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Lattice-Gas Modeling of Stiffness on fcc(111) Surfaces: General Results[1] T. L. EINSTEIN, T. J. STASEVICH, U. of Maryland, College Park — In a nearest-neighbor (NN) lattice-gas model of the island atoms on a (111) fcc surface,[2] the entropy of the leading term in the low-temperature expansion of the orientation-dependent free energyrelevant for understanding experiments on noble metals–comes exclusively from geometric considerations.[3] There are several remarkable consequences:[2] 1) The lowest-order stiffness (LOS) has no contribution from the energy. 2) Therefore, the step line tension cannot be extracted from the LOS. 3) The LOS has 6-fold symmetry, even though the line tension has only 3-fold symmetry. 4) The reduced LOS has the strikingly simple form $2\sqrt{3}/\sin(3\theta)$. Near close-packed orientations, the LOS is not adequate at these temperatures; by explicating the exact implicit solution for the hexagonal lattice gas,[4] we provide quantitative markers for where this breakdown occurs. Lastly, we show how to account for the energy difference between A and B steps by invoking a novel orientation-dependent trio interaction between atoms forming an equilateral triangle with NN legs.

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