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Effects of Sputtering Process Parameters for PVD Based MEMS Design

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Abstract: *MEMS or micro-electro-mechanical system is a widely used technology for manufacturing devices in micro range. This technology combines electrical and mechanical properties on a single chip. The most crucial step in MEMS fabrication process includes the deposition of device material on substrate by suitable deposition techniques [1]. So, present study intends to investigate the deposition of Ni, Ti and Cu based ternary thin film materials on Si (100) substrate for the fabrication of MEMS devices using classical molecular dynamics simulation, and also to study the variation of film structure and properties by varying its different process parameters like substrate temperature and substrate bias voltage etc [2-3]. For the deposition of this ternary thin film, PVD or physical vapor deposition technique is considered here. Physical vapor deposition (PVD) involves the deposition of thin film materials in vacuum by evaporation or momentum-transfer processes. From various types of PVD techniques, sputtering is considered here as it has high deposition rate, less possibility of contamination etc [6-8]. In this process, the material that is to be deposited is ejected from the source or target to the substrate by momentum exchange brought about by the impingement of energetic ions*.

I. Introduction

MEMS or micro-electro-mechanical system is a widely used technology for manufacturing devices in micro range. This technology combines electrical and mechanical properties on a single chip. The most crucial step in MEMS fabrication process includes the deposition of device material on substrate by suitable deposition techniques. The present study intends to investigate the deposition of Ni, Ti and Cu based ternary thin film materials on Si <100> substrate for the fabrication of MEMS devices using classical molecular dynamics simulation, and also to study the variation of film structure and properties by varying its different process parameters like substrate temperature and substrate bias voltage etc [4-5]. To deposit this ternary thin film, physical vapor deposition (PVD) technique is used here. The Physical vapor deposition (PVD) involves the deposition of thin film materials in vacuum by evaporation or momentum-transfer processes. There are various types of PVD techniques are available, among them the sputtering is considered as a comprehensive techniques, because it has high deposition rate, less possibility of contamination and high purity level.The computer based simulation and modeling of the atomic structures and models have become a powerful and widely used tool for obtaining basic knowledge of all materials and their properties. It is also useful for providing inputs to the designed models and process the inputs according to the instructions or codes given and obtaining the nearly desired outputs [9]. In this research, classical molecular dynamics simulator has been used to design a comprehensive sputtering based Physical Vapor Deposition (PVD) model and discussed its various properties. MEMS or micro-electro-mechanical system, also abbreviated as micro-system, are sophisticated devices that are produced using advanced micro-fabrication techniques. The steps of MEMS fabrication process are shown in the following figure.

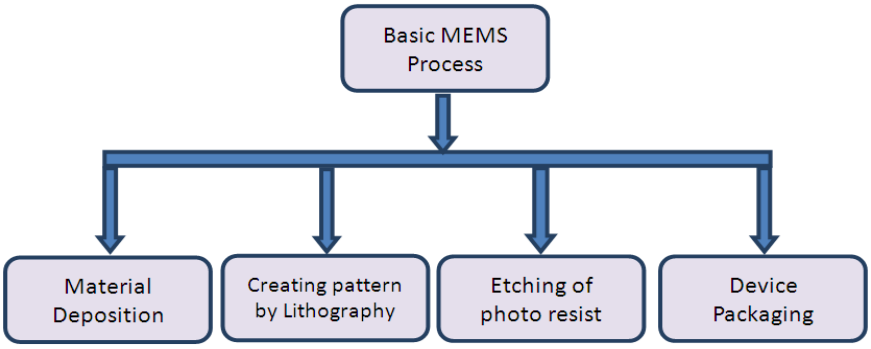

Figure 1: Flow chart of MEMS fabrication process**.**

The most crucial process in MEMS fabrication is the deposition of device material by suitable deposition technique. The present study is restricted to the deposition of thin film material which is aimed for MEMS based devices.

Film deposition is the most important part of the total MEMS fabrication. There are various processes by which materials can be deposited on the substrate like, CVD or chemical vapor deposition process, PVD or physical vapor deposition process, Electrochemical deposition process etc. From these numerous techniques, sputtering process is considered here.

Ti based sputter coating has been widely used for their wear and corrosion resistance, chemical and thermal stability and for the diffusion of barrier layers. For the fabrication of thin films, the deposition of Ni and Ti are quiet common and nickel-titanium based thin films sputtered by magnetron are gaining scientific interest day by day. Ni-Ti based films are used as shape memory alloy thin films for Micro-Electro-Mechanical System (MEMS) based models [13-15].

The functionality, behavior and application of Ni-Ti alloy thin films depend on its composition. To reduce this composition sensitivity and to make the hysteresis narrow, a third element Cu has been added and this further addition of Cu in the Ni-Ti matrix makes the material rigid. This shape memory alloy thin film characteristics are very much dependent upon the sputtering conditions i.e. substrate bias voltage, substrate temperature, pressure etc.

