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ASEE Abstract: Computational Modelling of Er^{3+}:Garnet Laser Materials

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The Er^{3+} ion has attracted a lot of interest for four reasons: 1) Its $^4I_{13/2} \rightarrow {}^4I_{15/2}$ transition lases in the eyesafe region near 1.5 μm 2) the $^4I_{11/2} \rightarrow {}^4I_{13/2}$ transition lases near 2.8 μm, an important wavelength for surgical purposes 3) It displays surprisingly efficient upconversion with lasing observed at 1.7, 1.2, 0.85, 0.56, 0.55, and 0.47 μm following 1.5 μm pumping, and 4) It has absorption bands at 0.96 and 0.81 μm and thus can be diode pumped. However, properties desirable for upconversion reduce the efficiency of 1.5 and 3 μm laser operation and vice versa. Since all of the processes are influenced by the host via the crystal field induced stark splittings in the Er levels, this project undertook modelling of the host influence on the Er lasinng behavior. While growth and measurement of all ten Er^{3+} doped garnets is the surest way of identifying hosts which maximize upconversion (or conversly, 1.5 and 3 μm performance), it is also expensive - costing ~\$10,000/material or ~ \$100,000 for the materials computationally investigated here.

The calculations were performed using a quantum mechanical point charge model developed by Clyde Morrison at Harry Diamond Laboratories. The programs were used to fit the Er:YAG experimental energy levels so that the crystal field parameters, B_{nm} could be extracted. From these radial factors, ρ_n, were determined for Er^{3+} in garnets. These, in combination with crystal field components, A_{nm}, available from X-ray data, were used to predict energy levels for Er in the other nine garnet hosts. The levels in Er:YAG were fit with an rms error of 12.2 cm^{-1} over a 22,000 cm^{-1} range. Predicted levels for two other garnets for which literature values were available had rms errors of less than 17 cm^{-1}, showing the calculations to be reliable. Based on resonances between pairs of calculated stark levels, the model predicts GSGG as the best host for 1.5 μm laser operation, GSGG or YSAG as the best host for 2.8 μm operation, and LuGG as the best host for an upconversion material.