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Simulation of Fracture Dynamics of Two-dimensional Titanium Carbide Ti_2C under Different Types of Tensile Loading

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Paper presents the results of the in-silico experiments concerning simulation of the tension and failure dynamics of two-dimensional (2D) titanium carbide Ti_2C under different types of tensile loading. The behavior of 2D nanosheet was studied within classical molecular dynamics (MD) methods. Two different loading methods, namely axial displacement and uniform tensile strain were considered in experiments. The first loading method consists in a consecutive shift of atoms in the right edge of the sample along the *x*-axis while atoms in the left edge of the sample are held fixed. The uniform tensile strain was performed by shifting left and right parts of the sample in opposite directions. During the simulations, atomistic configurations of the 2D Ti_2C nanosheet at different strain values were built for both loading methods. As it follows from the obtained data, different loading procedures lead to different fracture dynamics and crack formation in the studied sample. As calculated atomistic configurations show, in the case of axial displacement the fracture begins from the formation of cracks at the lateral edges of the sample. Cracks appear along the layers of constrained atoms at both fixed and shifted edges of the nanosheet, while at uniform tensile strain Ti_2C sample undergoes uniform stretching up to the critical strain where the crack starts to form. The strain-stress curves for both axial displacement and homogenous strain were calculated through the virial theorem. Strain-stress dependencies obtained for different loading procedures for Ti_2C sample overlap in the area of elastic deformation. Calculated data also show that plastic deformation and following destruction of the Ti_2C sample occur at strain $\varepsilon > 0.04$ for both methods of loading.

Keywords: Two-dimensional material, Molecular dynamics, Simulation, Fracture, Strain.

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1. INTRODUCTION

Two-dimensional (2D) materials attract much attention of many scientists nowadays. Among the mentioned materials is 2D titanium carbide Ti_2C –- one of the so-called MXenes. MXenes are novel nanomaterials with general chemical formula $M_{(n+1)}X_{(n)}$ where M represents the transition metal, and X can be either carbon or nitrogen [1]. Due to their unique structure, 2D MXenes have promising electrochemical properties and thus a wide area of potential applications, such as Li-ion batteries, supercapacitors, hydrogen storage and other [2-6]. Besides this, due to excellent physical properties and sheet-like structure they can be used as resonators in various nanoelectronic devices similarly to other 2D materials [7-9]. Ti_2C has a thickness of three atomic layers and hexagonal structure [1] where the plane of carbon atoms separates two planes of titanium as it is shown in Fig. 1.

Other distinguishing features of the MXenes are excellent mechanical properties, namely relatively high Young modulus [1]. However, information concerning mechanical properties of 2D carbides was mainly obtained by computational methods, as the experimental study of mechanical properties of nanomaterials is a very complicated task (see, for example, [10]). In the proposed paper, we report the results of the investigation of the failure dynamics of 2D titanium carbide Ti_2C within classical molecular dynamics (MD) methods. In this study, we aim to investigate the cracks formation and failure of the sample under two different loading procedures.

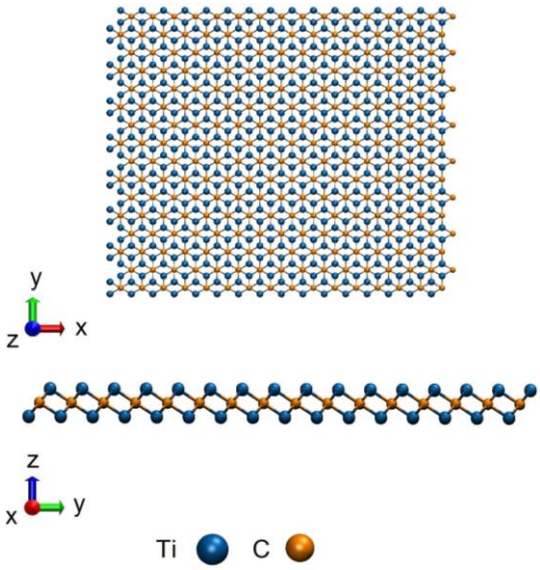

Fig. 1 – Atomic structure of 2D Ti_2C

It is worth to mention that elastic properties of 2D titanium carbides were studied by MD simulation for the first time in [11]. However, in [11], a single type of tensile load was used, and the study was focused on elastic properties and failure dynamics of three different samples $Ti_{n+1}C_n$ with $n = 1, 2, 3$. Also, a preliminary study of the deformation of Ti_2C under uniform tension was reported in [12]. In this paper, we report the failure dynamics of 2D Ti_2C under two different methods of tensile loading and compare the fracture evolution. Also, in this

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study, we compare the strain-stress curves obtained for both tensile methods and estimated values of critical strain and yield stress.

