ELASTIC PROPERTIES OF 1T-MX_2 TWO-DIMENSIONAL TRANSITION METAL DICHALCOGENIDES

ĐẶC TRƯNG ĐÀN HỒI CỦA CÁC TẤM VẬT LIỆU HAI CHIỀU DẠNG 1T-MX_2 (TRANSITION METAL DICHALCOGENIDES)

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ABSTRACT

This work studies elastic properties of 53 transition metal dichalcogenides 1T-MX_2 sheets using molecular dynamics finite element method with valence force field potential. Beside pristine structure, missing atom defects sheets are investigated. It is found that Young's modulus, shear modulus, and Poisson's ratio of 1T-MX_2 square shaped sheets saw an increase as its dimension increase. However, the figures nearly remain unchanged with the square sheets being larger than 160 × 160 Å. The results also show that the Young's modulus and Poisson's ratio of 1T-MX_2 square sheets are nearly isotropic in the zigzag and armchair direction. NiO_2 sheet possess the highest Young's modulus of 165.5 N/m while $TcTe_2$ have the lowest one of 29.2 N/m in the armchair direction. With missing atom defective sheets, the Young's modulus and shear modulus reduce by 26.2% and 47.4%, respectively, as percentage of defect incline to 10%. Our findings are good information for application of 1T-MX_2 in future.

Keywords: *Elastic properties; Nanomaterials; Transition metal dichalcogenides; Atomic finite element method.*

TÓM TẮT

Nghiên cứu này tính toán đặc trưng đàn hồi của 53 tấm vật liệu 1T-MX_2 (transition metal dichalcogenides) sử dụng phương pháp phần tử hữu hạn nguyên tử với hàm thế valence force field. Bên cạnh tấm nguyên thể, các tấm khuyết tật mất nguyên tử cũng được khảo sát. Kết quả chỉ ra rằng mô-đun đàn hồi, mô-đun trượt và hệ số Poisson của các tấm vuông 1T-MX_2 tăng khi kích thước tấm tăng. Tuy nhiên, các giá trị gần như không đổi khi kích thước tấm lớn hơn 160 × 160 Å. Kết quả cũng cho thấy, mô-đun đàn hồi và hệ số Poisson của các tấm vuông 1T-MX_2 xấp xỉ nhau theo cả hai phương zigzag và armchair. Mô-đun đàn hồi của tấm NiO_2 cao nhất với giá trị 165,5 N/m, trong khi đó tấm $TcTe_2$ thấp nhất với 29,2 N/m theo phương armchair. Ở tấm khuyết tật mất 10% nguyên tử ở trung tâm tấm, mô-đun đàn hồi và mô-đun trượt của tấm khuyết tật khi đó giảm 26,2% và 47,4% tương ứng. Những kết quả từ nghiên cứu này sẽ là thông tin hữu ích trong các ứng dụng của vật liệu 1T-MX_2 trong tương lai.

Từ khóa: *Đặc trưng đàn hồi; Vật liệu nano; Transition metal dichalcogenides; Phương pháp phần tử hữu hạn nguyên tử.*

1. INTRODUCTION

Two-dimensional (2D) materials such as graphene and transition metal dichalcogenides become an appealing topic because of their excellent characteristic and great potential applications. Graphene was the first developed 2D materials which are broadly used in range of applications from mechanics to electronics. However, having no bandgap, graphene's applications as a semiconductor are limited [1-4]. Transition metal dichalcogenides have proven to process a finite bandgap with 1-2eV [5] while maintaining the other interesting characteristics of 2D materials [6]. Two-dimensional transition metal dichalcogenides, MX_2, have been prepared by many methods such as electrochemical Li-intercalation and exfoliation, and chemical vapor deposition. They are made of planes of covalently bonded chalcogen X and metal M atoms. MX_2 monolayer has two types of structure, 1T-MX_2 and 1H-MX_2 [6]. Possessing unique optical properties and high specific surface area, MX_2 nanosheets are popularly used in biomedical applications [7, 8]. Studying elastic mechanical properties of MX_2 monolayers is necessary to their applications. Cooper et al. [9] used nano indentation in an atomic force microscopy to predict the in-plane Young's modulus of 1H-MoS_2 at 120 ± 30 N/m which was lower than 180 ± 60 N/m by Bertolazzi [10]. Generally, it is not easy to study mechanical properties of nanomaterials by the conventional experimental methods. Besides experimental works, mechanical properties of MX_2 was calculated by molecular dynamics [11], ab initio calculations (for some 1H-MX_2) [12, 13]. Recently, we have investigated elastic properties of 34 1H-MX_2 by using molecular dynamics finite element method (MDFEM) [14]. While shear modulus of 1T-MX_2 remain unexplored. In addition, influence of defects on elastic properties of most of 1T-MX_2 are not clearly explored.

