A microscopic model of the oxygen vacancies in Ca-doped YIG

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9.7 cm

Annealing experiments carried out on calcium doped yttrium iron garnet ($Ca:YIG$) in a reducing atmosphere, show decreases in the magnetisation over the entire temperature range. The electrical resistivity and the electric activation energy, however, increase. Charge carriers in $Ca:YIG$ are positive compensating holes. We compare with each other two situations, in which a compensating hole can be found. The first is the localization at an oxygen site which means the occupation of a hybridized eigen-energy level of an iron-oxygen cluster. The other is the localization of the hole in an attractive trap center. The latter is regarded as a result of a missing oxygen ion between the tetrahedral and octahedral iron-oxygen ionic clusters. For a sufficiently shallow trap, localized energy levels of the vacancy are considered to be eigen-energies of the hydrogen-like "atom". Assuming the Bohr radius equal to the calcium - oxygen distance, we can estimate the ground-state energy varying both the dielectric constant and the hole's effective mass. Communication between the tetrahedral and octahedral iron-oxygen clusters is maintained due to the $s-d$ hybridization. We find the energy-level structure of the pair of the clusters with either the ferro- or antiferromagnetic order of the spins. A difference in the respective ground states energies of the pair is equal to a superexchange parameter between the clusters' spins. Moreover, we find the current-voltage characteristics of the pair on the basis of the Landauer-like formula for the charge transfer.

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