2. SIMULATION SETUP

Tension and failure dynamics of 2D Ti_2C was studied on a sample with lateral sizes equal to 38×33 nm that was placed in the Cartesian coordinate system as it is shown in Fig. 1. Visual Molecular Dynamics software (VMD) [13] was used to build the atomistic configurations of the studied system. Interactions between atoms in the studied sample were calculated with the use of previously developed computer code for parallel computing [11]. Full description of the MD model of Ti_2C sample and simulation scheme are given in [11, 12], here we will only refer the interatomic potentials for MD simulations that were used in the model. To describe the metallic type of chemical bonding between titanium atoms the embedded atom method (EAM) [14] was used. Interactions between carbon and titanium atoms were described by combination of Lennard-Jones and Axilrod-Teller potentials as in [15]. System temperature was maintained at 300 K by the Berendsen thermostat [16].

3. RESULTS

Tensile loading of 2D materials in MD simulations can be implemented in several ways (see, for example, [17, 18]). In this work, we consider two different ways of stretching of the material (Fig. 2). First, we implement an axial displacement loading method that was applied to 2D graphene nanoribbons [17]. To implement mentioned procedure, Ti and C atoms in the first five layers of the left edge of the sample were held fixed during the simulation, while the first five atomic layers in the opposite part of the sample were constantly shifted in the x-direction. The displacement magnitude was set to provide a constant strain rate of 0.4 ns^{-1}. Schematic of the axial displacement tensile loading is shown in Fig. 2.

Obtained atomic configurations of the Ti_2C sample under axial displacement loading are shown in Fig. 3 and Fig. 4.

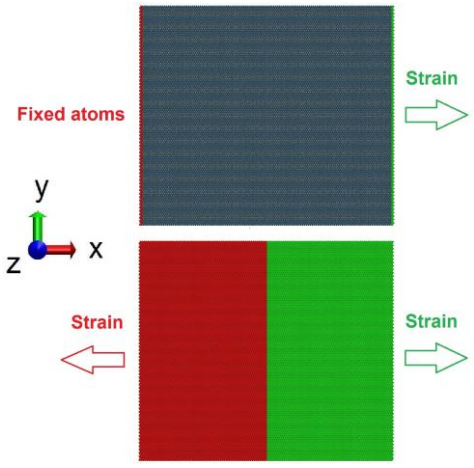

Fig. 2 – Schematics of the Ti_2C sample under axial displacement procedure of tensile loading (top panel) and uniform tensile strain (bottom panel)

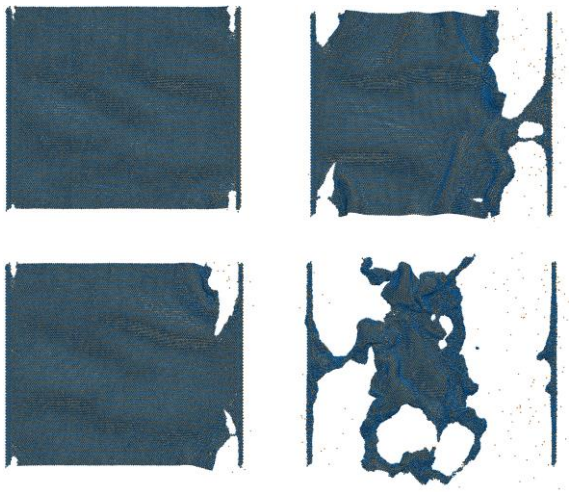

Fig. 3 – Fracture dynamics of the Ti_2C sample under axial displacement procedure of tensile loading (top view) at a strain of 0.025 (top left), 0.05 (bottom left), 0.06 (top right) and complete destruction of the sample at a strain of 0.1 (bottom right)

