

Abstract Submitted
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Structural evolution of Ag nanoparticles during electron driven synthesis of Ag filaments on Ag_2WO_4 : *In situ* observation and theoretical supporting evidence¹ EDISON Z. DA SILVA, Institute of Physics, University of Campinas, Unicamp, WYLLAMANNEY DA SILVA PEREIRA, INCTMN-UFSCar, 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_2WO_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_2WO_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.

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