Atomistic Study of Beam-Tilt Control of Channeling in Low-Energy Nitrogen Implantation into Diamond

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Precise control of implantation depth and lattice damage is essential for fabricating shallow nitrogen-vacancy (NV) centers in diamond for quantum sensing and nanofabrication. In diamond (100), low-energy nitrogen implantation is strongly influenced by crystallographic channeling, producing broad depth distributions and deep ballistic tails that degrade near-surface NV yield and process reproducibility. While small beam tilts are widely used to mitigate channeling, a quantitative, atomistic understanding of how implantation angle governs depth precision, damage localization, and process stability remains limited.

Here, we report a systematic molecular dynamics study of nitrogen implantation into diamond (100) as a function of beam tilt angle (0°, 7°, 15°, and 30°) and energy (1-5 keV). Simulations were performed in LAMMPS using a hybrid ZBL-Tersoff interaction potential with SRIM-calibrated electronic stopping. Multi-shot implantation sequences with statistical replicates were analyzed to quantify nitrogen depth distributions (median, interquartile range, and deep-tail metrics), near-surface disorder (sp^2 fraction within the top 2 nm), and shot-by-shot damage accumulation.

Normal incidence (0°) exhibits strong axial ⟨100⟩ channeling, leading to rapidly increasing depth spread and pronounced deep tails with increasing energy (*Figure 1*). Moderate tilts ($\sim 15^{\circ}$) suppress channeling and establish a collision-dominated stopping regime with tightly localized nitrogen depth distributions and minimal deep-tail risk. At larger tilts (30°), implantation becomes surface-skimming, producing shallower stopping but significantly increased near-surface sp^2 disorder indicative of enhanced graphitization risk. Shot-resolved analysis further reveals that channeling at 0° is dynamically unstable: near-surface disorder remains low for early shots and then increases abruptly as accumulated damage collapses channeling corridors, whereas the $\sim 15^{\circ}$ regime exhibits smooth, linear damage accumulation across shots (*Figure 2*).

These results establish beam tilt as a deterministic control knob that selects between axial channeling, collision-dominated stopping, and surface-skimming regimes in diamond (100). The resulting angle-energy process map provides practical guidance for shallow NV fabrication, identifying moderate tilt as an optimal window balancing depth precision, shallow vacancy localization, and surface lattice preservation. The predictions are directly testable experimentally and motivate crystallography-aware implantation recipes for atomically precise defect engineering in diamond nanofabrication.

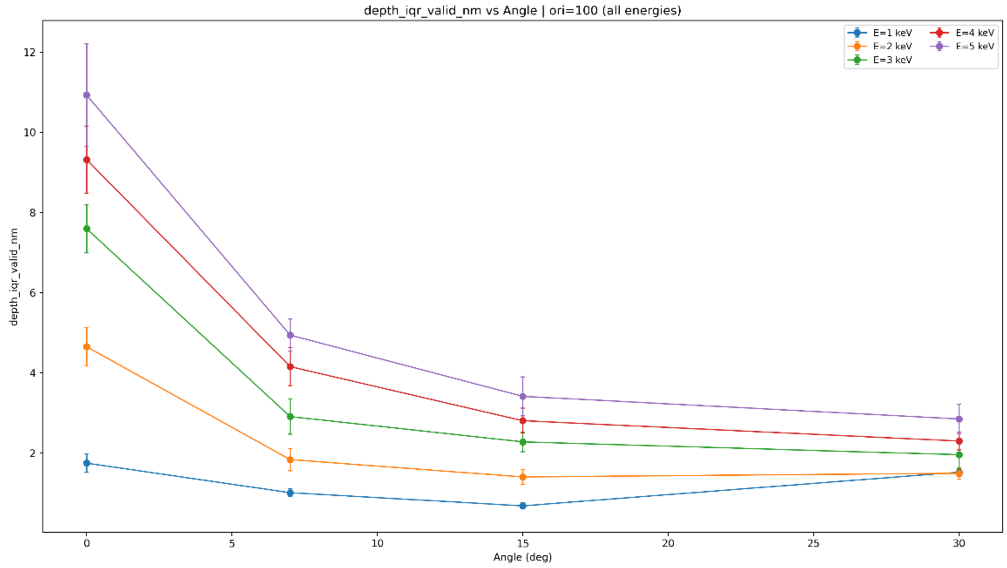

Figure 1: Interquartile range (IQR) of nitrogen implantation depth versus beam tilt for 1-5 keV implantation into diamond (100). Normal incidence shows strong channeling with rapidly increasing depth spread, while moderate tilt suppresses channeling and localizes stopping.

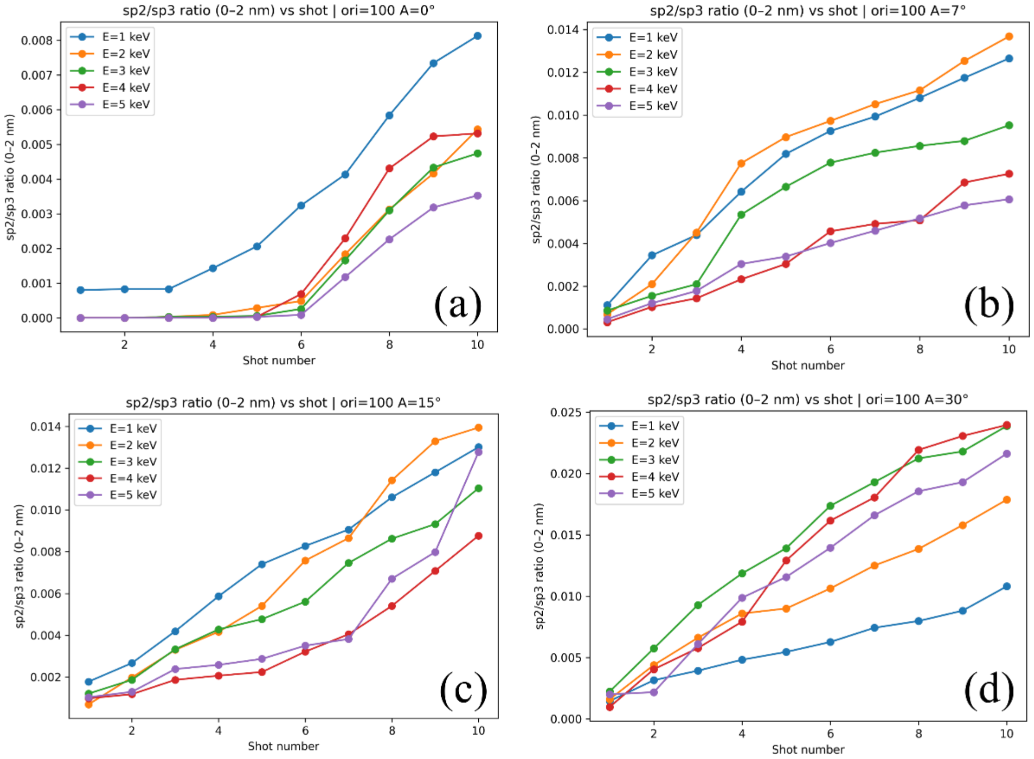

Figure 2: Shot-by-shot evolution of near-surface damage quantified by sp^2/sp^3 ratio (0-2 nm) for (a) 0°, (b) 7°, (c) 15°, and (d) 30° beam tilt. Normal incidence exhibits delayed damage accumulation due to channeling, whereas tilted implantation produces immediate and smoother near-surface damage growth.