DREXEL UNIVERSITY
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Monday May 21st 10 am
Hill Conference Room

Nanoindentation of Monolayer $Ti_{n+1}C_nT_x$ MXenes via Atomistic Simulations

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Abstract

Since their discovery in 2011, MXenes, two-dimensional transition metal carbides and/or nitrides, have been explored for uses in a wide range of applications due to their unique properties and facile synthesis methods. Despite this attention, there is a relative lack of understanding with regards to their fundamental mechanical properties. Here, nanoindentation of the MXene system $Ti_{n+1}C_nT_x$ was studied via atomistic simulations utilizing a parametrization of the ReaxFF interatomic potential, to understand the influence of point defects. From force-displacement curves, the Young's moduli of pristine $Ti_3C_2O_2$ and Ti_2CO_2 were calculated to be 466 GPa and 983 GPa, respectively. The influences of both titanium and carbon vacancies on $Ti_3C_2O_2$ were also quantified using simulated nanoindentation of a set of samples containing both 1% V_{Ti} and 10% V_C, resulting in a reduction of the calculated Young's modulus to 386 ± 31 GPa. Of particular importance, is that these results are in good agreement with recent experimental findings indicating the important role defects play in determining the mechanical behavior of MXenes. The calculated Young's modulus in this work for the defect-containing $Ti_3C_2O_2$ surpasses that of graphene oxide establishing it as a new benchmark in strength for solution-processed, 2D materials. Results here also indicate improvements can be made in current MXene processing methods to better approach the theoretical strength of pristine 2D materials.