

Two dimensional copper sheet. Experimental observation and theoretical investigation.

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Abstract

The high interest to atomically thin films initiated by investigation of graphene has recently triggered for the study of two-dimensional materials with nonlayered bulk like boron [1], sodium chloride [2] or iron [3]. Among all these materials the latter one attracts special attention because the formation of 2D layered metal is unexpected and controversial. 2D layer with metals is very difficult to form because metallic bonding leads to form 3D structures.

Here we present the report of existence of novel two-dimensional phase of copper studied by experimental and theoretical methods. Using *in situ* scanning transmission electron microscopy (STEM) it was observed special crystal lattice of 2D Cu on graphene which structure is principally different from the former reports.

Density functional theory allowed to elucidate the nature of the stability of observed Cu nanofilms. It was defined a critical role of the oxygen impurity atoms in the formation of stable 2D Cu cluster with unexpected orthogonal crystal lattice. It was found that the structure and stability of 2D Cu clusters strongly depends on the concentration and relative arrangement of oxygen impurities. Number of oxygen configurations was analyzed and the stable configuration was found corresponded well with experimental data.

Additional to separated clusters, the periodic 2D Cu crystal with embedded oxygen atoms was studied in details. Relative stability, features of elastic, electronic and magnetic properties were investigated. First-principles calculations explained the origin of the 2D phase formation and confirms the experimentally observed structures.

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