

Abstract Submitted  
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**Microscopic crystalline stability of SiC, III-V, and II-VI crystals: generation of Frenkel pairs**<sup>1</sup> PIOTR BOGUSLAWSKI, PAWEL JAKUBAS, Institute of Physics PAS — Applications of semiconductors in high-power/high-temperature devices require their structural robustness, which, at the microscopic level, is limited by generation of vacancy-interstitial Frenkel pairs (FPs). First principles calculations were used to analyze generation of FPs in SiC, GaN, ZnO, CdTe, ZnTe, and GaAs. Dramatic impact of injection currents on the process is stressed. We find that (i) in zinc blende crystals generation of FPs on cation sublattice is a few orders of magnitude more efficient than on the anion sublattice, while the opposite holds for GaN and ZnO, (ii) SiC, GaN, and GaAs are always structurally stable, with barriers of 5-10 eV. In contrast, in ZnTe and CdTe excess electrons reduce barriers from 3 to 1.4 eV, leading to degradation of II-VI light emitting diodes, (iii) in intrinsic ZnO the barriers are high, 5.5 eV. High p-type injection currents reduce the barrier to 3.5 eV, which is comparable to the band gap and may prevent high-power applications. A comprehensive analysis of the results is given.

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