The effects of substrate bias voltage on the properties of Ni-Ti thin film alloys are the subject matter of many recent studies and the application of this voltage on thin films causes the gain of high energy by the ions and this results the re-sputtering from the deposited thin film alloy leading to the formation of vacancies. In particular, the variation in deposition rate, crystallinity and composition occur due to re-sputtering which is caused by high ion-bombardment. So, the experimental observation of the deposition of magnetron sputtered Ni-Ti-Cu ternary thin film alloy on Si (100) substrate and the ion-assisted sputtering on that structure and for these reasons the variation of its properties are performed here [10]. This deposition process and film structure is also influenced by the substrate temperature. So, the effects of substrate temperature and depending upon it the changes in the properties of the film deposition are also investigated here.

In this paper, the experimental discussion that is based on the results of molecular dynamics simulation is presented. In this film deposition process, the negative substrate bias voltage controls the formation of crystalline phases. As the negative substrate bias voltage is applied the ions inside the sputtering chamber are attracted to the deposited film and strike the film surface with a very high kinetic energy and momentum. For this reason re-sputtering occurs from the deposited thin film.

It is found that the film deposition rate has been increased as well as decreased with increase in negative substrate bias voltage although it is expected to increase [11-12]. The reason behind it has not been explored. It can be dependent upon other sputtering parameters.

II. Materials And Methods

Film deposition is the most important part of total MEMS fabrication. There are various methods by which this process can be performed.

Table 1: Classification of deposition technologies is as given in the table.

Physical vapor deposition (PVD)	Thermal evaporation Electron beam evaporation (EBE) Sputtering Molecular Beam Epitaxy (MBE) Pulsed laser deposition (PLD) Ion plating Activated reactive evaporation Ionized cluster beam deposition
Chemical vapor deposition (CVD)	Plasma-enhanced CVD (PECVD) Atmospheric pressure CVD (APCVD) Metallorganic CVD (MOCVD) Atomic layer epitaxy Spray pyrolysis Liquid phase epitaxy
Electrochemical deposition	Electroless metal deposition Electroplating Anodization

From these various processes, Sputtering is considered here because of its high deposition rate, less possibility of contamination and high purity level.

Sputtering Deposition

Sputtering is a commonly used physical vapor deposition process that involves the ejection of neutral atoms from the target or source to the substrate by momentum exchange process performed by the impingement of energetic ions.

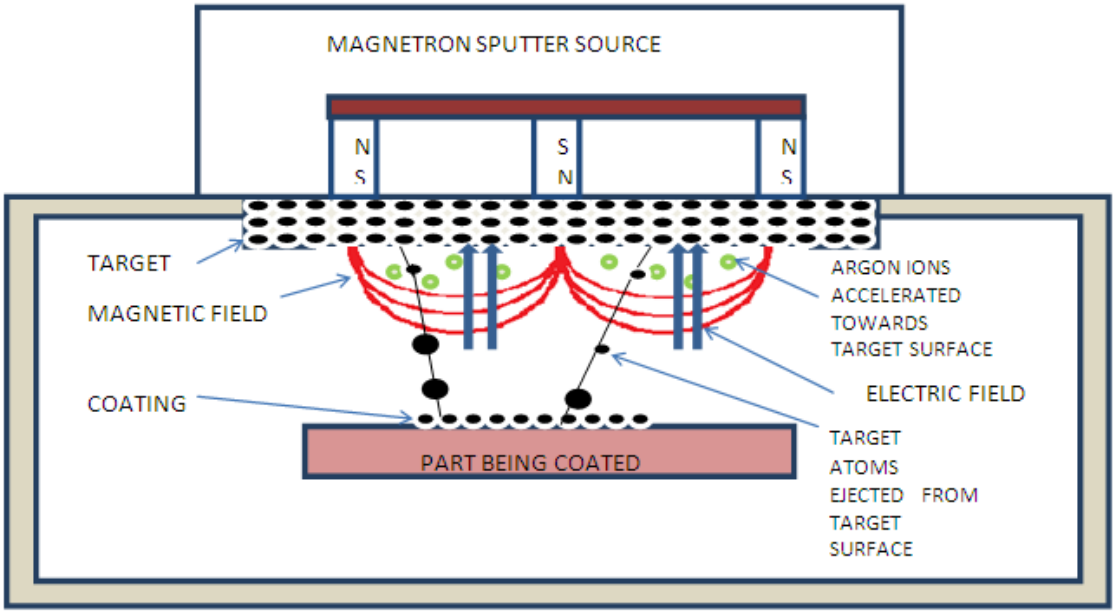

Figure 2: Sputter Deposition

Magnetrons are a class of cold cathode discharge devices used generally in a diode mode. The plasma or Ar^+ ions are initiated in the vacuum at pressures in the mTorr range by applying high DC or RF voltage. This plasma is sustained by the ionization of secondary electrons emitted from the cathode by ion bombardment. A magnetron cathode differs from a conventional diode cathode by the presence of a magnetic field. The magnetic field in the magnetron is oriented parallel to the cathode surface. Here the E×B drift of the emitted secondary electrons forms a closed loop. As the no. of secondary electrons increased, the plasma density will become higher than a conventional DC diode system. Magnetron sputtering is a low-cost and easy control method for film growth, especially suitable for large-scale film deposition. The whole process is performed by Molecular dynamics simulation.

