

Abstract Submitted
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First Principles Study of the Effect of Lattice Strain on Diffusion Barriers¹ HANDAN YILDIRIM, TALAT S. RAHMAN, University of Central Florida — To understand the three times larger values of the Erlich Schoewebel barriers for Ag on Cu(100) as compared to that for Cu on Ag(100) as obtained from our density functional theory calculations, we performed the diffusion of Ag adatom on Ag(100) and Cu adatom on Cu(100) under uniform lattice strain of 0-5%. We find the origin of the differences in the energetics to be the combination of Cu-Ag electronic coupling, relative atomic sizes and adsorbate-substrate lattice mismatch. The diffusion barriers on the ideal surfaces are found to decrease with increasing compressive strain and to increase with increasing tensile strain and almost a linear function of strain up to 5%. We show that this trend is universal and transferable to other metals. We will discuss the consequences of the modifications in the height of the ES barriers on growth modes.

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