Characterization and Applications of Titanium alloy with Nickel and Niobium based Shape memory alloys by Molecular Dynamic Simulation – A review

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Abstract. Characterization of Shape memory alloys using simulations like molecular dynamics (MD) approach is a difficult but at the same time it is an effective process. In this article, recent works on MD simulation of titanium-based shape memory alloys which can be used as nano sensors for sensing various properties like temperature, pressure and relative humidity were discussed. The accuracy of MD simulation is based on potentials like modified embedded atom method to study its mechanical behavior at different temperatures in atomic scale. Also, the force between individual particles of the alloy was calculated to determine the mechanical properties of shape memory alloys depending on the interparticle free space. Hence in this article authors were discussed various types of potentials and its effectiveness to characterize mechanical properties. Also, this article gives an overview of Nickel and Niobium based titanium alloy on various application.

1. Introduction
Shape memory alloys are smart materials which can regain its original state at transition temperature. Shape memory effect of titanium-based shape memory alloys are studied extensively by experiments. Titanium metal is alloyed with nickel and niobium as an alloying element to exhibit shape memory effect. The effect of Niobium content on mechanical properties and super elasticity was studied in Ti-Nb alloys fabricated by powder metallurgy [1-2]. The nickel–titanium based shape memory alloys have different applications in implants, springs and screws which were produced by investment casting and submitted to thermal and mechanical characterization [3]. Transformation temperatures of these shape memory alloys [4] have been compared with various materials. Significant interest is shown in titanium-based shape memory alloys and the molecular dynamic simulation of these alloys will be discussed.

Molecular dynamics (MD) simulations of Nickel-Titanium based alloys using the interatomic potential like second nearest neighbor modified embedded-atom method were performed to study mechanical behavior at atomic-scale and microstructural evolution at various temperatures [5]. Also, the effect of nano precipitate in Ni-Ti alloy is studied [6], which affects misfit in local atomic due to elastic disturbance fields at the precipitate-matric periphery. Niobium based titanium alloy [7] is studied as the alloying content of Nb was varied from 10 wt % to 50 wt %. The alloy with lower proportion (10%) of niobium acquires more hardness when compared to higher proportion (50%) of niobium. tin(Sn) is the another alloying element added to the Ti-Nb alloy [8]. The elastic modulus of Ti(75)-Nb(20)-Sn(5) alloy was 61 GPa, which is more suitable for human bone implant. The mechanical properties can be studied using molecular dynamic simulation [9] which will be helpful in
reducing the cost of experimentation also paves the way for simulating it for various application. One such application is nano sensor which will be discussed in this article.

2. SMAs in Sensors
SMAs properties [table 1] paves the option for being used as a prime element in sensors. Some of the properties for titanium based SMAs are listed [10-13].

| Composition | Transition temperature | Strain (%) | Recovery (%) | Inference                      |
|-------------|------------------------|------------|--------------|--------------------------------|
| Ti-Ni-Pd    | 100-530                | 2.6-5.4    | 90-100       | High work output and material cost |
| Ti-Ni-Pt    | 110-1000               | 3-4        | 100          | High work output and material cost |
| Ni-Ti-Hf    | 100-400                | 3          | 100          | Low material cost              |
| Ni-Ti-Zr    | 100-250                | 1.8        | 100          | Low material cost              |
| Ti-Nb       | 100-200                | 2-3        | 97-100       | Good ductility                 |
| Ti-Pd       | 100-510                | 10         | 88           | Good ductility                 |
| Ti-Au       | 100-630                | 3          | 100          | Good ductility                 |
| Ti-Pt-Ir    | 990-1184               | 10         | 40           | High yield strength            |

The Ni-Ti also used as a coating element in Optical fibers [Figure.1] to reflect a particular wavelength of light and transmits all other wavelengths [14]. Done by sputter deposition using a nickel-titanium shape memory alloy as thin film for Bragg grating on optical fiber surface. Centroid calculation to calculate the wavelength shifts are used to measure the strain in the optical fiber. These results show distinct and rapid changes in the optical fiber signal with respect to four related transformation temperatures in austenite-martensite forward and reverse phase transformations.

