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Simulated Scattering of Coherent X-rays from Dynamic GaN Crystal Surfaces¹ DONGWEI XU, Argonne Natl Lab, CAROL THOMPSON, Northern Illinois University, PETER ZAPOL, G. BRIAN STEPHENSON, Argonne Natl Lab — New techniques using coherent x-rays promise to reveal qualitatively new aspects of the arrangements and dynamics of atomic-scale features during materials synthesis. We present analysis of time-dependent speckle in the scattering of coherent x-rays from crystal surfaces, calculated from kinetic Monte Carlo simulations of atomic dynamics both at equilibrium in the growth environment at high temperature, and during non-equilibrium crystal growth. For equilibrium surfaces, standard single- q time correlation functions reveal the rates and power-law exponents of the q dependence for adatom/vacancy diffusion and surface step dynamics. For non-equilibrium surfaces undergoing growth, we calculate two-time correlation functions, and investigate how they can elucidate mechanisms of island nucleation and growth. During layer-by-layer growth, oscillatory correlations at integer monolayers appear at $q < q_{max}$, where q_{max} is the position of the island diffuse scattering peak. During 3-dimensional growth, correlations at non-integer-monolayer times appear at $q > q_{max}$. We will discuss the physical origins of these phenomena, to illustrate how coherent x-ray measurements of complex space/time correlations will be sensitive to atomic-scale mechanisms.

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