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Metallic bubbles nucleation and growth in VO2 nanofilms: insights from TDDFT+DMFT[1] VOLODYMYR TURKOWSKI, Dep. of Physics, Univ. of Central Florida, Orlando, FL 32816, JOSE MARIO GALICIA-HERNANDEZ, Inst. of Physics, Univ. of Puebla, Puebla 72550, Mexico and Univ. of Central Florida, Orlando, FL 32816 , GREGORIO HERNANDEZ-COCOLETZI, Inst. of Physics, Univ. of Puebla, Puebla 72550, Mexico, TALAT S. RAHMAN, Dep. of Physics, Univ. of Central Florida, Orlando, FL 32816 — We apply a time-dependent density-functional theory + dynamical mean-field theory (TDDFT+DMFT) approach to model the response of insulating nanofilms of VO2 to perturbations by ultrafast laser pulses. We focus on the spatially-resolved metallization of the systems, and especially on the process of nucleation and time-dependence of the size of the "surface" and "bulk" metallic domains (bubbles) as a function of film width. In particular, we find that the initial universal (parameter-independent) growth of the domains (radius $R \sim t^{1/2}$), changes by the bubbles shrinking ($R \sim t^{-a}$, $a \sim 1$) as a result of Coulomb scattering effects, and eventually by post-femto-second phonon-involved relaxation of the systems to the equilibrium accompanied by infrared photoemission. The time-dependent conductivity obtained from the above results is in a good agreement with available experimental data.[1,2] [1] D.J. Hilton et al., PRL 99, 226401 (2007); [2] T.L. Cocker et al., PRB 85, 155120 (2012).

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