Graphene growth on different sapphire crystal planes: A combined low-temperature PECVD and DFT study

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Graphene directly grown on sapphire via chemical vapor deposition (CVD) is a highly attractive candidate for optoelectronic devices, e.g., photodetectors or biosensors in medical applications [1,2]. It has been shown that the crystal orientation of the sapphire can significantly influence the thermal growth of graphene at elevated temperatures above 1000 °C, where plane-dependent surface reconstructions were the main contributors to different graphene qualities [3].

Here, we present a plasma-enhanced (PE) low-temperature CVD process for direct graphene growth on sapphire substrates with different crystal orientations. Systematically varying growth temperature and plasma power, respectively, we found that the growth rate strongly depends on the sapphire crystal plane: The highest growth rate is obtained for the ca-plane, followed by a-plane, c-plane and the finally r-plane. Depending on the growth conditions, $I_{2D}/I_G \sim 1$, $I_D/I_G \sim 0.71$ (Fig. 1a) and a sheet resistance down to 1.65 kΩ/□ are achieved at growth temperatures as low as 670 °C. Tuning growth time and plasma power, respectively, the graphene film thickness can be adjusted between ~ 1 to 12 layers with optical transmittances ranging from ~ 96.1 % to 74 % (Fig. 1b). Complimentary to the experiments, we conducted DFT simulations assuming a hit-and-stick mechanism of carbon complex adsorption on different sapphire crystal planes. The a-plane surface orientation shows considerably higher surface free energy than the other orientations, indicating high reactivity. By comparing the calculated adsorption energies, we found that adsorption is energetically favourable in the order of a-plane, c-plane and r-plane. This shows striking accordance to the experimentally observed growth rates, where graphene grew fastest in the same order of a-plane, c-plane and r-plane, linking the theoretical adsorption energies of carbon atoms to the plane-dependent differences in graphene thickness measured in the experiment (Fig. 1c).

References

[1] K.S. Novoselov et al., Science 353, aac9439, 2016
[2] S. Xu et al., Applied Surface Science 427 (2018) 1114–1119
[3] Y. Ueda et al., Appl. Phys. Lett. 115, 013103, 2019

Figures

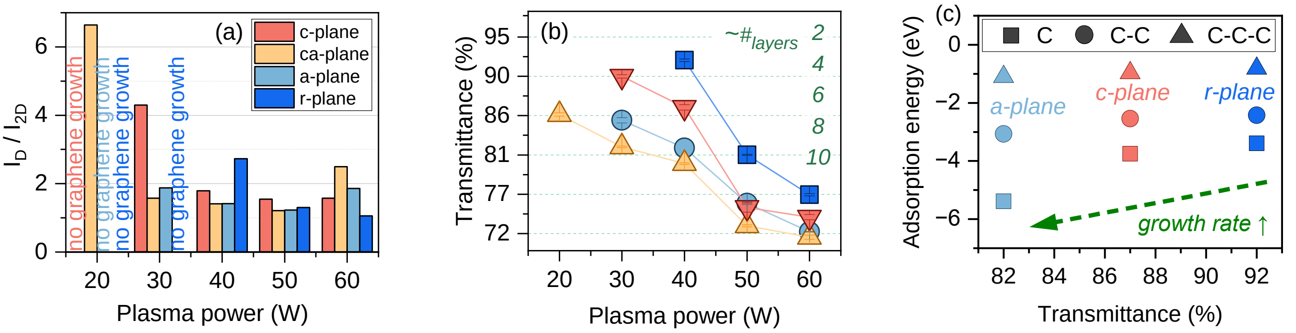

Figure 1: a) Plane-dependent I_D/I_{2D} ratios and b) transmittance vs. plasma power. c) Comparison of calculated adsorption energies of carbon species vs. transmittance (T_{opt} ↓ ~ growth rate ↑) of graphene layers on the a-plane, c-plane and r-plane of sapphire.