

Abstract Submitted
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Energetics of Cu Nanowires¹ MINE KONUK, Department of Physics, Istanbul Technical University, Maslak, 34469 Istanbul, Turkey, BERK ONAT, Informatics Institute, Istanbul Technical University, Maslak, 34469 Istanbul, Turkey, SONDAN DURUKANOGLU², Department of Physics, Istanbul Technical University, Maslak, 34469 Istanbul, Turkey — We have calculated activation energies for several single atom and vacancy diffusion mechanisms on the $\langle 100 \rangle$ and $\langle 110 \rangle$ axially oriented, rectangular Cu nanowires with a particular interest in determining the effect of varying cross-sectional area on the activation barriers for the investigated processes. The calculations are performed using the nudged elastic band technique based on the interaction potential obtained from the embedded atom method. Our results on activation barriers for adatom diffusion mechanisms indicate a clear dependence on the cross-sectional area of the nanowires. We, furthermore, find that the energy barrier for single vacancy diffusion is decreasing drastically near the outer wall compared to barriers for single vacancy diffusions taking place in the interior region of the nanowire.

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