Molecular Dynamics Simulation

Classical molecular dynamics simulation is a process for computing properties of a classical multi-atom system. It is concerned with the description of the atomic and molecular interactions that governs microscopic and macroscopic behavior of physical systems. Using this simulation process, the positions and velocities of the particles in the system and its variation with time can be easily obtained.

By solving Newton's second law, $(F = ma)$:

$$\frac{\partial^2 x_i}{\partial t^2} = \frac{F_{xi}}{m_i}$$

The motion of a particle (i^{th} particle) of mass m_i along one coordinate (x) with net force on the particle F_{xi} in that direction (x) can be obtained.

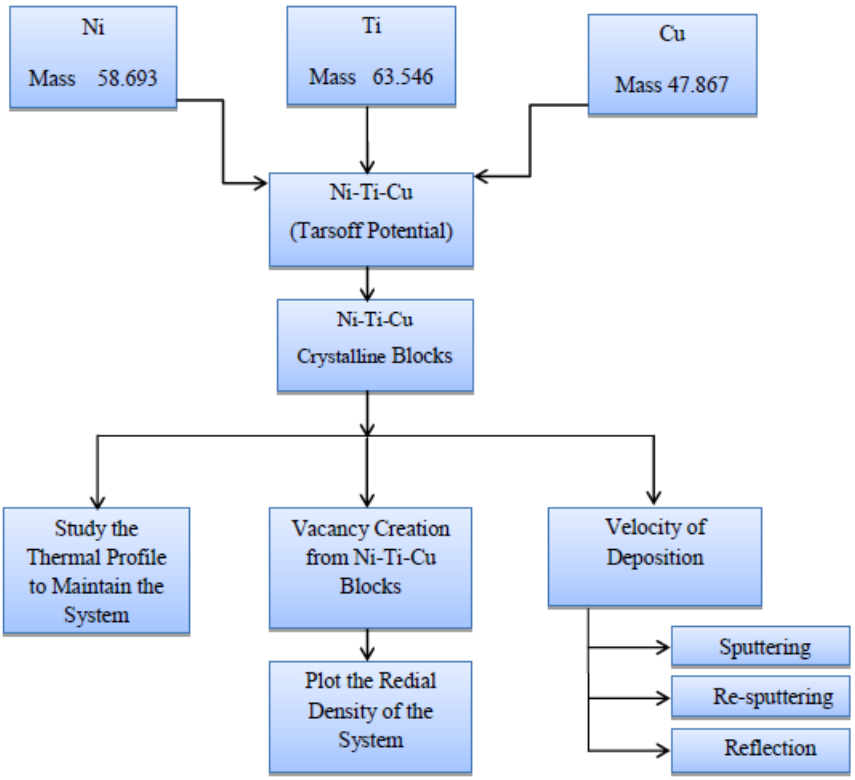

Figure 3: General steps performed in this research.

General Steps Of Molecular Dynamics Program

The general steps for designing the molecular dynamics simulation are discussed here. In this research, the classical molecular dynamics simulations were performed using Large Scale Atomic / Molecular Massively Parallel Simulator (LAMMPS) (Sandia et al,) platform. LAMMPS is a classical molecular dynamics code that models liquid, solid, or gaseous molecules in a desired manner. It can model atomic, polymeric, biological, metallic, granular, and coarse-grained systems.

At first the simulation is initialized. "units" command is used at first to set the style of units used for simulation. This command determines the units of all quantities mentioned in input script and data file. In this research, metal units are used. Then, the dimension of the simulation box is defined. For this purpose, dimension command is used. It basically set the dimensionality of the simulation. Here, 3 dimensions are required. Then the boundary of the simulation box is defined. "boundary" command sets the boundaries of the global simulation box in each dimension. A single letter is used for same style for both upper and lower face of the box. In this research, the boundary condition is taken as p p s (i.e. Periodic, periodic and shrink-wrapped). p is used in x and y direction. It means the box is periodic and the particles can interact across the boundary, and they can exit at one end of the box and can re-enter at other end. Using s, the face is set to encompass the atoms in that dimension (shrink-wrapping). In z direction, shrink-wrapping is used because the ad-atoms that are deposited on the substrate may cause reflection of the ad-atoms and re-sputtering of deposited atoms and the z direction box size should change accordingly. After that, style of atoms used for simulation is defined. For this, "atom_style" command is used. Here, atom-style is atomic, which denotes the default values generally used for coarse-grain liquids, solids, metals. Then input data are given using "read_data" command. It is used to read the data file containing information which LAMMPS needs to run a simulation.