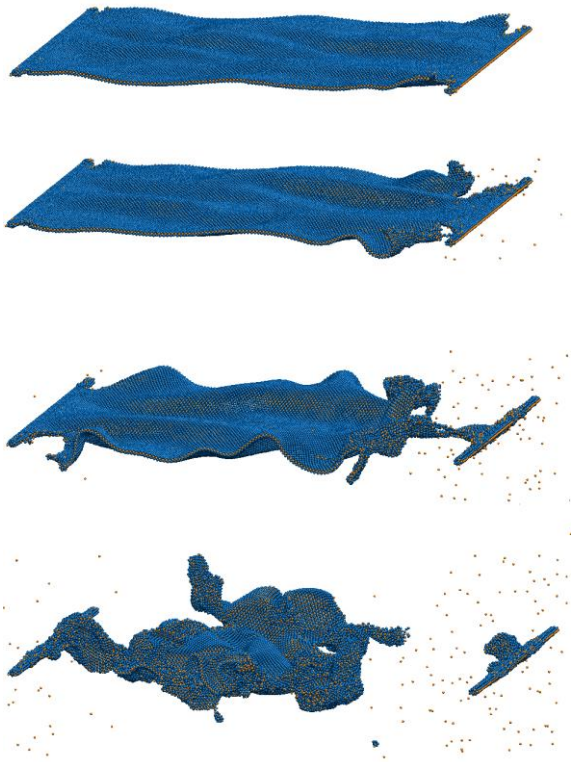

Fig. 4 – Fracture dynamics of the Ti_2C sample under axial displacement procedure of tensile loading (side view) at the same strain values as in Fig. 4 (from top to bottom)

As can be seen from the figures, the fracture begins from the formation of cracks at the lateral edges of the sample. Cracks appear along the layers of fixed atoms at both fixed and shifted edges of the nanosheet. At larger strain, cracks in the stretched area of the sample grow in sizes and propagate along the shifted layers of atoms. At the same time, free edges of the fractured parts of the sample are folding with the formation of additional cracks in the central area of the nanosheet.

As the strain increases, similar fracture mechanism is observed in the opposite edge of the sample, along the

layers of fixed atoms. As a result, at strain higher than 0.1, Ti_2C sample becomes completely separated from the edges with fixed atoms and loses its 2D sheet-like form. Thus, axial displacement loading method leads to complete fracture of the central part of Ti_2C sample from its edges with following folding and fracturing.

An alternative way of tensile loading of the sample in MD simulation is uniform tensile strain that is applied by displacement of the atoms located in the opposite parts of the Ti_2C sample in $+x$ and $-x$ directions, respectively (see bottom panel in Fig. 2). This procedure was also applied to the Ti_2C sample under investigation with the same strain rate as in the previous case of axial displacement.

Atomistic configurations of the studied sample that show the cracks formation are illustrated in Fig. 5 (top view) and Fig. 6 (side view).

At this type of tension, the sample undergoes uniform stretching up to the critical value of deformation where the crack starts to form. As the strain grows, small cracks occur in the center of the sample along the border between two parts shifted in opposite directions. At higher strain, formed cracks aggregate into bigger fractures which lead to a complete destruction of the sample.

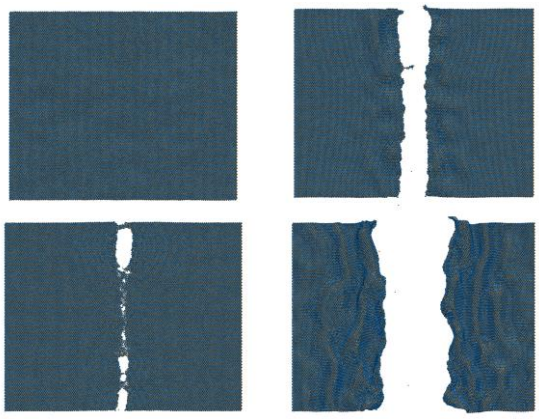

Fig. 5 – Fracture dynamics of the Ti_2C sample under uniform tensile strain (top view)

At both methods of tensile loading mechanical stresses in the sample were calculated through the virial theorem [19, 20] as:

$$\sigma_{ij} = \frac{1}{V}\sum_{\alpha=1}^{N}\left(\frac{1}{2}\sum_{\beta=1}^{N} r_{\alpha\beta}^{i} f_{\alpha\beta}^{j} - m^{\alpha} v_{i}^{\alpha} v_{j}^{\alpha}\right), \qquad (1)$$

where α and β are the indices of the atoms separated by distance $r_{\alpha\beta}^{i}$ and the force $f_{\alpha\beta}^{j}$ between them, i, j are the components of Cartesian coordinates, m is the mass of the atom, and V is a volume of the sample.

The strain-stress curves for both axial displacement and homogenous strain computed via equation (1) are presented in Fig. 7.

