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Field-enhanced vacancy diffusion in AlGaN[1] KEITH H. WARNICK, YEVGENIY PUZYREV, Dept. of Physics and Astronomy, Vanderbilt University, TANIA ROY, Dept. of Electrical Engineering and Computer Science, Vanderbilt University, DANIEL M. FLEETWOOD, Dept. of Electrical Engineering and Computer Science, Dept. of Physics and Astronomy, Vanderbilt University, RONALD D. SCHRIMPF, Dept. of Electrical Engineering and Computer Science, Vanderbilt University, SOKRATES T. PANTELIDES, Dept. of Physics and Astronomy, Vanderbilt University; Materials Science and Technology Division, Oak Ridge National Laboratory — Room-temperature (RT) native defect diffusion does not generally occur in semiconductors because of high activation energies (>1.5 eV). However, recent observations of plastic deformation in AlGaN/GaN High Electron Mobility Transistors (HEMTs) have been attributed to diffusive processes. Here we report first-principles density-functional calculations of the formation and migration energies of vacancies, including the effect of strain and electric fields. We find that triply-negatively charged cation vacancies are the enablers of self-diffusion, as follows: though strain alone is insufficient, we find significant activation barrier lowering due to the applied electric field acting on charged vacancies, reducing cation vacancy barriers in AlGaN to ∼1 eV or lower where RT diffusion becomes significant. The described mechanism of electric field enhanced vacancy diffusion is relevant for other materials, including several oxides that also feature charged vacancies with low formation energy.

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