"lattice" command is used to define a lattice which is a set of points in space used to determine a unit cell with basis atoms. Here the lattice style is dependent upon the dimension of simulation. In this research, the style 'fcc' is used to provide face centered cubic structure of the crystal.

Then three regions, lower region, middle region and upper region are defined respectively. The "region" command is used to specify the geometric region of space. This command is used typically to test whether an atom's position is contained in the region or not. For this, coordinates exactly on the region boundary are considered to be interior to the region. In this research, region "low block 0 50 0 50 -1 5 units box" is used to define the lower block and its corresponding x, y and z coordinates, "midl block 0 50 0 50 5 20 units box" is used to define middle block and "up block 0 50 0 50 20 221 units box" is used to define upper block of the total simulation. The individual groups are then identified using "group" command. It is used to identify a number of atoms as belonging to a group. The group ID can also be used then in other commands such as fix, compute,

dump or velocity to act on those atoms together. Using this command the individual groups can also be marked by different colors. If the group ID already exists, then group command adds the specified atoms to the group.

The "timestep" command is used to set the step size of time for subsequent molecular dynamics simulations. Here, timestep 0.001 is taken. Then the formulas which LAMMPS uses tocompute pairwise interactions are defined. For this purpose, pair_style command is used. Here, pair_styleeam/alloy is used to give alloy EAM type potential. pair_coeff command is then used to specify the pairwise force field coefficients for one or more pairs of atoms. The number and meaning of coefficients depends on the pair style. In this research, the pair coefficients are taken in NiTiCu.set file and mentioned in "pair_coeff" command with separating Ni Ti Cu. The radial distribution function is plotted using "compute" command. Using this command any kind of computation is performed in LAMMPS. The computed data calculated by this command are instantaneous values, meaning they are calculated from information about atoms on the current timestep or iteration.

Now the total process is dumped using"dump" command. It is normally used to take a snapshot of atom quantities to one or more files every N timesteps in different kind of styles.dump is performed here to render the output and to take several snapshots at each steps of the output.

