

# Qualitative Study of Nanoassembly Process: 2-D Molecular Dynamics Simulations

S.H. Mahboobi<sup>1,3,\*</sup>, A. Meghdari<sup>1,3</sup>, N. Jalili<sup>2</sup> and F. Amiri<sup>3</sup>

Abstract. Precise positioning of nanoclusters through manipulation in the presence of other clusters is one of the main challenging tasks in nanoclusters assembly. Currently, the size of clusters which are used as building blocks is decreasing to a few nanometers. As a result, the particle nature of the matter has a crucial role in manipulator/cluster/substrate interactions. In order to understand and predict the behavior of nanoclusters during the positioning process, it is, therefore, essential to have a deep insight into the aforementioned nanoscale interactions. In this research, 2-D molecular dynamics simulations are used to investigate such behaviors. Performing the planar simulations can provide a rather satisfactory qualitative instrument for our aim while the computation time is considerably decreased in comparison with 3-D simulations. The system considered here is made up of a tip, two clusters and a substrate. The main focus here is on metallic nanoclusters. In order to study the behavior of the above system which is made up of different transition metals, Nose-Hoover dynamics and Sutton-Chen interatomic potential are used. Furthermore, the effect of the material characteristics, tip form and manipulation scheme on the success of the process are examined. Such qualitative simulation studies can pave the pathway towards certain nanopositioning scenarios when considering different working conditions before consuming largescale computation time or high experimental expenses.

Keywords: Metallic nanoclusters; Nanomanipulation; Molecular dynamics simulations.

## INTRODUCTION

Currently, the interest for nanoassembly as a tool for creating nanometer scale sensors, actuators and mechanisms is receiving widespread attentions. Although two-dimensional micro fabrication can be performed by lithography, this approach is not satisfactory for creating complex nano-objects [1]. This goal can be achieved by either self-assembly or controlled nanoassembly. Self-assembly utilizes the inherent property of certain materials to self-assemble or self-organize into regular, crystal patterns [2]. Controlled nanoassembly is based on the controlled manipulation of individual atoms or nanoparticles [3].

Self-assembly has been researched comprehensively during the past decade [4-11]. It should be noted that many nanostructures and nanodevices have asymmetric structures, which most of them cannot be manufactured using self-assembly techniques [12]. This drawback in self-assembly calls for a controlled or robotic-based nanoassembly for creating a variety of patterns and structures. The core of this family of approaches is the nanomanipulation process.

Nanomanipulation includes lifting, placing, arranging, and pushing of nano-scale objects with nanometer precision. Nanomanipulation is one of the major appeals of the nano world [13]. Therefore, many researchers have dealt with nanomanipulation during the past decade [14-18]. In addition, controlled nanoassembly has gained comprehensive attention [12,19-22]. Some major applications are the fabrication of prototype nanoelectronic devices [3] and devices for photonics applications [22]. Controlled or

<sup>1.</sup> Institute for Nanoscience and Nanotechnology, Sharif University of Technology, Tehran, P.O. Box: 14588-89694, Iran.

<sup>2.</sup> Piezoactive Systems Laboratory, Department of Mechanical and Industrial Engineering, Northeastern University, Boston, MA02115, USA.

<sup>3.</sup> Center of Excellence in Design, Robotics and Automation, School of Mechanical Engineering, Sharif University of Technology, Tehran, P.O. Box 11155-9567, Iran.

 $<sup>*. \</sup> Corresponding \ author. \ E-mail: \ mahboobi@sharif.edu$ 

Received 9 February 2010; received in revised form 5 May 2010; accepted 18 May 2010

nanorobotic manipulation and assembly are in their infancy and the physical phenomena at this scale are not completely understood [2]. Being different from the macro-scale, inertial forces become negligible at the nanometer scale. On the other hand, continuum physics changes to molecular physics at the molecular scale.

Presently, employed modeling approaches for nanomanipulation assume bulk properties [13-15], which are based on continuum contact mechanics and long-rage atomic forces. Considering the rapid progress of the field and its applications, the demand for handling ultra-fine nanoparticles (having diameter less than 10 nm) seems to be inevitable. Accordingly, the atomistic features will appear. Moreover, manipulation modeling becomes more complicated if another cluster exists beside the target cluster (i.e. nanoassembly process).

Since Molecular Dynamics (MD) simulations play a significant role in thorough understanding of the nano-scale phenomena, it has been recently used to study nano-scale surface interactions despite the fact that it needs intensive computations [23-26].

