scintillation yield, decrease the afterglow, and improve the energy resolution.
Some properties of mixed crystal scintillators exhibit a non-linear concentration dependence, which differs from the linear Vegard's law. We interpret these non linear behaviors as the effect of the modulation of electronic structure by the fluctuation of spatial distribution of the substitutional ions in the crystals along 3 typical behaviors.
The simulation of ionic crystal solid solution allows us to extract several conclusions concerning the influence of the affinity between the substitutional ions on the observed scintillation properties. Without any affinity between the substitutional ions, the distribution of them is non-correlated and the maximum of the spatial fluctuations of the energy gap (bottom of the conduction band in case of substitution in the cationic sublattice) is achieved at a concentration of 50%. Such fluctuations result in the decrease of the mean free path for elastic above-barrier scattering of electrons, and therefore thermalization length for electrons decreases. When electron energy becomes lower than the height of fluctuations of the bottom of the conduction band, the localization can occur. This increases the probability of geminate recombination and increase the fraction of fast luminescence.
On the opposite, the account of the affinity between the cations substantially alters their distribution and the properties of the mixed crystal. In presence of affinity AA and BB, nanophase separation effects are already observed at concentration about 10% . Nanoclusters enriched with one type of the substitutional ions are formed. The clusters have sizes about a few lattice constants. The fluctuations of the potential become deeper and wider, which facilitate the localization at lower concentration of one of the components, about 30% (70%). This allows suggesting that in scintillator solid solutions showing a maximum LY at these concentrations, the affinity plays a major role. The absorption coefficient in this case is characterized by rather long tail in the transparency region.
The third behavior occurs in presence of cross affinity between cations (AB). In this case, the cation distribution is almost uniform at each concentration. The spatial variation of the energy gap is small; it is much narrow than at a random distribution. In such crystals the energy gap varies in proportion to the concentration (Vegard's law). There are practically no new localization levels, due to the small change of the potential at the non-uniformities.
In this presentation, we discuss the combination of theoretical calculations and experimental evidences to confirm this interpretation.

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