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PROCEEDINGS

Can Surface Structure Manipulate Mechanical and Thermal Properties of MXenes?

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ABSTRACT

As a novel type of transition metal-based 2D materials, the most popular MXene ($Ti_3C_2T_x$, where T is a surface termination, typically O, OH, and/or F) has been endowed amazing prospects in versatile fields, including energy storage, electromagnetic interference shielding, electronics and photon-detectors. At the same time, the inevitable oxidation structure observed in experiment also affect the property of MXene. With the help of the surface termination and surface oxidation, MXene showed diversity magnetic, electronic and optical behavior. However, our knowledge about the fundamental thermal and mechanical properties of MXene is limited, especially regarding the effect of surface structure on the mechanical and thermal properties. Without this knowledge, it is a big challenge to provide sophisticated design of the devices as well as evaluate the systematic risks. Atomistic simulation could contribute to this area by tracking the deformation and evolution of system. In this presentation, we will report the recent atomistic studies regarding the thermal and mechanical properties of MXene, with the emphasis on the effect of surface structure. It includes the following findings: 1) Surface oxidation modulates the interfacial and lateral thermal migration of MXene flakes in different ways: it boosts the interfacial thermal conduction, but suppress the lateral thermal dissipation. Our prediction is consistent with the experimental observation using ultrafast pump-probe technique which find two energy dissipation channels and these two channels are corresponding to the interfacial and lateral thermal dissipation path in the atomistic simulation. 2) the slight oxidation could not alter the fast energy migration from the MXene surface group to the binding water molecules due to the similar hydrogen bonds between water and interface. 3) The surface termination contributes to the mechanical properties. If the MXene terminated with oxygen atoms, it shows higher young's module comparing to the structure terminated with hydroxyl termination (OH). Besides the termination could also affect the maximum strength and the fracture path.

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