Supplementary information for

Stable partial dislocation complexes in GaN by molecular dynamics and first-principle simulations

Andrey Sarikov[1,2,3,*] and Ihor Kupchak[1,4]

[1] V. Lashkaryov Institute of Semiconductor Physics, National Academy of Sciences of Ukraine, 41 Nauky Avenue, 03028 Kyiv, Ukraine

[2] Educational Scientific Institute of High Technologies, Taras Shevchenko National University of Kyiv, 4-g Hlushkova Avenue, 03022 Kyiv, Ukraine

[3] National Technical University of Ukraine "Igor Sikorsky Kyiv Polytechnic Institute", 37 Beresteiskyi Avenue, 03056 Kyiv, Ukraine

[4] University of Rome "Tor Vergata", Via della Ricerca Scientifica 1, 00133 Rome, Italy

* Corresponding author. E-mail:sarikov@isp.kiev.ua

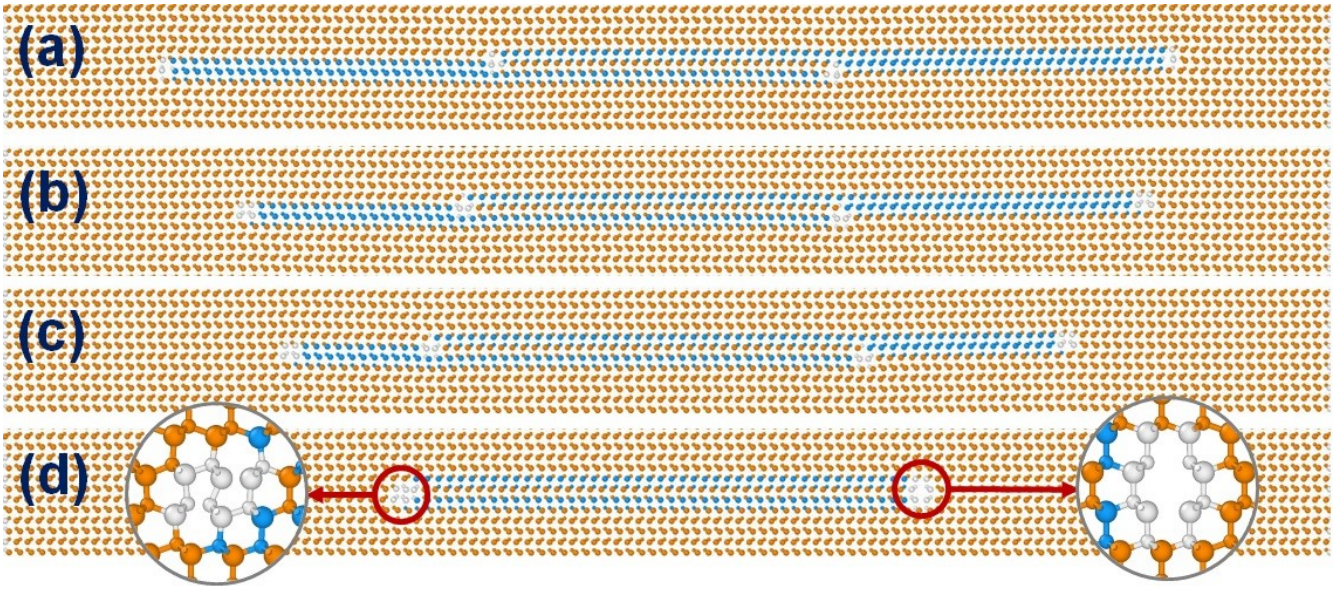

Figure 1. S. I. MD simulated evolution of the 90°-90° dislocation dipoles in wurtzite GaN. Simulated time: (a) – initial structure, (b) – 1.4 ns, (c) – 2.8 ns and (d) – 4.2 ns. The insets in panel (d) show enlarged atomic configurations of the formed stable dislocation complexes with zero total Burgers vectors.