As can be seen from the figure, the strain-stress curves obtained from different loading methods overlap in the area of elastic strain. Both methods give close values of failure strain. At the same time, yield stress estimated from simulation with homogeneous strain loading method has higher magnitude, most likely due to the larger number of atoms involved in tensile strain. At the strain $\varepsilon \approx 0.07$ both obtained dependencies start to decrease very fast due to the progressive destructions of the sample.

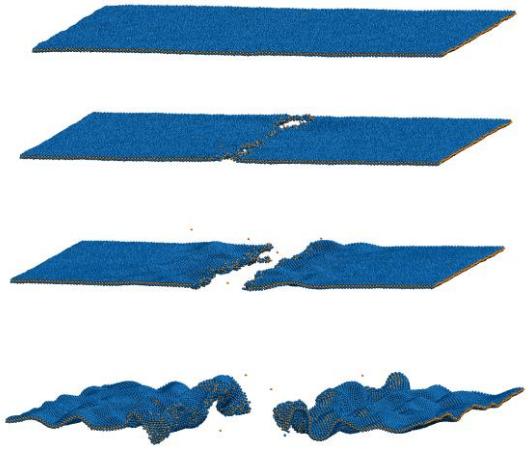

Fig. 6 – Fracture dynamics of the Ti_2C sample under uniform tensile strain (side view)

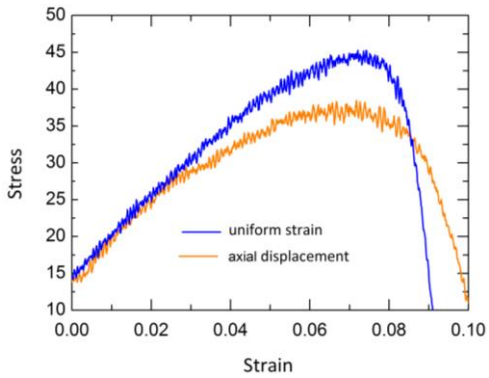

Fig. 7 – Obtained strain-stress dependencies of the studied Ti_2C sample for uniform tensile strain and axial displacement

4. CONCLUSIONS

The behavior of the 2D Ti_2C sample under tensile deformation by two different methods of tensile loading was investigated by classical MD simulations. Atomic configurations of the studied sample at both stretching procedures were calculated at different strains to track the differences in failure dynamics. Calculated atomic configurations and strain-stress curves suggest that plastic deformation and following destruction of the Ti_2C nanosheet under investigation occur at strain $\varepsilon > 0.04$ for both methods of loading. At the same time, different loading methods lead to different cracks evolution and failure dynamics.

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Моделювання динаміки руйнування двовимірного карбіду титану Ti_2C при різних типах навантаження розтягу

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У роботі представлені результати комп'ютерного моделювання динаміки розтягнення та руйнування двовимірного (2D) карбіду титану Ti_2C при різних процедурах навантаження розтягу. Поведінку зразка було досліджено в рамках методів класичної молекулярної динаміки (МД). В експериментах було розглянуто два різні способи навантаження, а саме осьове зміщення та рівномірне розтягування. Перший спосіб завантаження полягає в послідовному зміщенні атомів, що знаходяться у правому краї зразка вздовж осі x, за умови що атоми в лівому краї тримаються нерухомими. Рівномірний розтяг було реалізовано шляхом поступового зміщення лівої та правої частин зразка в протилежних напрямках. Під час моделювання були побудовані атомістичні конфігурації двовимірного зразка Ti_2C при різних значеннях деформації для обох методів навантаження. Як випливає з отриманих даних, різні процедури навантаження призводять до різної динаміки руйнування та утворення тріщин у досліднoму зразку. Обчислені атомістичні конфігурації показують, що у разі осьового зміщення руйнування починається з утворення тріщин на бічних краях зразка. Тріщини з'являються вздовж шарів нерухомих атомів як на фіксованому краю, так і на краю, що зміщується. В той час як при рівномірному навантаженні двовимірний зразок Ti_2C зазнає рівномірного розтягування до критичного значення деформації, коли починає утворюватися тріщина. Криві навантаження для осьового зміщення та рівномірного розтягування були обчислені за допомогою теореми віріалу. Залежності напружень від деформацій, отримані для різних процедур навантаження зразка, перекриваються в області пружної деформації. Обчислені дані також показують, що пластична деформація та наступні руйнування двовимірного зразка Ti_2C відбуваються при деформації $\varepsilon > 0.04$ для обох методів навантаження.

Ключові слова: Двовимірний матеріал, Молекулярна динаміка, Моделювання, Руйнування, Деформація.