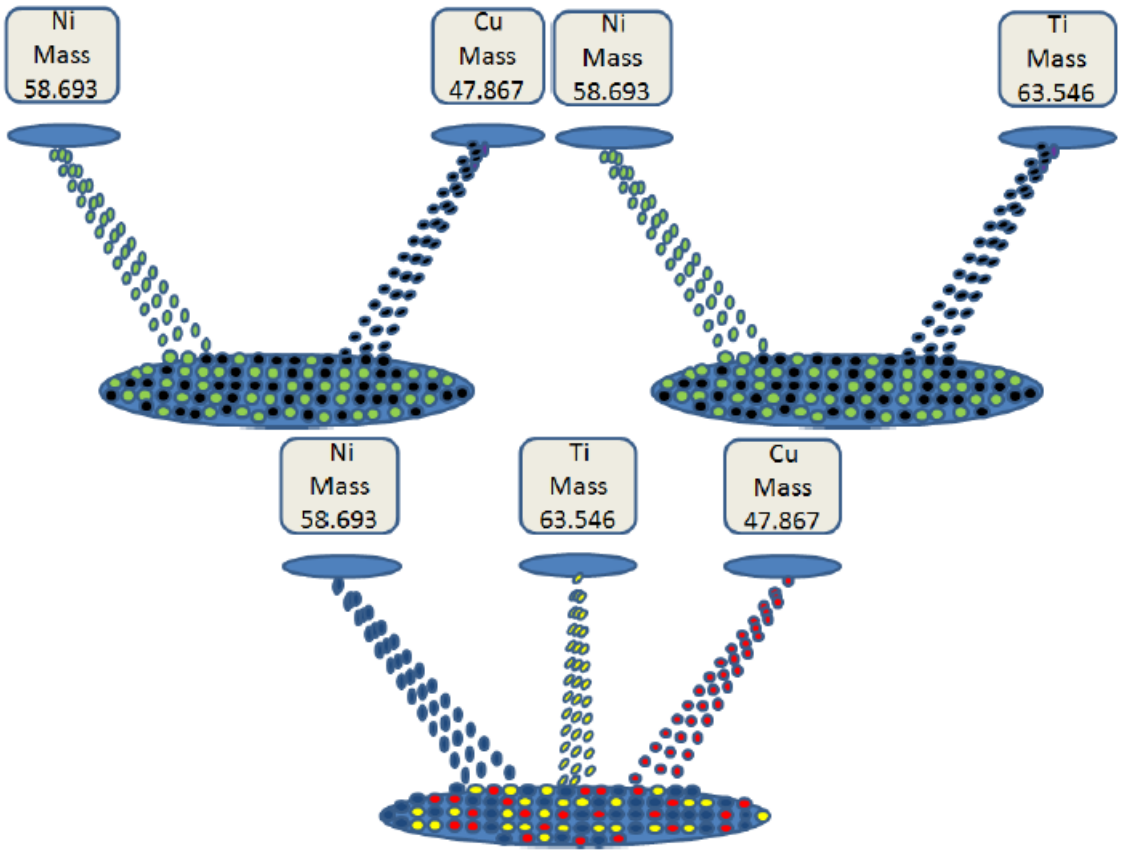

Figure 4: The schematic structure represents the Ni, Ti and Cu atoms striking a representative portion of Ni-Ti, Ni-Cu and Ni-Ti-Cu thin film.

III. Result & Discussions

Figure 5 suggests if the actual reflection and re-sputtering of ad-atoms have been counted with the increasing velocity of ad-atoms, it is found that when the velocity of the ad-atoms exceeded a critical value, the reflection and re-sputtering of the colliding atoms were observed. The variation of the critical value of this velocity is occurred due to different atomic densities of individual Ni, Ti and Cu atoms. The information in the figure 5 can be interpreted to control re-sputtering and reflection if the density of atoms just above the film and the velocities of ad-atoms corresponding to different bias voltages are provided. Basically the velocity of ad-atoms is totally dependent on the substrate bias which will provide in time of the fabrication process. Now, from the figure 5, it is clearly revealed that for a defined velocity (above critical velocity) the re-sputtering take place in a high domain than the actual reflection.

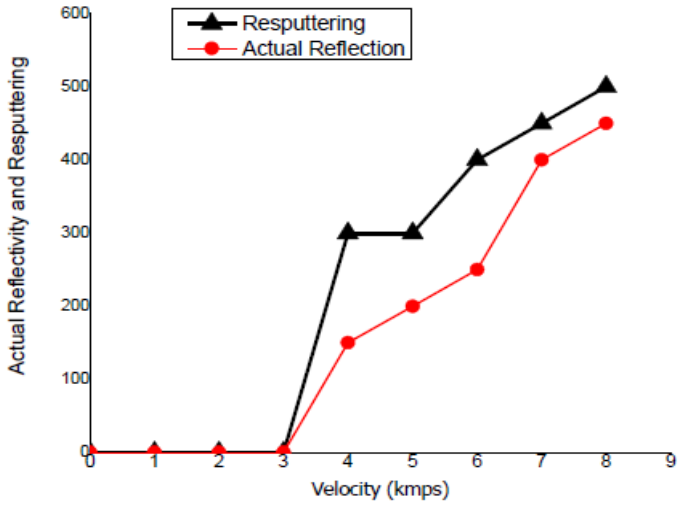

Figure 5: Variation of number of atoms which have been reflected and re-sputtered with colliding velocity.

In figure 6 and figure 7, the re-sputtering and actual reflection have been plotted separately against the velocity of ad-atoms and the two different plots also indicate the same kind of trend which has been found in figure 5 also.

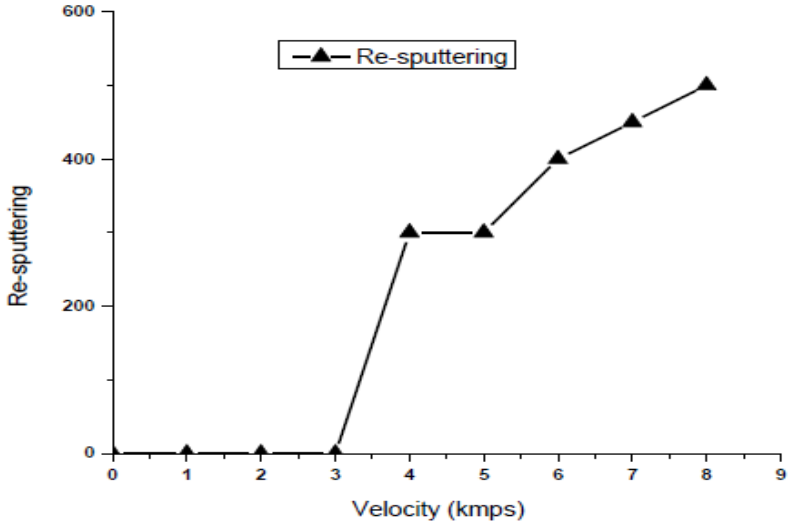

Figure 6: Variation of number of atoms which have been reflected with colliding velocity.

