Controllable Seeded Flux Growth and Optic-electric Properties of Bulk o-SiP Crystals

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Supporting information

Figure S1. The crystalline orientation of single-crystal flake was determined by single-crystal X-ray.
Figure S2. Oscilloscope traces of SHG signals for o-SiP with KDP as a reference.

Figure S3. DSC/TG data of o-SiP. Blue curve represents DSC and red curve represents TG. The sample decomposes at 1045 °C, where the endothermic peak in the DSC curve together with the dramatic weight loss indicates decomposition of the crystal.

Figure S4. Raman spectrum of o-SiP crystal grown by flux method.

Table S1. Crystallographic Data and Structure Refinement for o-SiP

<table>
<thead>
<tr>
<th>Empirical formula</th>
<th>SiP</th>
</tr>
</thead>
<tbody>
<tr>
<td>Formula weight</td>
<td>59.06</td>
</tr>
<tr>
<td>Temperature</td>
<td>293(2) K</td>
</tr>
</tbody>
</table>
Wavelength (Å) 0.71073  
Crystal system Orthorhombic  
Space group Cmc2₁  
Unit cell dimensions (Å)  
\[ \begin{align*} 
a &= 3.5255(6) 
b &= 20.563(4) 
c &= 13.666(2) 
\end{align*} \]  
Volume (Å³) 990.7(3)  
Z, Calculated density 16, 1.584 mg/m³  
Absorption coefficient 1.163 mm⁻¹  
F(000) 464  
Crystal size 0.18mm × 0.12mm × 0.11mm  
Theta range for data collection 1.98 to 27.47 deg.  
Limiting indices -4 ≤ h ≤ 4, -26 ≤ k ≤ 26, -17 ≤ l ≤ 17  
Reflections collected / unique 5513 / 1310  
R(int) 0.0254  
Completeness to theta = 27.47 99.3 %  
Refinement method Full-matrix least-squares on F²  
Data / restraints / parameters 1310 / 1 / 74  
Goodness-of-fit on F² 1.199  
Final R indices [I>2σ(I)]  \( R1 = 0.0215, \) \( wR2 = 0.0658 \)  
R indices (all data)  \( R1 = 0.0217, \) \( wR2 = 0.0660 \)  
Absolute structure parameter 0.4(3)  
Extinction coefficient 0.0001(4)  
Largest diff. peak and minimum 0.495 and -0.443 e.A⁻³  

Table S2. Hall effect measurements

<table>
<thead>
<tr>
<th>Test condition</th>
<th>Result</th>
</tr>
</thead>
<tbody>
<tr>
<td>I (nA) 10</td>
<td>Nb (cm⁻³)</td>
</tr>
<tr>
<td>B (T) 0.55</td>
<td>u (cm²·V⁻¹·s⁻¹)</td>
</tr>
<tr>
<td>Thickness (µm) 320.00</td>
<td>Rho (Ω·cm)</td>
</tr>
<tr>
<td>Delay Time (s) 0.100</td>
<td>RH (cm⁻³·C⁻¹)</td>
</tr>
<tr>
<td>Measure Time (h) 0.100</td>
<td>RHA (cm⁻³·C⁻¹)</td>
</tr>
<tr>
<td>T(K) 300</td>
<td>RHB (cm⁻³·C⁻¹)</td>
</tr>
</tbody>
</table>