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Structure, Vibrational Dynamics and Thermodynamics of silver thin-films on Cu(100) SAMUEL ROBERTS, JAMES WESTOVER, ABDELKADER KARA, University of Central Florida — We use a Real Space Green's function and the embedded atom method for interaction potentials, to examine the structural and vibrational properties of a silver thin-film (from one to four monolayers) on Cu(100). Due to the lattice mismatch, the first several layers of the substrate had major structural modification, in the form of buckling about 0.6A for the top two layers and 0.05A in the 6^{th} layer. For the case of a mono-layer, the vibrational densities of state of the silver atoms extend substantially beyond the maximum of the bulk density. The atoms in the first copper layer's density of state also show substantial enhancement of the high frequency end. These reflect the strong bonding between the monolayer and the substrate. The vibrational thermodynamic functions for these interface atoms will be presented

Abdelkader Kara
University of Central Florida

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