The complication of real-time feedback for cluster positions calls for feed-forward control based on precise models. As the physical phenomena at the nano-scale have not yet been entirely understood, the purpose of the present research is to carry out a 2-D qualitative atomistic investigation of nano-scale objects subjected to positioning tasks [27-29] in the presence of other clusters. The manipulator is assumed to be a Scanning Probe Microscope (SPM) tip that has become popular as a simple and accurate manipulation instrument for positioning, assembling, cutting, pushing/pulling, indenting or any other type of interactions [14,15].

#### MOLECULAR DYNAMICS

Molecular dynamics is considered as one of the most frequently utilized numerical methods for modeling material behaviors at the nanoscale. In MD, the motions of the molecules under the action of internal and external force fields are determined separately [30]. These motions are created by the potential energy existing between the atoms and external force fields. Here in this research, FCC metals are studied, and hence, a proper inter-atomic potential for this kind of materials must be selected. In nanomechanics, simple 2-body potentials like the Lenard-Jones potential cannot be utilized to study FCC metals as it does not provide satisfactory estimation of the physical properties of the materials with such structures. Therefore, a multibody long-range potential proposed by Sutton and Chen (SC) [31], which has been used in many physical investigations of FCC metals [32-35] is applied in our study. The general form of the SC potential is [31]:

$$U(r_{ij}) = \varepsilon \left[ \frac{1}{2} \sum_{i} \sum_{j \neq i} V(r_{ij}) - c \sum_{i} \rho_{i}^{\frac{1}{2}} \right],$$
  
$$V(r_{ij}) = \left( \frac{a}{r_{ij}} \right)^{n},$$
  
$$\rho_{i} = \sum_{j \neq i} \left( \frac{a}{r_{ij}} \right)^{m},$$
 (1)

where  $\varepsilon$  is a parameter with the energy dimension, a is a parameter with the dimension of length and is normally taken to be the equilibrium lattice constant, m, n(n > m) and c are positive constants.

In this paper, the modeling of interactions between unlike materials (e.g., between cluster and substrate) has been conducted using the extended SC potential which has been proposed for binary alloys by Rafii-Tabar and Sutton (RTS) [36]. The total energy for the combination of A and B atom types may be written as:

$$E^{\text{RTS}} = \frac{1}{2} \sum_{i} \sum_{j \neq i} V(r_{ij}) - d^{AA} \sum_{i} \hat{p}_{i} \sqrt{\rho_{i}^{A}} - d^{BB} \sum_{i} (1 - \hat{p}_{i}) \sqrt{\rho_{i}^{B}}.$$
 (2)

With:

$$V(r_{ij}) = \hat{p}_i \hat{p}_j V^{AA}(r_{ij}) + (1 - \hat{p}_i)(1 - \hat{p}_j) V^{BB}(r_{ij}) + [\hat{p}_i(1 - \hat{p}_j) + \hat{p}_j(1 - \hat{p}_i)] V^{AB}(r_{ij}),$$
(3)

$$\rho_i^A = \sum_{j \neq i} \phi^A(r_{ij})$$

$$= \sum_{j \neq i} \lfloor \hat{p}_j \phi^{AA}(r_{ij}) + (1 - \hat{p}_j) \phi^{AB}(r_{ij}) \rfloor,$$

$$\rho_i^B = \sum_{j \neq i} \phi^B(r_{ij})$$

$$= \sum_{j \neq i} \lfloor (1 - \hat{p}_j) \phi^{BB}(r_{ij}) + \hat{p}_j \phi^{AB}(r_{ij}) \rfloor, \qquad (4)$$

where the site occupancy operators are defined as:

$$\hat{p}_i = \begin{cases} 1 & \text{if site } i \text{ is occupied by an A atom} \\ 0 & \text{if site } i \text{ is occupied by a B atom} \end{cases}$$
(5)

Four parameters,  $\varepsilon^{AB}$ ,  $a^{AB}$ ,  $m^{AB}$  and  $n^{AB}$ , referring to the interaction between unlike atoms, can be obtained from the parameters from pure case by assuming the mixing rules:

$$m^{AB} = \frac{1}{2}(m^{AA} + m^{BB}),$$

$$n^{AB} = \frac{1}{2}(n^{AA} + n^{BB}),$$

$$a^{AB} = (a^{AA}a^{BB})^{1/2},$$

$$\varepsilon^{AB} = (\varepsilon^{AA}\varepsilon^{BB})^{1/2},$$
(6)

where the parameters  $\varepsilon^{AA}$ ,  $\varepsilon^{BB}$ ,  $a^{AA}$ ,  $a^{BB}$ ,  $m^{AA}$ ,  $m^{BB}$ ,  $n^{AA}$  and  $n^{BB}$  represent the parameters of the SC potentials for the pure A and pure B elements [36]. Parameter values to be used in the present research are listed in Table 1.

