Efficient and stable activation by microwave annealing of nanosheet silicon doped with phosphorus above its solubility limit

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SUPPLEMENTARY MATERIAL

The Si:P layer is grown epitaxially in a 300-mm-diameter single-wafer chemical vapor deposition tool (Applied Materials, CENTURA PRIME EPI) capable of cyclic deposition and etching. The tool is operated at 300 Torr and 670 °C with precursors of SiH_2Cl_2 (900 sccm) and PR_5 (240 sccm), reaction agent HCl (450 sccm), and carrier N_2 (6000 sccm). After epitaxial growth, the wafer is cut into 2 cm × 2 cm coupons before annealing.

RTA is performed in a Mattson Helios XP RTP tool from 580 to 750 °C for 5 min in N_2, whereas MSA is by a flash lamp annealing tool (SCREEN LA-3000-F). The sample is preheated to 750 °C before MSA at 1150 °C for 2 ms. HRXRD is by a triple-axis Bede D1 system with a copper $K\alpha_1$ source with a Ge (220) 2× monochromator. Rocking curves ($\Omega/2\theta$) around (004) are used to characterize lattice distortion and strain. PAS is performed by using a ^{22}Na source with 0–38 keV positrons. Doppler broadening of annihilation-generated photons around 511 keV is measured by a multichannel coincidence detector with an energy resolution of 1 keV and a peak-to-background ratio of 2×10^6. From the Doppler spectrum line, shape factors *W* and *S* are calculated.

Ab initio calculations are done with VASP code, PBE-PAW pseudopotentials, a plane wave energy cutoff of 450 eV, and a 4 × 4 × 4 Γ-centered Monkhorst-Pack k-point mess. A cubic supercell of 216 atoms is used, where P atoms are added as dopants and Si atoms are removed to form vacancies. Defect configurations are relaxed using a conjugate gradient algorithm until forces acting on atoms are smaller than 0.01 eV/Å. Dipole calculations are performed with CHARGEMOL software from the electronic density distribution of defects calculated with VASP. The calculation is at the absolute zero temperature without excitation or trapping of free electrons. In other words, charging states of the atoms or vacancies are not considered.

The electric field distribution in the MWA cavity is simulated by a finite-element full-wave electromagnetic simulator COMSOL Multiphysics. The dielectric constants of air, Si, and SiC are assumed to be 1, 11.7 and 9.7, respectively. The conductivities of air, Si, and SiC are assumed to be nil, 10 S/m, and nil, respectively. Because the microwave cavity is about a hundred times larger than the susceptor spacing, adaptive grids are used with approximately 0.3-mm grids between the susceptors and approximately 3-mm grids outside the susceptors.

SIMS is carried out in a Physical Electronics ADEPT-1010 tool with 500-eV Cs^+ ions at 60° incidence over a 400 μm × 400 μm area. The mass spectrum of $^{31}P^-$ is monitored from the center 20% of the sputtered area. The

sputter depth is calibrated by a stylus profiler assuming constant sputter rate. Concentrations of P in the Si are calculated using a relative sensitivity factor determined from a standard sample.

Sheet resistance is measured by a KLA-Tencor Rs100 inline four-point probe system, whereas carrier concentration is measured by a Swin 8800 Hall-effect system. For Hall measurements by the van der Pauw method, ohmic contacts are formed by indium on the four corners of the sample and wire-bonded to a printed circuit board. From the measured Hall coefficient R_H, the electron concentration is calculated by $n = 1/eR_H$, assuming unity Hall scattering factor for the heavily P-doped samples.

Based on *ab initio* calculations, Fig. S1 shows the net atomic charge distribution and Fig. S2 shows the magnitudes and directions of net atomic dipole components. Table SI lists the net atomic charge and Table SII lists the magnitudes and directions of net atomic dipole moments.