![Figure 1. Coating of optical fiber with Ni-Ti.](image)

Also, to find the relative humidity, Ni-Ti based sensors are employed [15]. The prime element was synthesized by electrospinning and calcination techniques. The correlation of RH sensing for different electrodes were studied and found that Ti based electrodes have higher sensitivity in RH sensing. Also, a lot of work carried out based on Ni-Ti in MEMS is explained [16]. The effect of doping Niobium with titanium in sensing the hydrogen gas [17] by delaying the anatase to rutile phase...
transformation during annealing which improves the homogeneity of sensing films. To improve the hydrogen sensing, a novel heterophase junction H\(_2\) sensors [18] are made. The Nb\(_2\)O\(_5\)-TiO\(_2\) nanofibers [19] exhibits greater sensing response to ethanol with higher performances, having lower operating temperature and detection limit. In future, SMAs prospects in nano-composites as sensors is studied [20] in various application with reference to aerospace, mechanical, medical and biomedical devices such as self-healing systems, self-deployable structures, actuators, sensors or their direct implementation in the industry are finally outlined. All these applications are succeeded because of the MD simulation tool, which reduced the experimentation time. For an accurate MD Simulation, the suitable interatomic potential is used. The development of potentials for MD simulation for a period of time will be discussed.

3. Evolution of Interatomic potential

To run MD simulations of NiTi shape-memory alloys, the accuracy of the interatomic potential is required. Various Interatomic potentials were developed on the basis of embedded-atom method (EAM) [24-27]. But these potentials could not be able to reproduce the accurate properties of the ternary alloys [28]. Saitoh et al. [29] and Ishida et al. [30] modified the existing Embedded Atom Method to reproduce the Ni-Ti phase transformations. This modified method could not produce accurate reversible temperatures, stress-induced phase transformation temperatures and crystallography phases. Because of the wrongly predicted martensite structure seen in [21-23] could not be reproduced. Recently, development of interatomic potential on the basis of second nearest-neighbor (2NN) MEAM model [33–35] and applied it to study the transition temperature of Nickel-Titanium shape-memory alloys and provided the expected results. So, the 2NN-MEAM model can be effectively used for the MD simulation Ni-Ti shape memory alloy. Using embedded atom method there are various works in MD simulation of Ni-Ti and Ni-Al alloys [36-39] and so it can be used for Ti-Nb based alloys.

![Figure 2. Machine learning for Interatomic potential.](image-url)

In future, these interatomic potentials can be enhanced by machine learning concepts as already an interatomic potential for Zirconium [40] was developed. Figure 2 shows the neural network configuration for predicting Interatomic potential.
4. Conclusion
The titanium-based shape memory alloys are characterized experimentally and so the characterization by molecular dynamics method is to be enabled. Their succession in Molecular dynamic simulation lead to decrease in time span for applying in wide variety of application. To have an accurate data, efficiency of the interatomic potential used to be studied. From the various works conducted the 2NN-MEAM model was more efficient and can give good results. In future these potentials can be enhanced by Machine learning concepts.

