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Simulation of Nanowires on Metal Vicinal Surfaces: Effect of Growth Parameters and Energetic Barriers AJMI B.H. HAMOUDA, University of Maryland & Univ. of Monastir, SONIA BLEL, Univ. of Monastir, T.L. EINSTEIN, University of Maryland, MRSEC, MARYLAND TEAM, LAB. OF QUANTUM PHYSICS OF MONASTIR TEAM — Growing one-dimensional metal structures is an important task in the investigation of the electronic and magnetic properties of new devices. We used kinetic Monte-Carlo (kMC) method to simulate the formation of nanowires of several metallic and non-metallic adatoms on Cu and Pt vicinal surfaces. We found that mono-atomic chains form on step-edges due to energetic barriers (the so-called Ehrlich-shwoebel and exchange barriers) on step-edge. Creation of perfect wires is found to depend on growth parameters and binding energies. We measure the filling ratio of nanowires for different chemical species in a wide range of temperature and flux. Perfect wires were obtained at lower deposition rate for all tested adatoms, however we notice different temperature ranges. Our results were compared with experimental ones [Gambardella et al., Surf. Sci.449, 93-103 (2000), PRB 61, 2254-2262, (2000)]. We review the role of impurities in nanostructuring of surfaces [Hamouda et al., Phys. Rev. B 83, 035423, (2011)] and discuss the effect of their energetic barriers on the obtained quality of nanowires. Our work provides experimentalists with optimum growth parameters for the creation of a uniform distribution of wires on surfaces.

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