Role of defect relaxation for trap-assisted tunneling in high-κ thin films: A first-principles kinetic Monte Carlo study

Abstract:
We assess the impact of structural relaxation of defects upon charging on trap-assisted tunneling in high-κ dielectric materials. ZrO$_2$/Al$_2$O$_3$/ZrO$_2$ thin films are taken as an exemplary system. In our completely different approach, a first-principles defect model is derived from Hedin's GW approximation calculations, which is then coupled to kinetic Monte Carlo charge transport simulations. Comparison between simulation and experiment demonstrates that it is often imperative to take structural relaxation processes into account when modeling nanoscale transport across defect states.

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