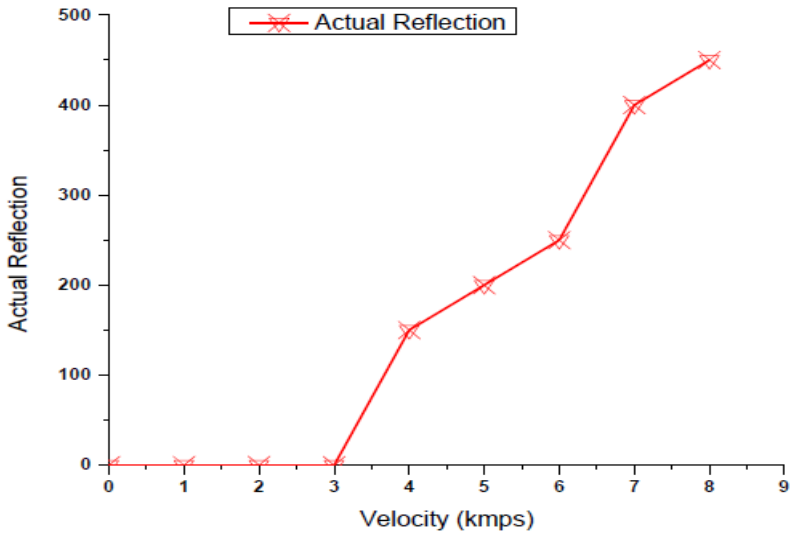

Figure 7: Variation of number of atoms which have been re-sputtered with colliding velocity.

In figure 8, the deposition of thin films for different time steps have been rendered and the figure suggests that after a certain amount of time a film have been developed with a certain amount of thickness.

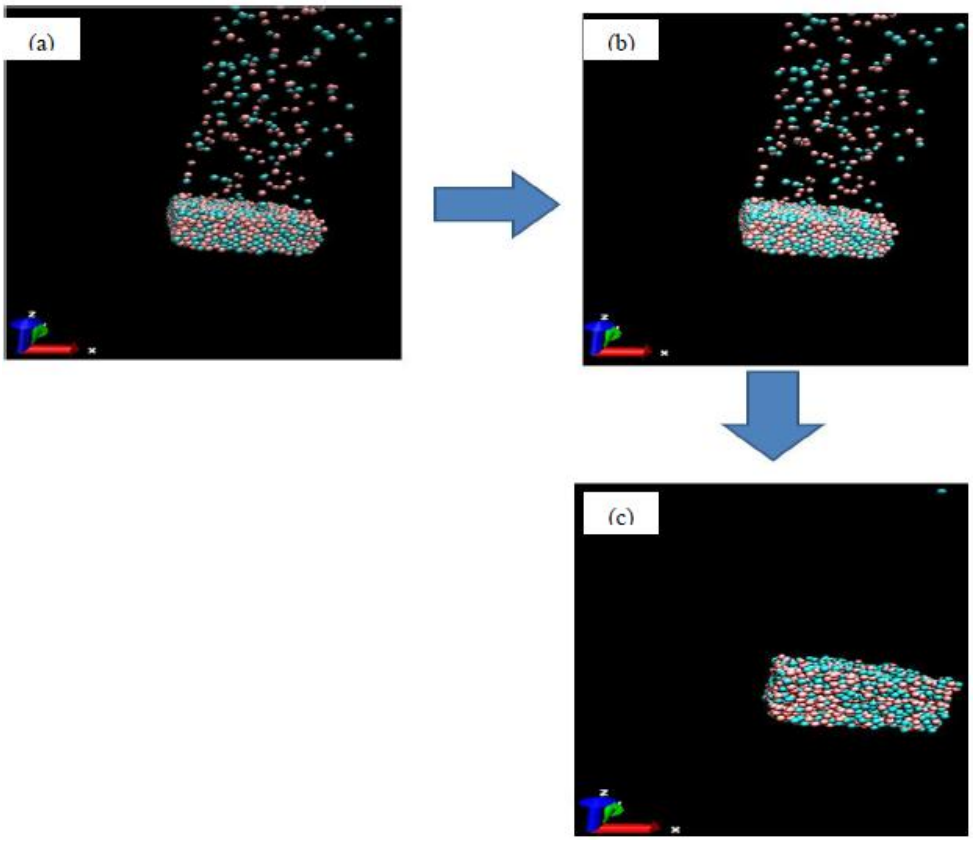

Figure 8: The development of the thin film at different time intervals (a) for time t = 10Ps, (b) for time t = 15Ps, (c) for time t = 20Ps.

The figure 8 also suggests that, as the time increases from t = 10Ps to 20Ps, the thickness of the film will also increase in a linear way. The figure 9 suggests the final structure of the film developed for different composition at 20Ps.