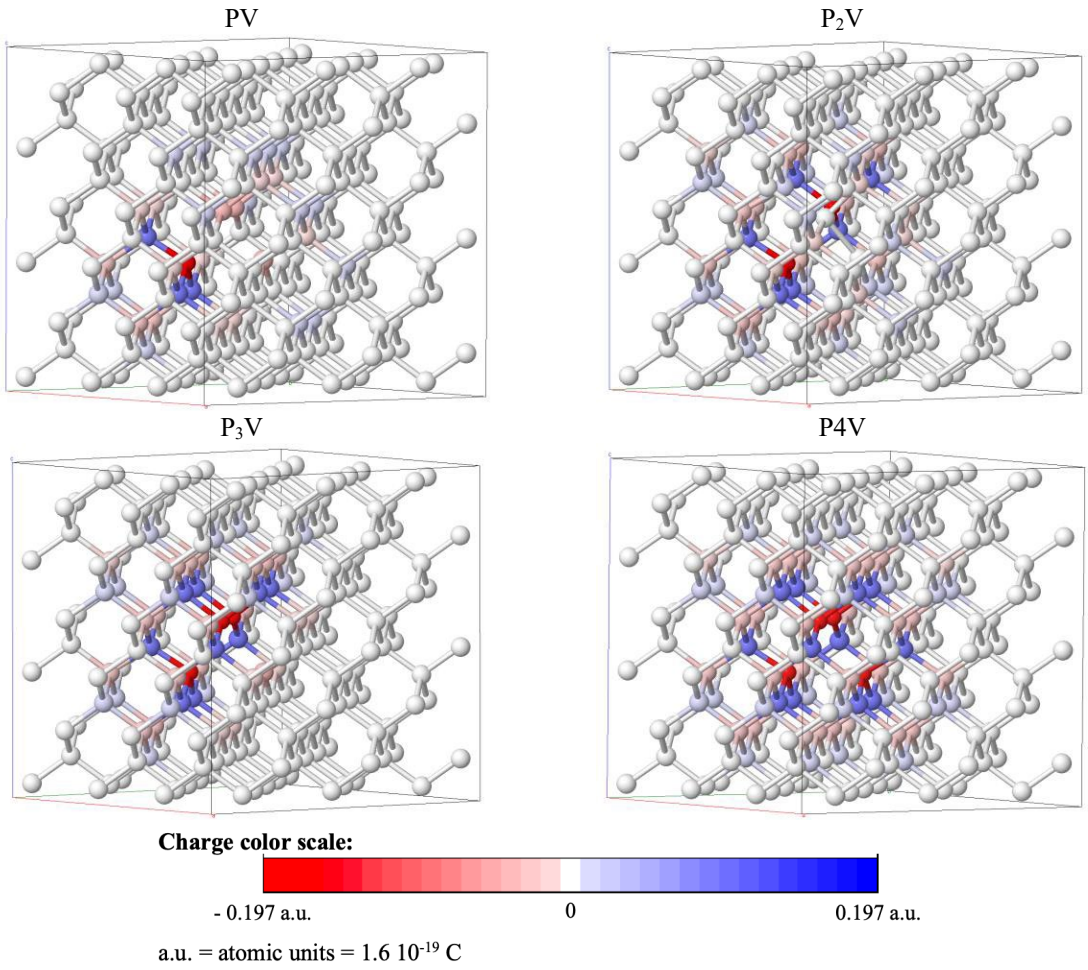

FIG. S1. Atomic structure of Si:P. Red atoms are P with negative charge, blue atoms are Si with positive charge, and white atoms are Si without charge.

Table SI. Atomic charge distribution

Cluster	Minimum Charge (P)	Maximum Charge (nearest Si to P)
P1V	−0.197 a.u.	0.0898 a.u.
P2V	−0.192 a.u.	0.0918 a.u.
P3V	−0.172 a.u.	0.0912 a.u.
P4V	−0.166 a.u.	0.0886 a.u.

