

Atomic-Scale Mechanisms of Mg Oxidation

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Magnesium (Mg) is the lightest structural metal with medium strength and remarkable friendliness to the environment including biocompatibility. Despite abundancy, Mg is one of the most critical materials for the EU, which contributes to many sustainable development goals. Its reactivity and susceptibility to degradation is well known for many years, and the bulk body of studies can be found in the literature. Nevertheless, fundamentals of physical processes around the interface of Mg alloys with gaseous and aqueous environments and oxide film formation at early stages is surprisingly scarcely studied. Main reasons for this stem from objective difficulties associated with high magnesium reactivity in normal atmospheric conditions.

In this talk, we focus on fundamental mechanisms of Mg oxidation at early stages. In the experimental part, high-resolution X-ray photoelectron spectroscopy (HR-XPS) in ultra-high vacuum conditions was used. It is a synchrotron-based surface sensitive technique, which reveals local chemical environments of near-surface atoms in a sample. Based on the analysis of energy shifts in the core-level electrons, it allows revealing surface states and the kinetics of oxide formation from the very first interaction of O₂ molecules with Mg surface. Nevertheless, HR-XPS cannot provide information on the geometric characteristics of Mg-O units.

Therefore, the experimental HR-XPS studies need to be complemented with theoretical density-functional theory (DFT) based simulations which we did using Quantum Espresso code. The DFT simulations enable unrevealing local structures of MgO units and their evolution into oxide layer. The theoretically feasible atomic configurations in the oxide units are then used for calculating energy shifts in the core-level electrons of respective surface atoms. These energy shifts are eventually compared to experimentally found values, and coherent mechanisms of Mg oxidation depending on the crystallographic orientation of surface are reconstructed.

As main results, we demonstrate that Mg reactivity and kinetics of oxidation strongly depend on the crystallographic orientation of surface, while some surfaces even reconstruct prior to oxidation.