

Estimation of the degree of surface defectiveness of the $Ti_3C_2T_x$ films

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Two-dimensional (2D) nanomaterials with chemical and structural diversity have attracted research interest due to their unique photonic, mechanical, electrical, magnetic, and catalytic properties that distinguish them from bulk materials [1]. Among them, 2D titanium carbide with the following chemical formula $Ti_3C_2T_x$ (T can be O, OH, or F), known as MXene, is being intensively researched for various applications. The properties of MXene $Ti_3C_2T_x$ can vary depending on the synthesis methods. The work aims to compare the surface defects of MXenes $Ti_3C_2T_x$ obtained from Ti_3AlC_2 after an aggressive dissolution of aluminum in HF and a milder treatment in LiF/HCl [2]. A convenient method for monitoring the concentration of defects – carbon and titanium vacancies – is electron spin resonance (ESR) spectroscopy. In the MXene $Ti_3C_2T_x$ samples, spin-localized states related to the MXene $Ti_3C_2T_x$ surface were detected: carbon vacancies with a captured electron (V_C) and Ti^{3+} ions in coordination with the cation vacancy ($Ti^{3+}-V_{Ti}$). It is shown that a wide signal with $g_{iso} = 1.94-1.95$ from $Ti^{3+}-V_{Ti}$ centers can indicate the presence of titanium vacancies, and ESR spectroscopy can be a tool for assessing the defectiveness of the surface of MXenes $Ti_3C_2T_x$. The concentration of centers ($Ti^{3+}-V_{Ti}$) is an order of magnitude higher in the sample after treatment in HF than in LiF/HCl, which is experimental evidence of higher defectiveness and heterogeneity of the chemical composition and surface structure of MXenes $Ti_3C_2T_x$ obtained by treating Ti_3AlC_2 in an HF solution in comparison with LiF/HCl. For applying MXenes in various fields, controlling the concentration of surface vacancies in these materials is important. The presence of vacancies is an advantage of these materials when used in adsorption and photocatalysis, but vacancies are undesirable for use, for example, in optics. The ability to quantitatively monitor the concentration of titanium vacancies and carbon in MXenes $Ti_3C_2T_x$ using ESR spectroscopy is an important result of this study.

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