5. References
[1] Kalita D, Rogal Ł, Czeppe T, Wójcik A, Kolano-Burian A, Zackiewicz P, Kania B and Dutkiewicz J 2019 Journal of Materials Engineering and Performance 7 1-8
[2] Yahaya and Mazyan 2016 Materials Science Forum 863 14–18
[3] de Brito Simões J and de Araujo CJ 2018 Journal of Intelligent Material Systems and Structures 29(19) 3748-57
[4] Van Humbeeck J 2012 temperatures Materials Research Bulletin 47(10) 2966-8
[5] Xiang Chena and Teng Liu 2016 Shape Memory Alloy 146 61-69
[6] Piyas Chowdhury, Luca Patriarca, Guowu Ren and Huseyin Sehitoglu 2016 International Journal of Plasticity 81 152-167
[7] Thoemmes A, Bataev IA, Belousova NS and Lazurenko 2016 11th International Forum on Strategic Technology (IFOST) 26-29
[8] Li P, Ma X, Wang D and Zhang H 2019 Metals 9(6) 712
[9] Nikonov AY 2017 InAIP Conference Proceedings 1909(1) 020152
[10] Ma J, Karaman I and Noebe RD 2010 International Materials Reviews 55(5) 257-315
[11] Hee Young Kim, Satoru Hashimoto, Jae Il Kim, Hideki Hosoda and Shuichi Miyazaki 2004 Material transactions 45 2443-2448
[12] Noebe R, Gaydosh D, Santo Padula II, Garg A, Biles T and Nathal M 2005 InSmart Structures and Materials 2005: Active Materials: Behavior and Mechanics 5761 364-375
[13] Morawiec H, Le’tko J, Koval Y and Kolomytzev V 2000 Materials science forum 327 291-294
[14] Mohanchandra KP, Karnani S, Emmons MC, Richards WL and Carman GP 2008 Applied Physics Letters 93(3) 031914
[15] S.Batool, Z.Imran, M.Israr Qadir, M.Usman, H.Jamil, M.A.Rafiq, M.M.Hassan and M.Willander 2013 Journal of Materials Science & Technology 29 411-414
[16] Mehrpouya M and Cheraghi Bidsorkhi H 2016 Micro and Nanosystems 8(2) 79-91
[17] Zhong Li, ZhengJun Yao and Azhar Ali Haidry 2019 Journal of Alloys and Compounds 806 1052-1059
[18] Bao Y, Wei P, Xia X, Huang Z, Homewood K and Gao Y 2019 Sensors and Actuators B: Chemical 301 127143
[19] Gang Lia, Xin Zhang, Huan Lu, ChaoYan, 2019 Sensors and Actuators B: Chemical 283 602-612
[20] Krishan Kumar Patel and Rajesh Purohit 2018 Materials today proceedings 5 20193-20200
[21] Otsuka K and Ren X 2005 Progress in Materials Science 50 511-678
[22] Waitz T, Tsuchiya K, Antretter T and Fischer FD 2009 MRS bulletin 2009 11 814-21
[23] Greer JR and De Hosson JT 2011 Progress in Materials Science 56(6) 654-724
[24] D. Farkas, D. Roqueta, A. Vilette, and K. Ternes 1993 Modell. Simul. Mater. Sci. Eng. 4 359
[25] M. S. Daw and M. I. Baskes 1984 Phys. Rev. B 29 6443
[26] W. S. Lai and B. X. Liu 2000 J. Phys.: Condens. Matter 12 53
[27] M. W. Finnis and J. E. Sinclair 1984 Philos. Mag. A 50 45
[28] D. Mutter and P. Nielaba 2010 Phys. Rev. B 82 224201
[29] K. Saitoh, K. Kubota, and T. Sato 2010 *Tech. Mech.* **30** 269
[30] H. Ishida and Y. Hiwatari 2007 *Mol. Simul.* **33** 459
[31] M. I. Baskes 1992 *Phys. Rev. B* **46**, 2727
[32] Y. Zhong, K. Gall, and T. Zhu 2011 *J. Appl. Phys.* **110** 033532
[33] B.-J. Lee and M. I. Baskes 2000 *Phys. Rev. B* **62** 8564
[34] B.-J. Lee, M. I. Baskes, H. Kim and Y. K. Cho 2001 *Phys. Rev. B* **64** 184102
[35] B.-J. Lee, W.-S. Ko, H.-K. Kim and E.-H. Kim 2010 *CALPHAD* **34** 510
[36] Lu HY, Chen CH and Tsou NT 2019 *Materials* **12(1)** 57
[37] Pun G and Mishin, Y 2010 *Journal of physics* **22** 395403
[38] G.P. Purja Pun and Y. Mishin 2009 *Philosophical Magazine* **89** 3245-3267
[39] W S Ko, B Grabowski, and J Neugebauer 2015 *Physical Review B* **92(13)** 134107
[40] Zong H, Pilania G and Ding X 2018 *npj Comput. Mater.* **4** 48