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Molecular Dynamics Simulations of Upward Diffusion of Adatoms and Clusters on Facetted fcc Metal (110) Surfaces[1] HAILI YANG, QIANG SUN, Zhengzhou University, Zhengzhou, Henan, China, SONGYOU WANG, Fudan University, Shanghai, China, SHUNFANG LI, Zhengzhou University, Zhengzhou, Henan, China, ZHENYU ZHANG, Oak Ridge National Laboratory, The University of Tennessee, YU JIA, Zhengzhou University, Zhengzhou, Henan, China — We study upward self-diffusion of adatoms and small clusters across the outer edges of the mounds formed in fcc metal(110) homoepitaxy using molecular dynamics simulations with interatomic potentials described by the embedded-atom method. Our results show that both single adatoms and small clusters on the (111) and (100) facets of Al and Cu(110) can readily diffuse upwards and cross the outer edge of the mounds, but with different atomistic mechanisms. An adatom crosses the outer edge via a simple place exchange or indirect exchange mechanism. In contrast, the upward diffusion and outer-edge crossing of small clusters is realized by their dissociation at the edge of the mound after one or two cluster atoms are incorporated into the edge. Our simulations reveal that there truly exists efficient upward mass transport in homoepitaxy on facetted fcc metal (110) surfaces.

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