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Application of Learning Methods to Local Electric Field Distributions in Defected Dielectric Materials[1] KIM FERRIS, Pacific Northwest National Laboratory, DUMONT JONES, Proximate Technologies, LLC. — Local electric fields reflect the structural and dielectric fluctuations in a semiconductor, and affect the material performance both for electron transport and carrier lifetime properties. In this paper, we use the LOCALF methodology with periodic boundary conditions to examine the local electric field distributions and its perturbations for II-VI (CdTe, Cd(1-x)Zn(x)Te) semiconductors, containing Te inclusions and small fluctuations in the local dielectric susceptibility. With inclusion of the induced-field term, the electric field distribution shows enhancements and diminishments compared to the macroscopic applied field, reflecting the microstructure characteristics of the dielectric. Learning methods are applied to these distributions to assess the spatial extent of the perturbation, and determine an electric field defined defect size as compared to its physical dimension. Critical concentrations of defects are assessed in terms of defect formation energies.

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