Cohesive energy of each material and adhesive energy of material pairs are among the most fundamental aspects of cluster behavior in the performed simulations. Data of cohesive energy per atom for bulk material conditions are listed in Table 1 for ten metals. These data are based on the definition of the SC potential parameters.

Based on the definition of this potential, the cohesive energy per atom is given by:

$$E_c = \frac{\varepsilon S_n^f}{2m} (2n - m). \tag{7}$$

In a perfect FCC crystal,  $S_n^f$  is defined by the following sum [31]:

$$S_n^f = \sum_j \left(\frac{a}{r_j}\right)^n. \tag{8}$$

However, it must be noted that the value of cohesive energy must be corrected for non-bulk materials [37]. Generally, cohesive energy of surface atoms is less than those amounts for bulk materials. Nonetheless, cohesive energy is related to the nominal value depending on the geometry and regardless of material [38]. Thus, we can consider the values reported in Table 1 as a comparison tool for cohesive energy of nanoparticles made of different materials provided that they have the same configurations.

In order to impose the environmental temperature on the system in the simulations, Nose-Hoover dynamics [39,40] is used as a heat bath. Consequently, the equations of motions in the velocity Verlet form have been used for the simulations [30]. The time step is set to 2 femtoseconds.

### SIMULATION METHODOLOGY

Figure 1 displays the form of the tip/clusters/substrate system for assembly purpose by a SPM as a manipulator during the nanomanipulation process. The motion of each atom is limited to the (111) plane in the FCC lattice since the simulation is two-dimensional. Therefore, the simulation time decreases in comparison to its 3-D counterpart [41] and most of the qualitative



Figure 1. Tip/clusters/substrate configuration in assembly process.

**Table 1.** Parameters of the Sutton-Chen potentials and cohesive energy per atom  $(E_c)$  [31].

Element	m	n	a(A)	$arepsilon( extbf{eV})$	c	$c\ (1\ 1\ 1)$	$E_c \ (\mathrm{eV})$
Ni	6	9	3.52	$1.5707 \times 10^{-2}$	39.432	28.798	4.44
Cu	6	9	3.61	$1.2382 \times 10^{-2}$	39.432	28.798	3.50
Rh	6	12	3.80	$4.9371 \times 10^{-3}$	144.41	107.759	5.75
Pd	7	12	3.89	$4.1790 \times 10^{-3}$	108.27	78.762	3.94
Ag	6	12	4.09	$2.5415 \times 10^{-3}$	144.41	107.759	2.96
Ir	6	14	3.84	$2.4489 \times 10^{-3}$	334.94	183.572	6.93
Pt	8	10	3.92	$1.9833 \times 10^{-2}$	34.408	24.411	5.86
Au	8	10	4.08	$1.2793 \times 10^{-2}$	34.408	24.411	3.78
Pb	7	10	4.95	$5.5765 \times 10^{-3}$	45.778	32.936	2.04
Al	6	7	4.05	$3.3147 \times 10^{-2}$	16.399	11.453	3.34

properties and physical phenomena can also be revealed by these 2-D tests.

Because of the limited number of atoms in the system, for performance reasons, shock wave reflection from boundaries will be an inevitable phenomenon that may lead to local melting on the substrate surface [42]. Although this artifact is observed more in impacts of large or high energy clusters, it can be an undesirable issue in our simulations. An immediate solution is enlarging the substrate size as large as possible for computational facilities. However, some other systematic approaches have been used by researchers especially in simulation of surface bombardment and cluster penetration [43]. Naming a few, we can mention the usage of the generalized Langevin equation approach [44,45] and other schemes to prevent the reflection of the pressure wave from the fixed boundaries [46]. Application of a proper heat bath, as used in our simulations, can also reduce this effect by dissipating the excessive energy of the system based on a certain temperature. Nonetheless, since the dynamics equations of the system act on the temperature of the whole substrate, some local heat rises may appear in contact areas.