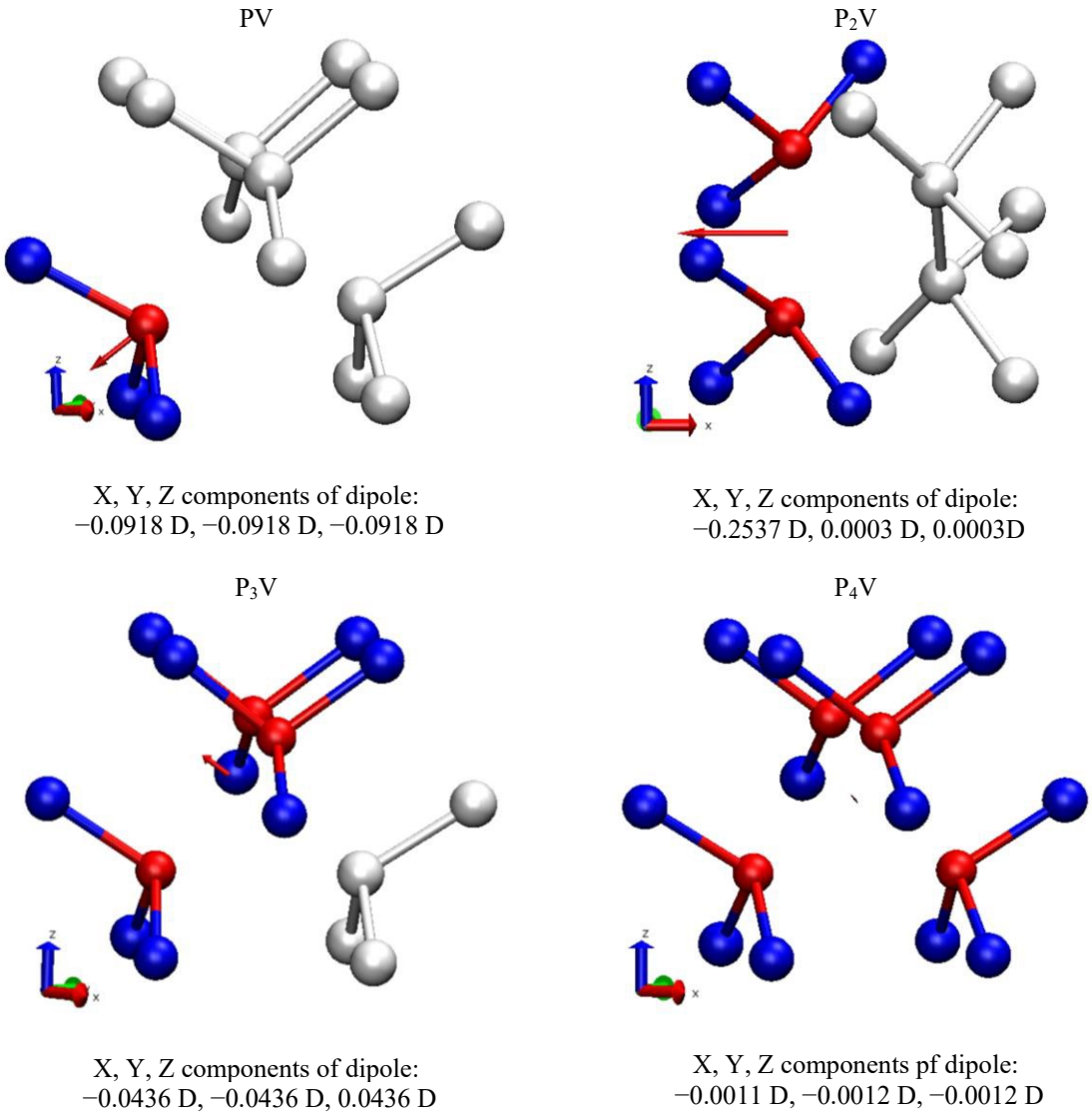

FIG. S2. Dipole magnitudes and directions. Only atoms up to the 2nd neighbors of the vacancy are shown. Net dipoles are represented by red arrows.

Table SII. Dipole magnitude and direction

Cluster	Dipole Moment	
	Magnitude	Direction
P_1V	0.16 D	[−1 −1 −1]
P_2V	0.25 D	[−1 0 0]
P_3V	0.08 D	[−1 −1 1]
P_4V	0	-