Direct Measurement of the Ehrlich-Schwoebel Barrier and Herringbone Potential Energy Fluctuations via Three-Dimensional Atomic Force Microscopy

Bugrahan Guner[1], Mehmet Z. Baykara[2], and Omur E. Dagdeviren[1]*

[1] Department of Mechanical Engineering, École de technologie supérieure, University of Quebec, Montreal, QC, Canada, H3C 1K3
[2] Department of Mechanical Engineering, University of California Merced, Merced, CA, USA, 95343
* Presenting author's e-mail: omur.dagdeviren@etsmtl.ca

Thin film growth processes are governed by atomic-scale mechanisms that dictate material morphology, properties, and function. Among these, the Ehrlich–Schwoebel (ES) barrier plays a central role by impeding interlayer mass transport at step edges, yet no direct measurements of this energy barrier have been reported to date. Here, as Figure 1 shows, we present the first direct quantification of the ES barrier on monoatomic step edges of the Au(111) surface using three-dimensional atomic force microscopy (3D-AFM). By mapping tip-sample interaction forces in three dimensions with sub-nanometre resolution, we reconstruct the local potential energy landscape near step edges, revealing an energy barrier of ~150 meV at the upper edge and a corresponding potential well of ~200 meV at the lower edge. These measurements confirm the presence of asymmetric energetic features that hinder downhill diffusion and promote three-dimensional island growth, providing long-sought experimental validation of the ES mechanism. In addition to step-edge barriers, our measurements uncover how the Au (111) herringbone reconstruction modulates local chemical reactivity. We find enhanced interactions near elbow sites, attributed to undercoordinated surface atoms, and diminished interactions along ridges, consistent with overcoordination. This spatial heterogeneity in reactivity reflects subtle variations in atomic coordination imposed by the reconstruction, with implications for site-selective adsorption and catalysis.

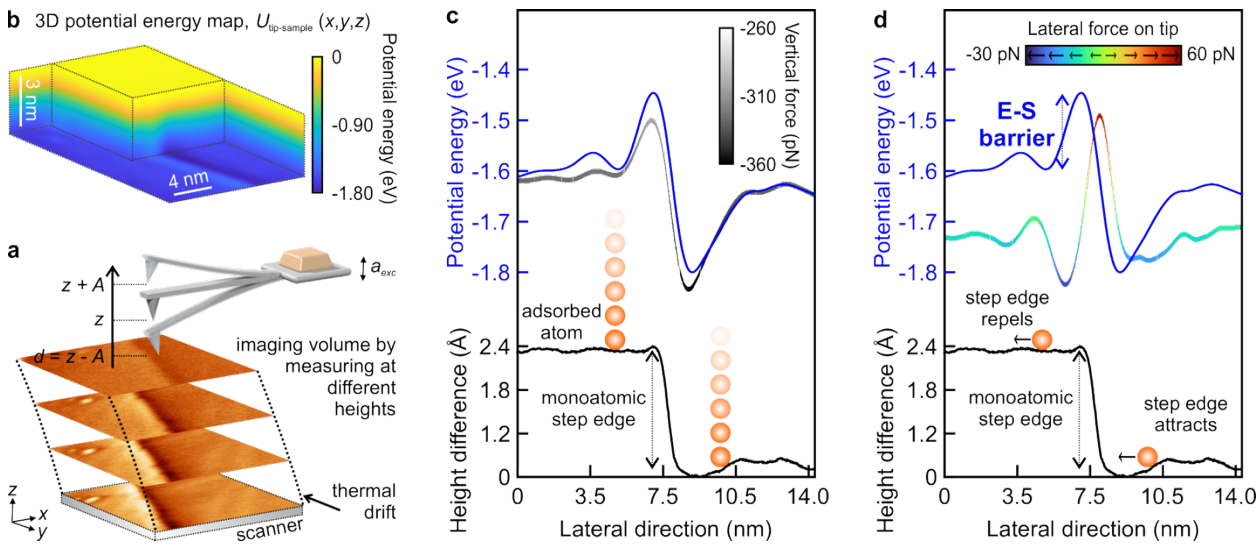

Figure 1. Three-dimensional mapping of tip–sample interaction energy and force. (a,b) Constant-height measurements at 41 z-positions enabled reconstruction of the $U_{tip–sample}$ (x, y, z) and corresponding force fields via spatial derivatives. (c,d) Vertical and lateral energy and force profiles across a step edge reveal site-specific interactions with adsorbates.