In this study, we will investigate elastic properties of 53 1T-MX_2 (M = Sc, Ti, V, Mn, Co, Ni, Zr, Nb, Mo, Tc, Rh, Pd, Sn, Hf, Ta, W, Re, Ir, Pt; X = O, S, Se, Te) sheets using MDFEM. Effects of size and missing-atom defects on Young's modulus, Poisson's ratio, and shear modulus of 53 1T-MX_2 sheets are estimated and discussed.

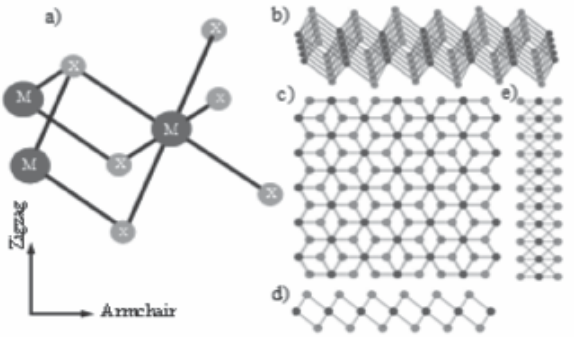

Figure 1. Atomic structure of 1T-MX_2 sheet: a) zoom in of the nine nearest atoms; b) 3D view; c) top view; d) front view; e) side view of the sheet. Blue and magenta balls represent the M and X atoms, respectively.

2. MODEL AND NUMERICAL METHOD

Figure 1 shows the puckered configuration of 1T-MX_2 sheet. Each metal M atom is surrounded by six chalcogen X atoms, which are divided into the top and bottom groups. The initial bond length between neighboring M and X atoms is l_0 and the initial angles (M-X-M) and (X-M-X) are the same angle of θ_0 which are taken from Ref. [11], These geometric parameters are used to establish the pristine structure of 1T-MX_2 sheets. The number of atoms on circular areas at center of the sheet are removed to create defected sheets (see Fig. 5).

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The valence force field (VFF) model is the fastest numerical simulation to study linear phenomena. Therefore, it is used to simulate the atomic interactions in the 1T-MX_2 sheets in this work. In VFF potential, the energy variations for the bond stretching and the angle bending are described by quadratic forms:

$$E_b = \frac{1}{2}C_b.\left(\delta l_{ij}\right)^2, E_a = \frac{1}{2}C_a.\left(\delta\theta_{ijk}\right)^2 \quad (1)$$

Where C_b and C_a are two force constant parameters corresponding to the bond-stretching and the angle-bending, respectively (Fig. 2). The bond stretching describes the energy variation for a bond due to a bond variation δl_{ij}. The angle bending gives the energy variation for an angle resulting from an angle variation $\delta\theta_{ijk}$. The VFF potential parameters of 53 1T-MX_2 sheets are taken from Ref. [11].

Molecular dynamic finite element method, which was used to successfully investigate the mechanical properties of various hexagonal sheets in our previous works [14-16], is here adopted to study the elastic properties of the 1T-MX_2 sheets. Further detailed numerical procedure of MDFEM and VFF potential is available in our previous works [14, 15].

Uniaxial tension and pure shear experiments are conducted to calculate Young's modulus Y, Poisson's ratio, and shear modulus G. Yt and Gt denoting 2D Young's modulus and 2D shear modulus, respectively (t is the sheet's thickness) will be used in this work.

