Structural evolution of Ag nanoparticles during electron driven synthesis of Ag filaments on Ag$_2$WO$_4$: In situ observation and theoretical supporting evidence$^1$ EDISON Z. DA SILVA, Institute of Physics, University of Campinas, Unicamp, WYLLAMANNEY DA SILVA PEREIRA, INCTMN-UFGS, Universidade Federal de São Carlos, JUAN ANDRÉS, LOURDES GRACIA, Departament de Química Física i Analítica, Universitat Jaume I, MIGUEL SAN-MIGUEL, Institute of Chemistry - University of Campinas, ELSON LONGO, INCTMN-UNESP, Universidade Estadual Paulista, VALERIA M. LONGO, INCTMN-USP, Universidade de São Paulo, Instituto de Física de São Carlos — α–Ag$_2$WO$_4$ crystals irradiated by an electron beam from an electron microscope under high vacuum, nucleate metallic Ag, and form Ag metallic nanowires on the α crystals surface. In order to understand this interesting and complex behavior of the formation and growth of Ag nanowires on α–Ag$_2$WO$_4$ we investigated by detailed in situ transmission electron microscopy (TEM), field emission scanning electron microscopy (FE-SEM) studies, density functional theory calculations and ab initio molecular dynamics (MD) simulations. First principle calculations point out that Ag-3 and Ag-4 atoms, located on the (100) surface, are the most energetically favorable to undergo the diffusion process to form metallic Ag. Ab initio MD simulations and nudged elastic band (NEB) method were used to investigate the minimum energy pathways for diffusion of Ag atoms to outward sites on the (100) surface. The results point out that the injection of electrons decreases the activation barrier for this diffusion step and this unusual behavior results from the presence of a lower energy barrier process.

$^1$Financial support FAPESP, Project 2010/16970-0, grant (2013/02032-7), calculations performed at CENAPAD-SP.

Edison da Silva
Institute of Physics, University of Campinas, Unicamp

Date submitted: 03 Nov 2014