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XANES study of copper nanoclusters grown on *p*-GaAs (100) by electrochemistry: refined analysis by MS calculations

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Full multiple-scattering (FMS) XANES calculations were performed to study the cluster structure investigating an early stage growth of copper clusters on *p*-GaAs(001) by electrochemical method [1]. Based on the structural parameters extracted from refined EXAFS analysis, realistic model structures of small Cu clusters were considered. The influence of the GaAs(001) substrate and the contribution of oxygen atoms with various geometric arrangements were also taken into account. A comparison of the FMS calculations with experiment shows that, in the early stage of electrochemical deposition, copper atoms predominantly form Cu dimers with some preferential orientation relative to the substrate and coordinated with O atoms [1]. Possible existence of Cu trimers and tetramers is excluded.

[1] K. Tamura *et al.*, J. Phys. Chem. B 2000, 9017-9024.
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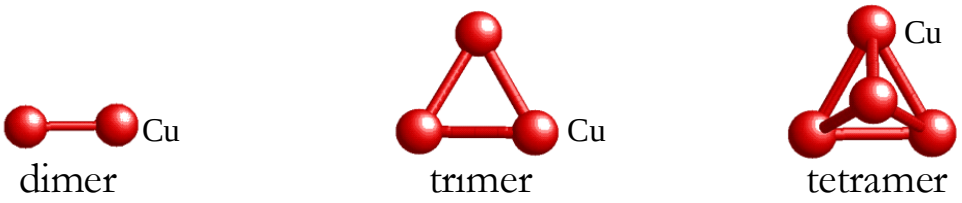

Figure 1: Schematic structure of dimer, trimer and tetramer.