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Effects of Steering and Shadowing in Epitaxial Growth

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While shadowing has been known to play a role in some thin-film deposition processes, until recently it has been assumed that in epitaxial growth the effects of steering and shadowing are negligible. Here we present analytical and molecular dynamics results describing the effects of steering due to the short-range and long-range van der Waals (vdW) attraction in metal (100), (111) and (110) epitaxial growth. Our results lead to a general picture of the process of deposition near step-edges^{1,2} which is quite different from the standard downward funneling picture. In particular, we find that short-range attraction plays an important role not only *before* but also *after* collision with the step. As a result, it can significantly enhance the uphill current, selected mound angle, and surface roughness in epitaxial growth. In the case of deposition on metal (111) and (110) surfaces we also find a significant asymmetry between the interaction at A and B steps which may be explained by differences in the step geometry. General expressions for the surface current and selected mound angle valid for arbitrary crystal geometry are also presented. We have also calculated the vdW constant describing the long-range interaction between a Cu atom and a Cu(100) surface.³ Our result is large enough to explain recent observations⁴ of a significant increase in mound angle in Cu/Cu(100) growth for large angles of incidence ($\theta > 50^\circ$) and also indicates that for smaller angles of incidence the dominant effects are due to the short-range rather than to the long-range interaction. Finally, we discuss the effects of shadowing in oblique incidence epitaxial growth and its implications for the control of nanoscale patterning.

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