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Initial Growth of Nb on Cu(100) studied by STM and Density Functional Theory

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Initial growth mode of Nb on Cu(100) is studied by scanning tunneling microscopy (STM) and density functional theory. Nb/Cu is immiscible at room temperature, but isolated Nb atoms are expected to be incorporated up to the second layer by DFT. STM shows that Nb atoms mix with Cu atoms in the first layer at room temperature and diffuse into the second layer upon annealing. In the second layer, Nb-induced features are preferentially found at step edges and appear as bright dots surrounded by dark rings. Details of comparison between experiment and theory will be discussed.