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Molecular Dynamics Study of the Mechanical Properties of the Grapheme-like Titanium Carbide Ti_2C

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Molecular dynamics simulations have been performed to study the mechanical properties of two-dimensional titanium carbide under tensile deformation. Young modulus was calculated from the linear part of strain-stress curve. From the radial distribution function it is found that the structure of the simulated samples is preserved during the deformation process. Calculated values of the elastic constants are in good agreement with the DFT data.

Keywords: Two-dimensional material, Titanium carbide, Strain-stress curve, Young modulus

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A new, large family of two-dimensional transition metal carbides and nitrides, known as MXenes has recently been discovered [1, 2]. Their unique properties suggest large area of potential applications [3, 4]. Since the discovery, MXenes are intensively studied by different methods and techniques [5-7] with computational studies making a large part of these efforts. Here we report the results of an atomistic simulation of the two-dimensional titanium carbide Ti_2C.

Atomistic simulations were carried out within classical molecular dynamic techniques. To describe the different types of bonding in the Ti_2C monolayer we use the embedded atom model (EAM) [8], Axilrod-Teller (AT) [9] and Lennard-Jones [10] potentials.

During the simulations potential energy of the particles, system temperature and the velocities were recorded. The system temperature was maintained at 300 K, using Berendsen thermostat [11].

Mechanical properties of the samples were studied under the tensile deformation with different strain rates. Strain was applied to the Ti_2C monolayer by pulling one edge of the sheet while the opposite edge was fixed. Tension was applied to the system up to the destruction of the samples. To detect the changes in the Ti_2C structure the radial distribution functions (RDF) were calculated.

In the process of tensile load the overall stress in the material was calculated by the virial theorem [12], and the strain-stress curves were obtained.

Obtained strain-stress curves have a similar form with a linear region, related to elastic deformation. At a higher strain, stress continues to increase up to the threshold point of a yield stress, followed by a sharp drop related to the sample destruction. Tensile deformation was applied to the system at different strain rates. All the strain-stress curves demonstrate the linear region of elastic deformation, with the slope being independent from the strain rate.

The Young's modulus values were obtained from the strain-stress curves with the strain $\varepsilon < 0.01\%$ by linear regression with the average value $E = 597 \pm 55 GPa$. These results are in good agreement with the DFT calculations [5].

Our simulations have shown that the classical molecular dynamics approach correctly describes mechanical behavior of the two-dimensional titanium carbide and may be used in further investigations of the structural and mechanical properties of the MXenes terminated by oxygen containing functional groups produced experimentally.

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