At the beginning of the test, atoms of nanocluster and substrate possess their minimum-energy form while passing through the relaxation phase. Afterwards, the nanocluster will be subjected to a certain assembly strategy which is applied by the manipulator tip. While the manipulator travels with a constant speed, the nanocluster is pulled or pushed in the same way and toward the other cluster. For simplicity, the tip atoms are tightened together and form a rigid body. In order to go through realistic conditions regarding the bulk material properties, the outer layers of substrate are confined to have no motion in both vertical and horizontal axes (the atoms which are colored in black in Figure 1).

While the nanoclusters are made of different transition metals such as Ni, Cu and Pt (having diameters of 43, 44 and 48 Angstrom respectively), the substrate and tip are made of Au and Ag, respectively. The temperature has been held constant at 1 K during all of the simulations. Other simulation parameters include assembling scheme and the tip form. The major purpose of the executed simulations has been the qualitative analysis of the manipulation-based assembly process plus making decisions on their level of success.

#### NANOASSEMBLY SCENARIOS

There are various practical strategies for positioning tasks. Here we deal with three major scenarios to be used in nanocluster manipulation in the presence of another cluster to be adhered to the first one. These schemes are shown in Figures 2a-2c. Two different



Figure 2. Different strategies for positioning in the assembly process. (a) Push-pull; (b) push-up; and (c) pull-up.

phases are assumed: positioning and releasing. They are schematically depicted in these figures by a singleline releasing. They are schematically depicted in these figures by a single-line and double-line arrow, respectively. The latter usually possesses higher speed than the former. We consider two types of positioning, as well as two types of releasing. The first cluster maybe pushed or pulled by the tip (see Figures 2a and 2b for pushing and Figure 2c for pulling). The tip stroke in the first phase equals the initial distance between clusters. After the push-type positioning, the cluster can be released either by high speed pulling back or tip-lifting. It should be mentioned that because of the existence of the second cluster, only the second separation approach is practical for the releasing phase after pull-type positioning. Each scenario has its own characteristics which considerably affect the process success addressed in the performed simulations.

## SIMULATION RESULTS

As mentioned earlier, our main objective here is to qualitatively study and determine various assembly cases. Therefore, the effect of versatile factors on the manipulation quality will be revealed. According to the nanopositioning purpose of the process, to have a successful assembly, the average distance traveled by

the atoms of the nanoparticle during the first phase should be very close to the distance traveled by the manipulator tip. The last location of the positioning phase must remain unchanged during the release phase. Furthermore, the location of the second nanocluster must stay unchanged during the process to provide the desired pattern. The intactness of the particle during the process is another success criterion. A variety of simulations have been carried out to investigate the nanomanipulation process considering different material types, tip forms and assembly scenarios. Τwo employed tip forms are triangular and circular. In all of the simulations, the position of each cluster is determined by the average position of its atoms. At the beginning of the simulation, the clusters are positioned with a 50 A gap between them. The second phase starts when the tip travels as much as the gap between clusters (50 A in the performed simulations).

#### Strategy 1 (Push-Pull)

The first scenario includes a pushing phase and a high speed pulling back release phase. Figure 3 illustrates some snapshots of the simulated process at the final point of the second phase for different conditions. Figures 3a and 3b depict the assembly by triangular tip for Ni and Pt clusters, respectively. Both of these cases were considered as failure but in different ways. In the case of Ni clusters, adhesion of the first cluster to the tip and the other cluster in the returning phase leads to process failure. Referring to cohesive energy data, usage of the RTS formalism predicts the adhesion of Ag-Ni and Ag-Cu pairs to be higher than cohesive energies of Ni and Cu, respectively. However, long



Figure 3. Cluster pairs at the final point of the second phase of strategy #1 for different materials and tip shapes. (a) Ni clusters and triangular tip; (b) Cu clusters and triangular tip; (c) Pt clusters and triangular tip; (d) Ni clusters and circular tip; (e) Cu clusters and circular tip; and (f) Pt clusters and circular tip.

contact line to the tip can lead to the pulling of the assembled clusters. This occurs because the Pt doesn't find the opportunity to adhere to the second cluster. On the other hand, in the case of Pt clusters, the adhesion only occurs between the first cluster and the tip.

