

Multicomponent TMD Phase-field model with elastic heterogeneity

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Abstract

A generalized semi 2D-model for the structural transformations under mechanical strains of multi-components transition metal dichalcogenide (TMD) monolayers were manipulated. In this model, not only the chemical and structural but also elastic heterogeneity, through the eigen strain method, were introduced. Basing on this model, some experimental observation can be simulated and understood better. Some qualitatively pre-results related to these phase transformations were obtained by this model, some of them are interesting and still need further study.

1 Introduction

Transition metal dichalcogenide (TMD) monolayers, as two-dimensional materials, have a wide variety of interesting physical and electronic properties [1–4]. Structural transformations can occur in TMD with appropriate mechanical strain. These transformations lead to large or qualitative changes in electronic transport properties [5–7]. If we can precisely control these transformations of these 2D materials, they will be able to be used to develop some new technologies such as ultrathin, flexible, nanoelectronic and optoelectronic devices [8–10]. One way to realize this is using strain engineering. Recent first-principles and experimental work suggest that it is possible for Group VI TMDs to exploit rapidly and possibly reversibly, switch between crystal structures with largely different transport properties through strain induced structural transformations. As examples, the first-principles [11] results indicate that the 2H to 1T' phase transformation can be expected under 1-2% of uniaxial strains for MoTe₂ and experiments [12] also demonstrate a room temperature semiconductor-metal transition under a tensile strain of 0.2% for MoTe₂ thin film at room temperature. This approach holds promise for the creation of heterostructures in which crystal structure is controllably varied within a single monolayer or across multiple layers.

In this work, we focused on simulating the transformations in bendable 2D layers of multi-component Group VI TMDs between semiconducting 2H and metallic/semimetallic 1T' phases. Because we are interested in direct view of microstructural morphologies, mechanical response, and instances of localized transformation behavior in the mesoscale, we employed the diffuse-interface phase-field microelasticity (PFM) model [13–16]. Diffuse-interface here means we do not treat the interfaces as infinitely thin, or sharp, regions but use continuous variation of order parameters to

represent them. Basing on the quantitative results from both DFT calculations and experimental observations [17], the PFM quasi-2D model for multi-component TMD monolayers was built. In this model, for different chemical components, not only various chemical potential and misfit strain introduced from the phase transformations but also different elastic moduli were used, which gave not only chemical and structural but also elastic heterogeneity. With the help of this model, it is possible to study the phase transformations in TMD monolayers under strain engineering with lots of different conditions. For examples, macroscopic strains, indenter morphology and substrate attraction with different prefix chemical components are all interesting conditions that may related to controlling phase transformations of TMD monolayers.

2 Diffuse-Interface Model

In this model, we use the diffuse-interface phase-field model, which treat different phases with continuously changing variables. Order parameter $\phi(\vec{r})$ was assumed to describe two different chemical components. $\phi(\vec{r})$ equals 0 for component 1 and 1 for component 2. If more kinds of chemical components are needed (which is required when we want to introduce the free boundary as the third chemical components), other order parameters can be introduced to represent the extra chemical components.

Within the same chemical component, the phase transformation from 2H to 1T' can also happened in six different orientations or configurations. Thus, we use η_p ($p = 1, 2 \text{ or } 3$) to describe the six 1T' variants, where η_p could be -1 or 1 to represent different 1T' phases and 0 for 2H phase.

The free energy of this two-component and inhomogeneous monolayer could be expressed as a functional F_{tot} . This free energy could be divided as stress free energy density f_{chem} and elastic energy density f_{elas} as $F_{tot} = \int_A (f_{chem} + f_{elas}) dA$, where $f_{chem} = f_{bulk}(\eta_p) + 1/2 \sum_p |[\phi\beta_1 + (1 - \phi)\beta_2]\Delta\eta_p|^2$. β_1 and β_2 in this model are constants proportional to interfacial energy of component 1 and 2 because we adopt the simulation at length scales above the morphological crossover length using interfacial isotropy.

The form of f_{elas} for chemically heterogeneous but elastically homogeneous systems can be easily derived based on Berry's chemically homogeneous model [17] by adding the order parameter $\phi(\vec{r})$ to denote different chemical components.

In order to obtain the expression of the elastic energy density f_{elas} with elastic heterogeneity, the eigen strain method [18] were employed to transfer this elastically heterogeneous system to an elastically homogeneous system at the price of adding an unknown eigen strain to the system. Using the computational methods, this unknown eigen strain can be determined for this certain type of system. So the system now is similar to the chemical heterogeneous but elastic homogeneous one as we discussed above, then the form of the energy density is available.

3 Example results

Some qualitative pre-result will be shown here, these are some interesting phenomenon and still need further study to get the quantitative conclusions and better understanding.

For Figure. 1, as we expect, the phase transformation will first start from MoTe₂ due to the smaller transformation strain. And the amplitude of strain required to trigger this transformation is larger than the prediction from DFT calculation due to the energy barrier of this transformation.