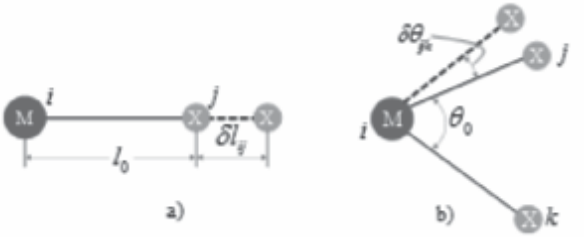
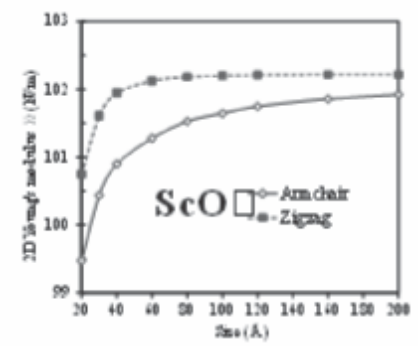


Figure 2. Two types of elements in VFF potential: a) Two-body (bond-stretching) element and b) Three-body (angle-bending) element.

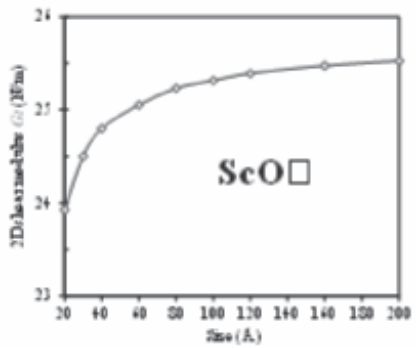
3. RESULTS AND DISCUSSION

To begin, the square shaped 1T-ScO_2 sheet with size between 20 × 20 Å and 200 × 200 Å are chosen to investigate size effect on its elastic properties. The size effect on Young's modulus, shear modulus, and Poisson's ratio of 1T-ScO_2 sheet is shown in Fig. 3. It can be seen that 2D Young's modulus of 1T-ScO_2 sheet in both zigzag and armchair direction increases when its size increases with the former are always higher than the latter. With size of square sheet being lager than 160 Å, the figure nearly remains unchanged at 102.2 N/m in the zigzag direction and 101.9 N/m in the armchair direction. Therefore, we can say that 2D Young's modulus of 1T-ScO_2 sheet is isotropic in the armchair and zigzag direction. The similar pattern can be seen in 2D shear modulus of 1T-ScO_2 sheet with an incline from 23.9 to 25.5 N/m as size of sheet increase from 20 Å to 200 Å. In similar way, Poisson's ratio of 1T-ScO_2 sheet nearly plateau at 0.141 and 0.146 in zigzag and armchair direction, respectively, when the size is larger than 160 Å. These results well agree with that come from molecular dynamics [11]. Form above results, 52 remain sheets with dimension of 160 × 160 Å are established to estimate their elastic properties. Like 1T-ScO_2, Young's modulus and Poisson's ratio of 1T-MX_2 sheets are isotopic in armchair and zigzag direction so the ☞

results in the armchair direction were chosen to show in Fig. 4. Our results agree well with those from molecular dynamics [11] and first-principle calculations [17].



(a)



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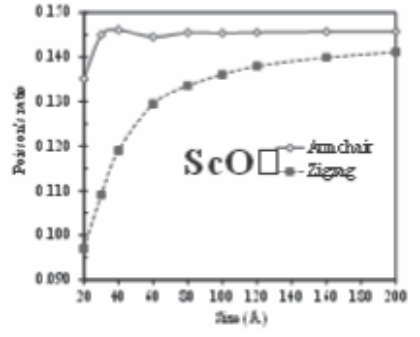

(c)

Figure 3. Size effects on (a) Young's modulus; (b) shear modulus and (c) Poisson's ratio of square shaped 1T-ScO_2 sheet.

Figure 4a shows that 2D Young's modulus of NiO_2 sheet is the highest with the figure of 165.5 N/m while that of $TcTe_2$ sheet is the lowest with the figure of 29.2 N/m. Poisson's ratio shown in Fig. 4c with some value being negative which was explained in Ref. [17] . Through modeling pure shear test, this is the first time 2D shear modulus of 53 1T-MX_2 sheets has been estimated and given in Fig. 4b.

