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First-passage time approach to kinetic Monte Carlo simulations of metal(100) growth[1] GIRIDHAR NANDIPATI, YUNSIC SHIM, JACQUES AMAR, University of Toledo — One of the difficulties in carrying out realistic kinetic Monte Carlo simulations is the existence of rapid, repetitive low-barrier processes which can dramatically slow down the simulation. For example, in metal(100) growth the rate for edge-diffusion can be very fast even at moderate temperatures, while the barriers for edge-detachment and corner rounding are relatively high. While one approach to this problem is to artificially reduce the rate of edge-diffusion, such an approach can significantly alter the thin-film evolution. To address this problem while still preserving the relative rates for all processes, we have developed a modified KMC method in which edge-diffusion and corner-rounding are treated using a first-passage time formalism, while the remaining processes are treated as in normal KMC. In simulations of an effective-medium theory (EMT) based model of Cu/Cu(100) growth at $T = 200$ K and above we find that a speed-up of several orders of magnitude is possible, without sacrificing accuracy. Preliminary results for Cu/Cu(100) growth at high temperatures will also be presented.

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