Abstract Submitted
for the NES06 Meeting of
The American Physical Society

Random and Non-Random Placement of Rare Earth Ions in an Yttrium Aluminum Garnet ($Y_3Al_2(AlO_4)_3$) Crystal JEREMY TUDISCO, JOHN COLLINS, Wheaton College — When ionic insulating solids are doped with rare earth or transition metal ions, the spectroscopic properties of those ions depend on their concentration and distribution in the crystal. The efficiency of some processes, such as non-radiative energy transfer among the ions, depends on the details of their distribution, and interpreting the data requires an explicit or implicit assumption regarding that distribution. Their distribution is often assumed to be either random, or less realistically, spread evenly throughout the crystal. In this work, we construct a virtual crystal, and place dopant ions in randomly and nonrandomly, and then study the resulting distributions. We constructed a laser crystal, Yttrium Aluminum Garnet (YAG), containing up to 160,000 atoms (1000 unit cells). The doping process was simulated by selecting particular Yttrium ions, and substituting them with ions of a different type. This simulates the doping of rare earth ions, which are known to favor substituting at Yttrium sites. This doping was done at various concentrations. The random distribution was simulated with a "random" number generator. Non-random substitution of ions was also accomplished in a way that mimicked attractive and repulsive forces among dopant sites. For each ion we found the distance to its nearest neighbor and plotted the occurrence of each nearest neighbor distance. We batch-processed (1000 runs) the program in order to find an average distribution of the ions.

John Collins
Wheaton College

Date submitted: 17 Mar 2006 Electronic form version 1.4