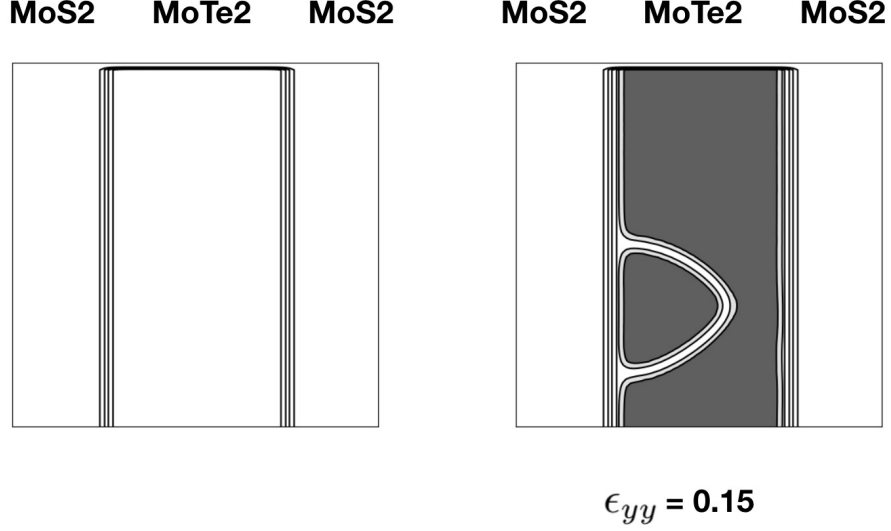


Figure 1: Two components system under uniaxial strain in y direction, the middle stripe between the black lines is MoTe_2 and outside MoS_2 . White regions means 2H phase, grey represent 1T' phase with certain orientation. The transformation strain ϵ_{yy} here is 0.15.

As for Figure. 2, the indenter not only trigger the phase transformations inside the indent region, but also outside, which provide another way to control the phase transformations process of TMD monolayers. The shape of the indenter or the morphology of the monolayers will also have influences on the phase transformations, which worth further study.

4 Concluding Remarks

In this work, a PFM model for the structural transformations of TMD monolayers was constructed with both chemical and elastic heterogeneity by adding a new order parameter $\phi(\vec{r})$ to describe different components and using eigen strain method to deal with changing elastic moduli. Some qualitative results were obtained by simulating different approaches to control strains in this system and observing the phase transformation pattern combined with these approaches. The following directions for this work are further studying this system with more complicated or various conditions to get better understanding and quantitative results to reveal the potential of this strain engineering phase transformation technique of multi-components TMD monolayers.