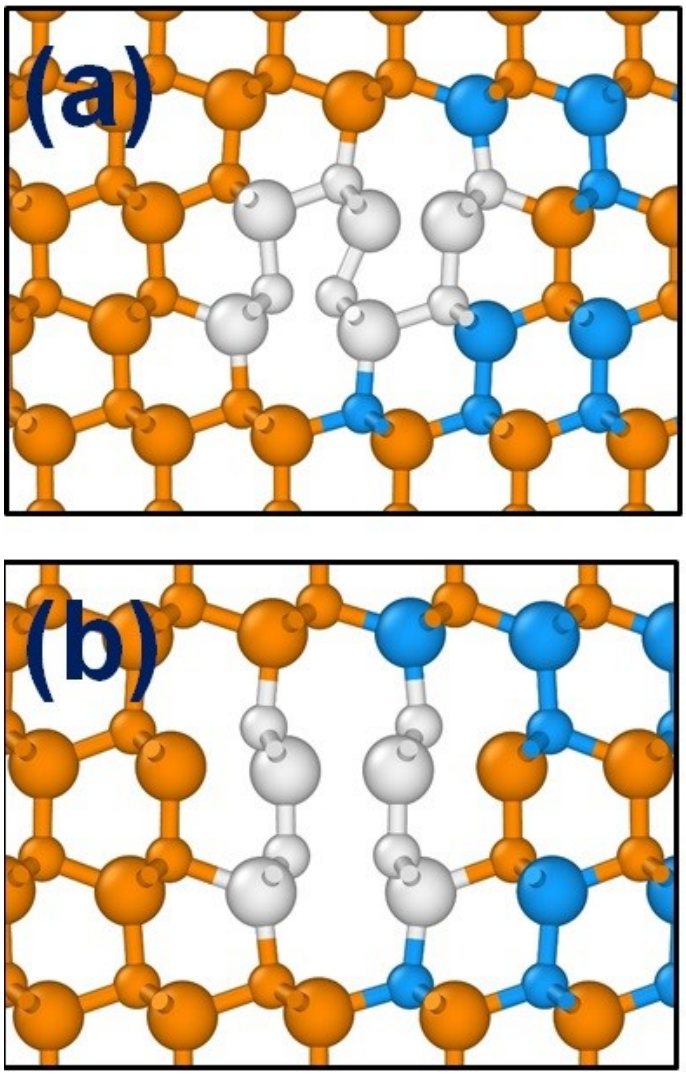

Figure 2 S. I. Atomic configuration of a flower-like 90°-90° Shockley partial dislocation complex obtained by molecular dynamics (a) and DFT (b) calculations.

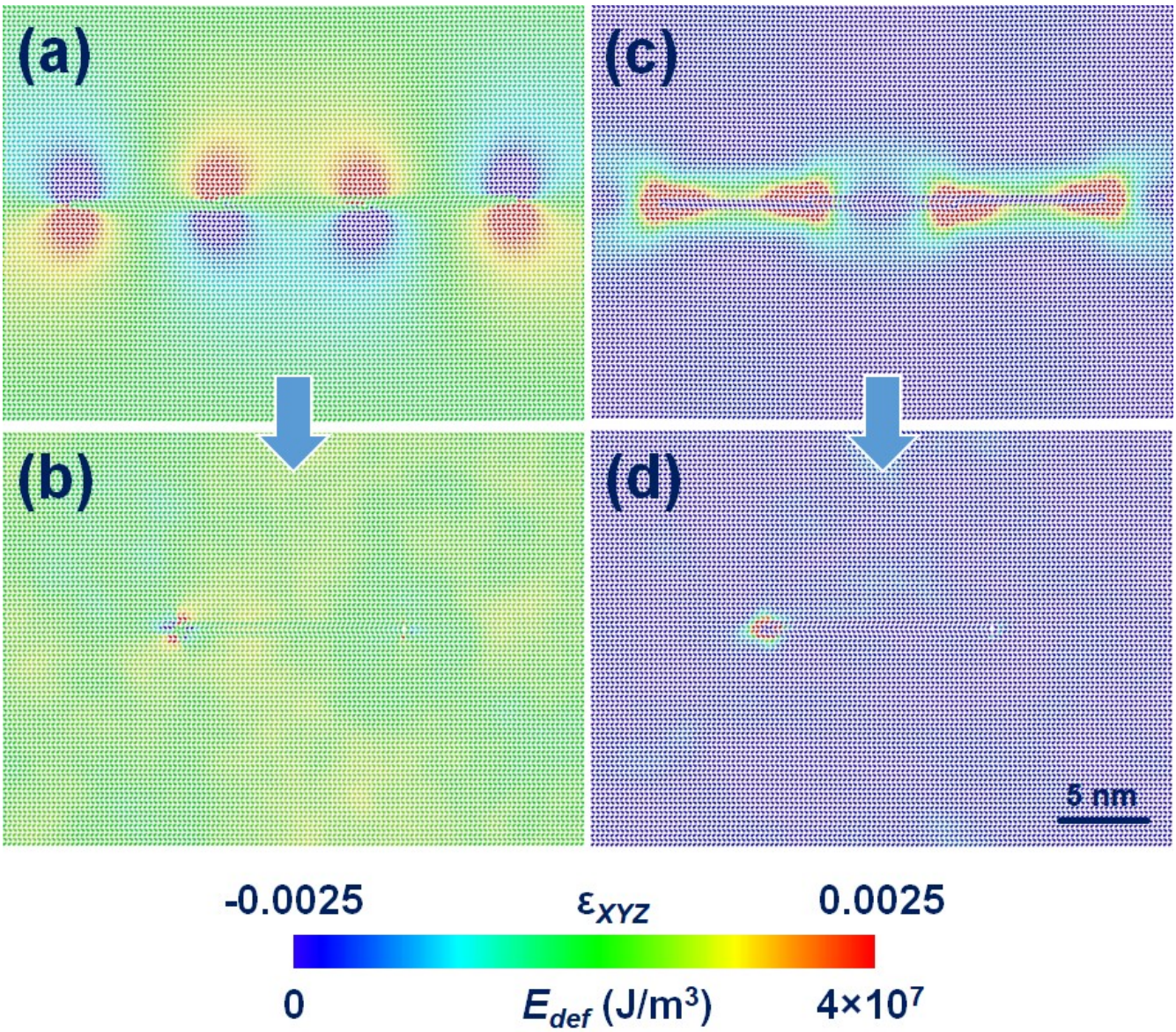

Figure 3 S. I. Distribution of volumetric strain (a, b) and elastic energy density (c, d) in the wurtzite GaN cell with 90°-90° dislocation dipoles before (a, c) and after (b, d) formation of double partial dislocation complexes.