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**Large-scale simulations of glancing-angle deposition**[1]

JACQUES AMAR, XUEJING LIU, University of Toledo — While thin-films grown via glancing-angle deposition have interesting structural, mechanical, and optical properties, the large range of time- and length-scales makes realistic simulations difficult. Accordingly, while activated relaxation processes may be important at long time-scales, here we focus on the deposition process since we expect the effects of shadowing and deposition-induced relaxation to dominate for large deposition angles. In particular, by taking advantage of the speed of recently developed graphical-processing-units (GPUs) we have carried out "large-scale" GPU-enhanced MD simulations of Cu/Cu(100) growth up to 20 monolayers (ML) for deposition angles $\theta$ (corresponding to the angle with respect to the substrate normal) ranging from 50° to 85° and for both random and fixed azimuthal angles. In general, we find good agreement with experimental results for the dependence of thin-film porosity on deposition angle and film-thickness. Results for the dependence of the surface roughness, lateral correlation length and microstructure (e.g. defect density, vacancy density, and strain) on the deposition angle and film thickness will also be presented.

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[X] Prefer Oral Session
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