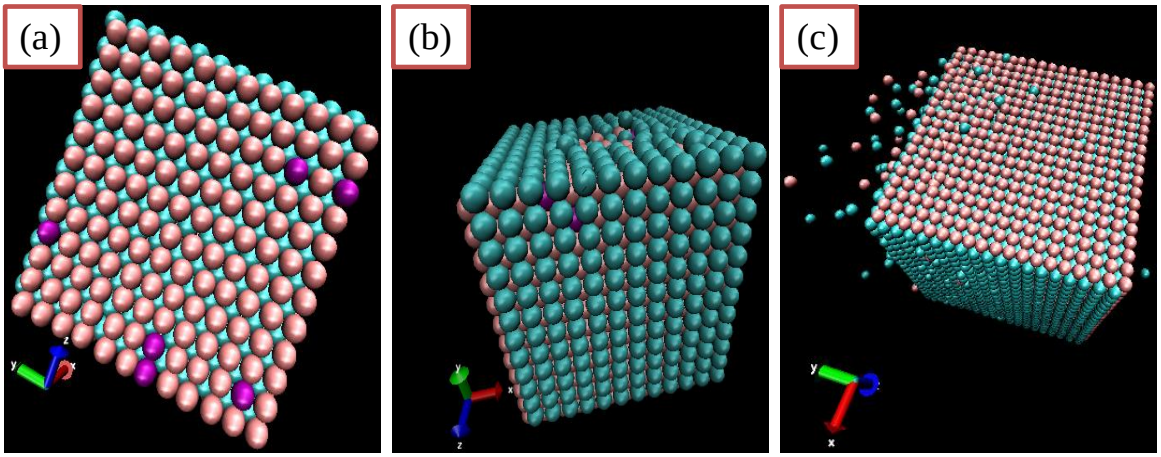

Figure 9: Final film structure at 20Ps (a) Ni-Ti-Cu, (b) Ni-Ti, (c) Ni-Cu.

Now, when the substrate bias for deposition of the film increases, the ad-atom velocity of the film will also increases. Now, for the effect of increasing of ad-atom velocity, the resputtering and reflection will start. Due to this resputtering, the density of ad-atoms differs. As the density of ad-atoms decreases, the thickness of the film will also decreases. Figure 10 shows the different structures of the film at different time intervals.

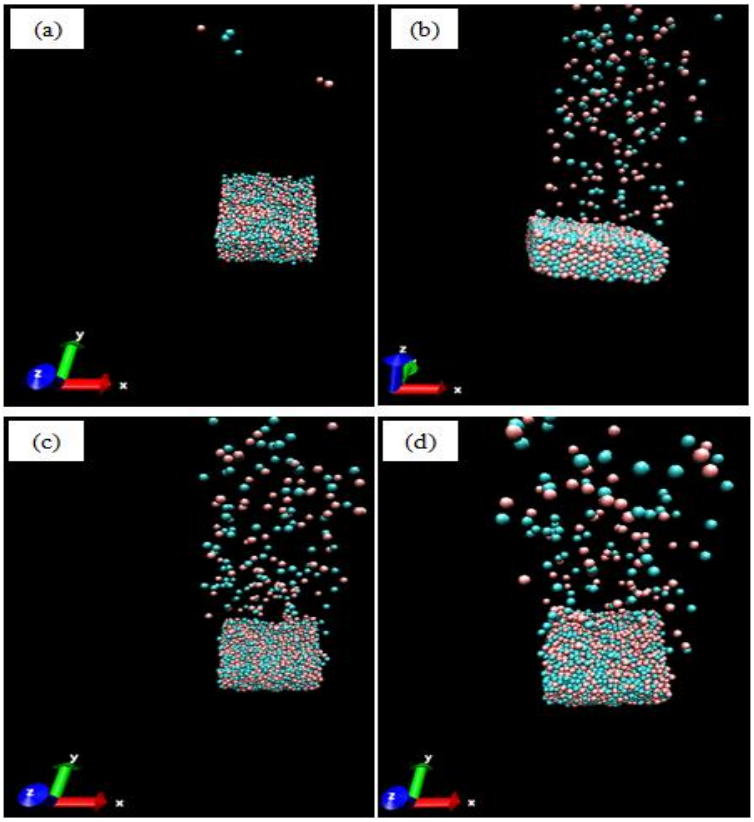

Figure 10: Film Structure of resputtering process started as the negative substrate bias voltage is increasing at different time intervals (a) for time t = 5Ps, (b) for time t = 10Ps, (c) for time t = 15Ps, (d) for time t = 20Ps.

By observing the radial distribution functions, it can be found that, when the sputtering process starts, the atoms from the source or target are deposited on the substrate and the structure becomes more stable. After a certain time, when the resputtering starts, the stability of the film structure is becoming unstable from its previous stable state.Figure 11 shows the radial distribution functions of Ni-Ti, Ni-Cu and Ni-Ti-Cu respectively. The peaks are seems to be dissolved in the graphs which indicates that the stability is decreasing as the time passes by.

