

论文

铜的电化学腐蚀过程的红外光谱电化学及量子化学方法研究

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摘要:

设计了一种超薄层红外光谱电化学池,对铜电极的电化学腐蚀过程的现场监测表明,该电解池有较好的电化学性质和红外光谱响应性;铜电极在1.0 mol/L KCl溶液中的电化学腐蚀过程伴随铜的氯化物生成.以量子化学方法(ab initio 和arguslab)计算软件对形成的化合物及其红外光谱进行了理论计算.结果表明,在KCl支持电解质水溶液中,铜氧化生成的铜(I)离子易与氯离子形成较稳定的三配位化合物,并获得了与实验结果一致的红外光谱.

关键词: 红外光谱电化学 超薄层电解池 铜腐蚀 量子化学计算

STUDY ON ELECTROCHEMICAL CORROSION OF COPPER BY IR SPECTROELECTROCHEMISTRY AND QUANTUM CHEMISTRY METHODS

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Abstract:

An ultra-thin layer IR spectroelectrochemical cell was designed for in-situ monitoring the electrochemical corrosion of copper. The cell shows a very good electrochemical properties and response of IR spectroelectrochemical behavior. In 1.0 mol/L KCl aqueous solution, copper corrosion was accompanied with the formation of a series copper(I) chlorides. By means of quantum chemistry calculation (ab initio and arguslab), it has provided that among several copper chlorides, the one with three chlorides is the stable one. The calculated IR spectra are accord well with the experimental results.

Keywords: IR spectroelectrochemistry ultra-thin layer spectroelectrochemical cell corrosion of copper quantum chemical calculations

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