Usage of circular tip leads to same problem for the Ni cluster (see Figure 3c) while it solves the issue for Pt clusters (see Figure 3d). On the contrary, for the Cu clusters, the assembly cannot be performed. This may be because of the low adhesion energy between the clusters (the same as the cohesive energy) or missing the opportunity of adhesion as a result of the inaccurate positioning phase. Regarding the manipulation of Pt by the circular tip, we can observe a proper performance and formation of the desired assembly (see Figure 4c). In contrast to the manipulation by the triangular tip, in this case, usage of the circular tip leads to the more accurate positioning and less adhesion to the tip in the release phase. Another observed phenomenon is the piled-up surface in the space between the clusters because of the confining nature of 2-D simulations.

Distances traveled by the clusters in comparison with the desired position (indicated by solid line) in the case of triangular and circular tips are illustrated in Figures 4a to 4d. It should be noted that the desired position for the second cluster is stationary. Although all three examined materials (Ni, Cu and Pt) show an acceptable behavior in the pushing phase, the high speed pulling back may not be promising for releasing purposes.

#### Strategy 2 (Push-Up)

The second scenario includes a pushing phase and a tip-lifting release phase. Figures 5a to 5d depict some illustrative examples of the results gained by this positioning scheme. In Figures 5a and 5b one can see the Ni and Pt clusters, respectively, while manipulated by a triangular tip at the final point of the second phase. The former case is qualitatively successful while the latter case fails based on the fact that the clusters are not adhered together. Similar phenomena occur when using the circular tip for Ni clusters (see Figure 5c). In contrast to the case of the triangular tip, adhesion of the Pt cluster to the circular tip in upward motion leads to the process failure (see Figure 5d).

Distances traveled by the clusters in comparison to the desired position (indicated by solid line) in the case of triangular and circular tips are illustrated in Figures 6a to 6d. The main drawback of this scheme is due to the offset caused by the attraction to the tip in the second phase. This can be solved by a proper change in the trajectory of the tip by pushing the tip farther than the desired position. The simu-



Figure 4. Distances traveled by the clusters in comparison with the desired position for different materials and tip shapes in strategy #1. (a) First cluster (triangular tip); (b) second cluster (triangular tip); (c) first cluster (circular tip); and (d) second cluster (circular tip).



Figure 5. Cluster pairs at the final point of the second phase of strategy #2 for different materials and tip shapes. (a) Ni clusters and triangular tip; (b) Pt clusters and triangular tip; (c) Ni clusters and circular tip, and (d) Pt clusters and circular tip.

lations were repeated, incorporating offsets in the tip motion target. Consequently, the first cluster will be moved farther than the desired position to compensate for the backlash occurred in the detachment phase. The illustrated results in Figures 7a and 7b are the evidences for the improvement of the process caused by the implemented approach. Although one may think of feedback compensation to solve this issue, lack of realtime sensing calls for feed-forward control approaches in such cases.

#### Strategy 3 (Pull-Up)

The third positioning method includes a pulling stage followed by lifting the tip for detachment. The simulations have been repeated for this last scheme as well as for others. Some of the simulation results are illustrated in Figures 8a to 8d. These snapshots are captured at the final point of the second phase. Based on the obtained results, Ni and Cu clusters showed an acceptable capability to be manipulated by a triangular tip but not by a circular one. In contrast, the Pt cluster adheres to both types of tip. Such



Figure 6. Distances traveled by the clusters in comparison with the desired position for different materials and tip shapes in strategy #2. (a) First cluster (triangular tip); (b) second cluster (triangular tip); (c) first cluster (circular tip), and (d) second cluster (circular tip).



Figure 7. Distances traveled by the clusters in comparison with the desired position for different materials and tip shapes in strategy #2 with compensation. (a) First cluster (triangular tip), and (b) second cluster (triangular tip).



Figure 8. Cluster pairs at the final point of the second phase of strategy #3 for different materials and tip shapes. (a) Ni clusters and triangular tip; (b) Pt clusters and triangular tip; (c) Ni clusters and circular tip; and (d) Pt clusters and circular tip.

results make this approach unreliable. However this was predictable for the circular tip case because of the high amount of space prevention caused by this tip form.

Distances traveled by the clusters in comparison with the desired position (indicated by solid line) in the case of triangular and circular tips are illustrated in Figures 9a to 9d. Similar to the second approach, the main drawback of this scheme, in addition to adhesion to the tip, is the offset caused by the attraction to the tip in the second phase that can be solved by a proper change in the trajectory of the tip. Here in contrast with the second scenario, the compensation can be realized by pushing the tip less than the desired distance.