To investigate the influence of missing atom defect on elastic properties of 1T-MX_2, once again, ScO_2 sheet is chosen. Atoms in circular area at center of the sheet are removed to form defective sheet. Rate of missing atom are taken from 1% to 10%. Results are shown in Fig. 5. The 2D Young's modulus and shear modulus of ScO_2 sheet significantly decrease when proportion of missing atom increases. The 2D Young's modulus see a decrease by 26.2% (from 101.9 to 75.1 N/m) while the 2D shear modulus decline by 47.4% (from 25.5 to 13.4 N/m). The trendline of both Young's modulus and shear modulus is nearly linear with a constant negative slope of 265 N/m and 119 N/m, respectively.

4. CONCLUSIONS

The elastic properties of 53 two-dimensional 1T-MX_2 sheets have been investigated by using MDFEM with VFF potential. Our results show that NiO_2 is the hardest 1T-MX_2 sheet while $TcTe_2$ is the softest one. The Young's modulus is isotropic in zigzag and armchair direction and increases by 2.5% while the shear modulus increases by 6.7 % as the size of square sheet increase from 20 × 20 Å and 200 × 200 Å. For defective sheet, it is found that the Young's modulus and shear modulus linearly reduced by 26.2% and 47.4%, respectively, when proportion of missing atom increase to 10%.

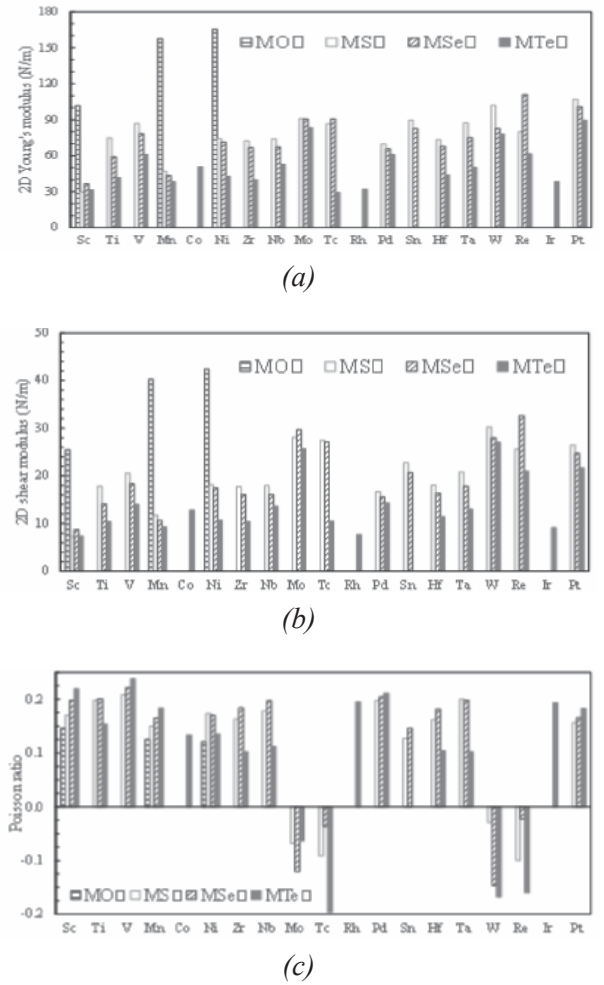

Figure 4. Elastic properties: (a) Young's modulus; (b) shear modulus; and (c) Poisson's ratio of 53 square shaped 1T-MX_2 sheets.

