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Initial Stages of Nb Growth on Cu(100)

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Heteroepitaxial metal on metal systems have attracted attention by its characteristic structural, electronic, and magnetic properties. But essential prerequisite is the understanding of the initial growth mode for the determination of such properties. We have studied the initial growth mode of Nb on Cu(100) using Scanning Tunneling Microscopy(STM) and density functional theory(DFT). Cu is immiscible against Nb in bulk at room temperature, and the atomic radii differ from that of Nb by 15%. STM measurements are carried out at RT and 78 K under UHV. Initially deposited Nb atoms are immediately incorporated subsurface. Upon annealing, Nb substitutionally replaces the first layer Cu atom. They are preferentially found at step edges and appear as bright dots surrounded by dark rings. Ordering emerges from step edges as annealed. Ordered $(\sqrt{5}\times\sqrt{5})R26.6^{\circ}$ phase Nb structure is formed at θ <0.2 ML after annealing to 783K. At higher coverage, θ >0.25, annealing leads to $p(2\times2)$phase. Due to the large mismatch in lattice parameters, the domain size is limited to a few tens of nm^2. Possible physical mechanism responsible for such behavior, and drastic differences in their growth mode will be discussed.