MoS₂ MoTe₂ MoS₂

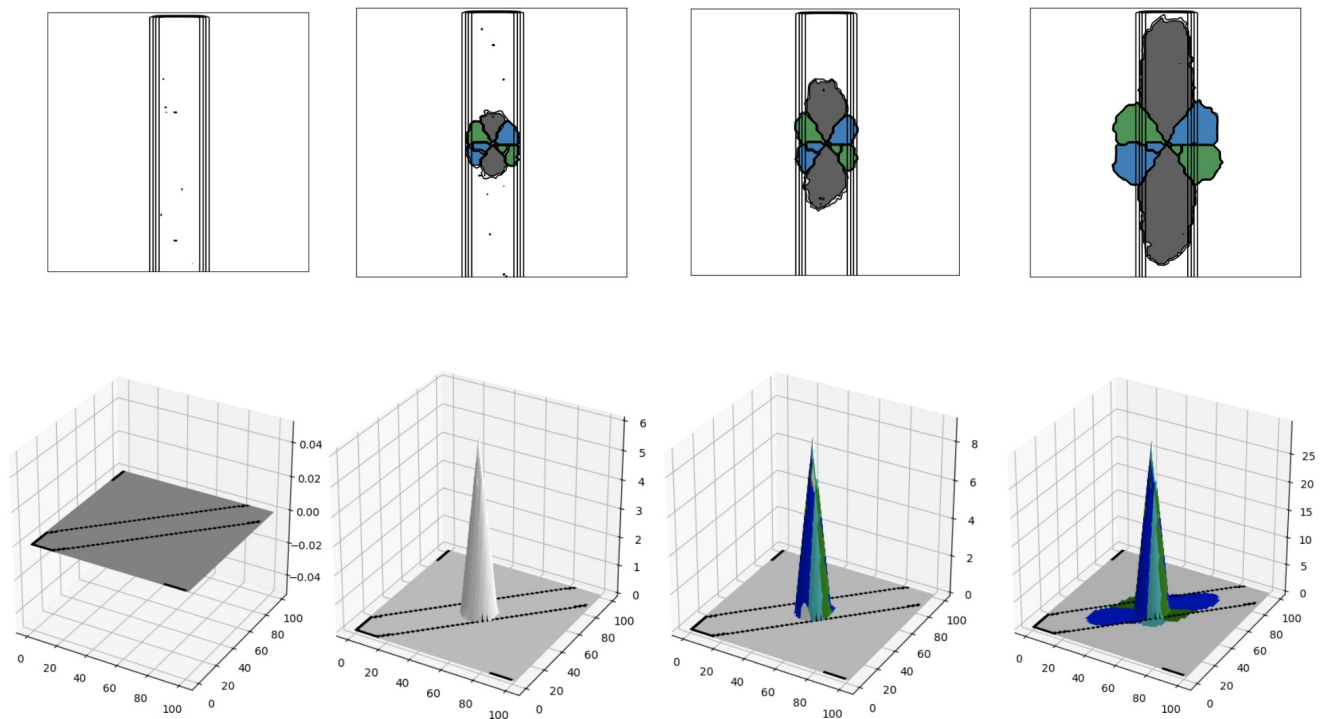


Figure 2: Two components system under the compression of indenter, the middle stripe between the black lines is MoTe₂ and outside MoS₂. White regions means 2H phase, other colors represent 1T' phase with different orientations.

References

- [1] M. Chhowalla, H.S. Shin, G. Eda, L.J. Li, K.P. Loh, and H. Zhang. The chemistry of two-dimensional layered transition metal dichalcogenide nanosheets. *Nature Chemistry*, 5:263275, 2013.
- [2] A.K. Geim. Graphene: Status and prospects. *Science*, 324(5934):1530–1534, 2009.
- [3] A.K. Geim and I.V. Grigorieva. Van der waals heterostructures. *Nature*, 499:419425, 2013.
- [4] X. Qian, J. Liu, L. Fu, and J. Li. Quantum spin hall effect in two-dimensional transition metal dichalcogenides. *Science*, 346(6215):1344–1347, 2014.
- [5] A. Castellanos-Gomez, R. Roldn, E. Cappelluti, M. Buscema, F. Guinea, H.S.J. van der Zant, and G.A. Steele. Local strain engineering in atomically thin mos₂. *Nano Letters*, 13(11):5361–5366, 2013.
- [6] P. Johari and V.B. Shenoy. Tuning the electronic properties of semiconducting transition metal dichalcogenides by applying mechanical strains. *ACS Nano*, 6(6):5449–5456, 2012.
- [7] Q. Yue, J. Kang, Z. Shao, X. Zhang, S. Chang, G. Wang, S. Qin, and J. Li. Mechanical and electronic properties of monolayer mos₂ under elastic strain. *Physics Letters A*, 376(1213):1166–1170, 2012.
- [8] A. Allain, J. Kang, K. Banerjee, and A. Kis. Electrical contacts to two-dimensional semiconductors. *Nature Materials*, 14:11951205, 2015.
- [9] R. Kappera, D. Voiry, S.E. Yalcin, B. Branch, G. Gupta, A.D. Mohite, and M. Chhowalla. Phase-engineered low-resistance contacts for ultrathin mos₂ transistors. *Nature Materials*, 13:11281134, 2014.
- [10] A. B. Kaul. Two-dimensional layered materials: Structure, properties, and prospects for device applications. *Journal of Materials Research*, 29:348–361, 2014.
- [11] K.A.N. Duerloo, Y. Li, and E.J. Reed. Structural phase transitions in two-dimensional mo- and w-dichalcogenide monolayers. *Nature Communications*, 5(4214), 2014.
- [12] S. Song, D.H.Keum, S. Cho, D. Perello, Y. Kim, and Y.H. Lee. Room temperature semiconductor?metal transition of mote₂ thin films engineered by strain. *Nano Letters*, 16(188), 2016.
- [13] A. Artemev, Y. Jin, and A. Khachaturyan. Three-dimensional phase field model of proper martensitic transformation. *Acta Materialia*, 49(7):1165–1177, 2001.
- [14] A. Artemev, Y. Wang, and A. Khachaturyan. Three-dimensional phase field model and simulation of martensitic transformation in multilayer systems under applied stresses. *Acta Materialia*, 48(10):2503–2518, 2000.
- [15] Y. Wang and A. Khachaturyan. Three-dimensional field model and computer modeling of martensitic transformations. *Acta Materialia*, 45(2):759–773, 1997.
- [16] A. Khachaturyan. *Theory of Structural Transformations in Solids*. Dover Publications, 2013.

- [17] J. Berry, S. Zhou, J. Han, D.J. Srolovitz, and M.P. Haataja. Dynamically programmable two dimensional materials. *Nano letters*, 2017.
- [18] Y.U. Wang, Y.M. Jin, and A.G. Khachaturyan. Phase field microelasticity theory and modeling of elastically and structurally inhomogeneous solid. *Journal of Applied Physics*, 92(1351), 2002.