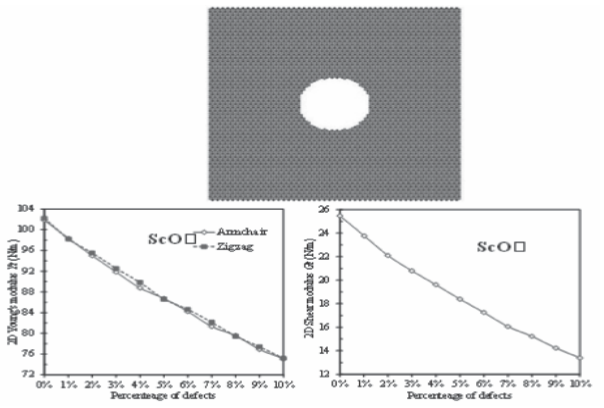

Figure 5. Snapshot of a missing atom defective 1T-MX_2 sheet and changes of Young's modulus and shear modulus with changing percentage of defects.

References:

[1]. Singh, S., et al., "*Graphene nanomaterials: The wondering material from synthesis to applications*". Sensors International: p. 100190 (2022).

[2]. Radisavljevic, B., et al., "*Single-layer MoS2 transistors*". Nature Nanotechnology. 6(3): p. 147-150 (2011).

[3]. Lopez-Sanchez, O., et al., "*Ultrasensitive photodetectors based on monolayer MoS2*". Nature Nanotechnology. 8(7): p. 497-501 (2013).

[4]. Mak, K.F., et al., "*Atomically Thin MoS2: A New Direct-Gap Semiconductor*". Physical Review Letters. 105(13): p. 136805 (2010).

[5]. Huo, N., Y. Yang, and J. Li, "*Optoelectronics based on 2D TMDs and heterostructures*". Journal of Semiconductors. 38(3): p. 031002 (2017).

[6]. Huang, X., Z. Zeng, and H. Zhang, "*Metal dichalcogenide nanosheets: preparation, properties and applications*". Chemical Society Reviews. 42(5): p. 1934-1946 (2013).

[7]. Liu, T., et al., "*Drug Delivery with PEGylated MoS2 Nano-sheets for Combined Photothermal and Chemotherapy of Cancer*". Advanced Materials (Deerfield Beach, Fla.), 26(21): p. 3433-3440 (2014).

[8]. Yin, W., et al., "*High-Throughput Synthesis of Single-Layer MoS2 Nanosheets as a Near-Infrared Photothermal-Triggered Drug Delivery for Effective Cancer Therapy*". ACS Nano. 8(7): p. 6922-6933 (2014).

[9]. Cooper, R.C., et al., "*Nonlinear elastic behavior of two-dimensional molybdenum disulfide*". Physical Review B. 87(3): p. 035423 (2013).

[10]. Bertolazzi, S., J. Brivio, and A. Kis, "*Stretching and Breaking of Ultrathin MoS2*". ACS Nano. 5(12): p. 9703-9709 (2011).

[11]. Jiang, J.-W. and Y.-P.J.a.p.a. Zhou, "Parameterization of Stillinger-Weber potential for two-dimensional atomic crystals" (2017).

[12]. Çakır, D., F.M. Peeters, and C.J.A.P.L. Sevik, "*Mechanical and thermal properties of h-MX2 (M= Cr, Mo, W; X= O, S, Se, Te) monolayers: A comparative study*". 104(20): p. 203110 (2014).

[13]. Alyörük, M.M., et al., "*Promising piezoelectric performance of single layer transition-metal dichalcogenides and dioxides*". 119(40): p. 23231-23237 (2015).

[14]. Nguyen, D.-T., "*Elastic Mechanical Properties of Transition Metal Dichalcogenides Monolayer Using Atomic Finite Element Method*". In The AUN/SEED-Net Joint Regional Conference in Transportation, Energy, and Mechanical Manufacturing Engineering. 2022. Singapore: Springer Nature Singapore.

[15]. Le, M.-Q. and D.-T. Nguyen, "*Atomistic simulations of pristine and defective hexagonal BN and SiC sheets under uniaxial tension*". Materials Science and Engineering: A. 615: p. 481-488 (2014).

[16]. Nguyen, D.-T., et al., "*Effects of various defects on the mechanical properties of black phosphorene*". Superlattices and Microstructures. 112: p. 186-199 (2017).

[17]. Ruzsinszky, L.Y.a.Q.Y.a.A., "*Negative Poisson's ratio in 1T-type crystalline two-dimensional transition metal dichalcogenides*". Nature Communications. 8 (2017).