178. Title: Experimental and ab initio study of vibrational modes of stressed alumina films formed by oxidation of aluminium alloys under different atmospheres

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Abstract: A comprehensive study of the alumina films formed from heating Fe3Al under different oxidizing atmospheres is conducted using Fourier transform IR spectroscopy in the complete mid-IR and far-IR ranges on the IR/THz synchrotron beamline of the SOLEIL facility. In addition, density functional theory is used to simulate alpha-alumina vibrational spectra for both bulk structure and thin slabs. The experimental absorbance spectra of films extend in a narrow energy range and present characteristic features similar to crystalline alpha-alumina (corundum structure). Moreover, the films spectra show a very good general agreement with the ab initio calculations for the alpha-alumina bulk structure. Nevertheless, in addition to transverse vibrations, extra modes, compared to the sapphire spectrum, can originate from either remnant transition alumina or from intense longitudinal-like modes present in the thin slab simulations. Furthermore, the dependence of film dynamical properties on oxygen and water partial pressures is addressed, and the strain induced by the film growth on the metal substrates is evaluated. This combination of simulated and measured absorbance spectra allows the precise determination of the crystalline nature of alumina thin films grown by oxidation under different atmospheres.