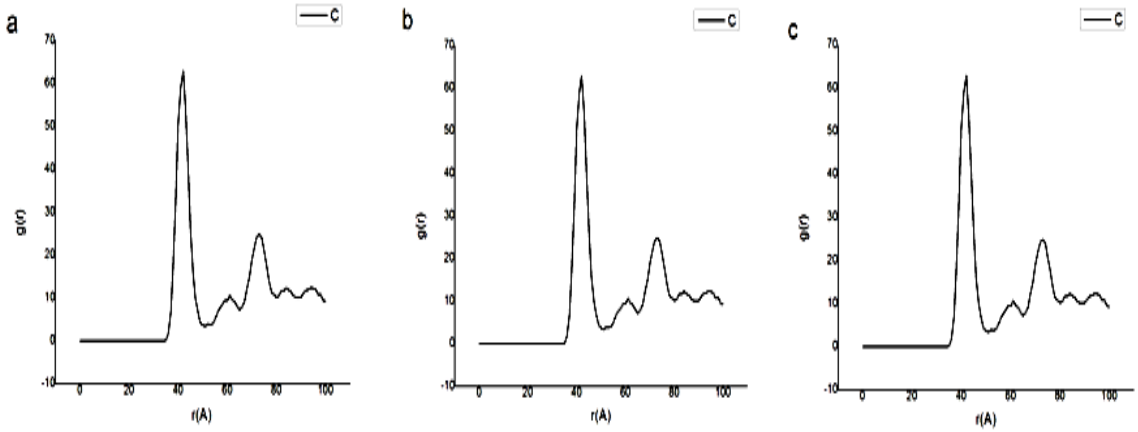

Figure 11: The Radial Distribution Function of (a) Ni-Ti (b) Ni-Cu and (c) Ni-Ti-Cu respectively.

From the Simulations, it is also found from the three processes that the change in the Average temperature of the film occurred as the resputtering starts. Below are the outputs showing increase in the Average temperature of the Film. As the time increases, due to the increase in the number of ad-atoms, the Average Temperature also increases. The thermal profiles of the three processes shows that the thermal stability is less at initial stage and increases as time increases and become quiet linear after a certain time. Figure 12 shows the thermal profiles of Ni-Ti, Ni-Ti-Cu and Ni-Cu respectively.

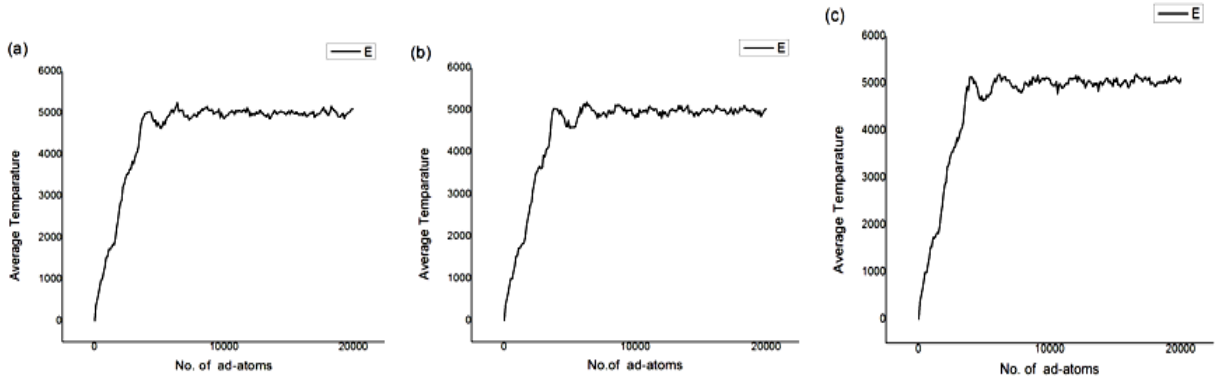

Figure 12: The Thermal Profile of (a) Ni-Ti (b) Ni-Ti-Cu and (c) Ni-Cu respectively.

IV. Conclusion

It can be concluded by performing this research and observing the output that the sputtering process parameters that are substrate bias voltage and temperature play crucial role in this total material deposition process of MEMS fabrication.

As the sputtering process starts, the positive Ar^+ ions are initiated towards the source or target and due to bombardment, the target atoms are deposited onto the substrate material. Now, as the negative substrate bias voltage is applied, the positive ad-atoms are bombarded on the substrate material that causes reflectivity and resputtering from the surface of the substrate. For this resputtering the film becomes unstable. So, for the application of negative substrate bias voltage, the stability decreases drastically.

From the thermal profile it is observed that, due to this bombardment the temperature increases and thermal profile also changes and when bombardment is not take place, thermal profile is nearly stable.

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