

Abstract Submitted
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Strain-Induced Modification on Diffusion Barriers: An Ab-initio Study¹ HANDAN YILDIRIM, TALAT S. RAHMAN, University of Central Florida — While it is known that adatom diffusion barriers via hopping mechanism increase with increasing tensile and decrease with increasing compressive strain, we show that the extent of variation in the barriers is system specific. In particular, our DFT based calculations for the self-diffusion of Cu, Ag and Pd adatoms on strained (100) terraces and near step edges show that the variation for Pd on Pd(100) is much smaller than that for Ag on Ag(100) and Cu on Cu(100). Electronic structure analysis, particularly the shift in the d-band center, shows that the electronic structure of Pd is the most affected. Although this perturbation is expected to induce the highest deviation in the barriers for Pd, our analysis shows the opposite. This contradiction is traced to the dissimilarity in their elastic responses. We find that the elastic response to strain is the least for Pd. We compare the relative importance of strain induced changes in surface electronic structure and atomic relaxations in determining the changes in diffusion barriers.

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