## CONCLUDING REMARKS

The present research deals with an atomistic study of the controlled robotic nanoassembly process that is carried out by applying a series of planar molecular dynamics simulations. The decision on the success level of the above process under different circum-



Figure 9. Distances traveled by the clusters in comparison with the desired position for different materials and tip shapes in strategy #3. (a) First cluster (triangular tip); (b) second cluster (triangular tip); (c) first cluster (circular tip); and (d) second cluster (circular tip).

stances can be made using this approximate qualitative approach. In fact, in comparison with more detailed 3-D simulations, this approach can decrease the computation time significantly. Three different manipulation schemes, namely, push-pull, push-up and pull-up were examined to realize the assembly process. The SPM tip and the substrate were made of Ag and Au, respectively. Ni, Cu and Pt clusters were selected to be manipulated. The tip appears in two forms: triangular and circular. All possible combinations were examined and the molecular placements were recorded and depicted as snapshots. These illustrative outcomes and a comparison between real and desired cluster positions lead to a comprehensive knowledge about the role of each factor in the success or failure of the whole procedure.

According to the simulation results, the pulling approach possesses a more satisfactory positioning capability in comparison to pushing. It should be mentioned that while adhesion due to the pulling process may be promising for positioning task in some cases, it leads to poor outcomes for pulling-based detachment. Taking into account some prescribed corrections, the tip lifting approach can be a suitable candidate for the release phase. Cluster position change during the second phase (which is created by tip attraction) can be regarded as the major weakness of the lifting approach. This existing offset can be compensated for by drifting the positioning final point back and forth for pulling and pushing approaches, respectively. Moreover, the characteristics of the materials can play an important role in the process. As the simulation results demonstrated, Ni and Cu clusters have quite acceptable behavior under the test circumstances while the attachment of Pt clusters to the tip results in failure in some test examples. These behaviors were affected not only by the tip form but also by the positioning strategy.

Generally, cohesive energy of materials and adhesion energy of cluster/substrate pairs play fundamental roles in the behavior observed in the manipulation. In this viewpoint, more commensurate pairs show the more adhesive behavior which shows its extreme form for completely similar pairs. Nonetheless, some contradictory behaviors observed in the obtained results makes us aware of the dangers of predicting the test results solely based on various limited theoretical aspects. On the other hand, this is the essence of these sorts of computational tests whose results are dependent on a wide range of connecting parameters and individual atomistic configurations, and which sometimes do not have any straight-forward interpretation. For example, the great dependence of cohesion and adhesion behavior of the system parts on their geometrical aspects and their mutual interfaces, as well as, values for the cohesive energy per their individual

atoms makes the interpretation and explanation of some behaviors highly complicated.

The knowledge gained through this dissertation is highly beneficial for further experiments in order to be able to plan the conditions and routines which guarantee more effective nanomanipulation. Nonetheless, we must be aware of the drawbacks of the simulation methodology and the possible inaccuracies. Some of the observed behavior and deformations are artifacts due to simulation conditions. Mentioning a few of the limiting issues, we can name the tip rigidity, limited size of substrate, high pushing speed and the inherent limitation of 2-D tests. In addition, the approximations due to the interatomic potential are other sources of imperfect simulations.

#### REFERENCES

- Rubio-Sierra, F.J., Heckl, W.M. and Stark, R.W. "Nanomanipulation by atomic force microscopy", *Advanced Engineering Materials*, 7(4), pp. 193-196 (2005).
- Pereira, G.G. "Towards nano-scale devices via selfassembly", Current Applied Physics, 4(2-4), pp. 255-258 (2004).
- Requicha, A.A.G. "Nanorobots, NEMS, and nanoassembly", Proceedings of the IEEE, Special Issue on Nanoelectronics and Nanoprocessing, 91(11), pp. 1922-1933 (2003).
- Heister, K., Frey, S., Ulman, A., Grunze, M. and Zharnikov, M. "Irradiation sensitivity of self-assembled monolayers with an introduced 'weak link' ", *Langmuir*, **20**(4), pp. 1222-1227 (2004).
- Krupke, R., Malik, S., Weber, H.B., Hampe, O., Kappes, M.M. and Löhneysen, H.V. "Patterning and visualizing self-assembled monolayers with low-energy electrons", *Nano Lett.*, 2(10), pp. 1161-1164 (2002).
- Harnett, C.K., Satyalakshmi, K.M. and Craighead, G. "Low-energy electron-beam patterning of aminefunctionalized self-assembled monolayers", *Appl. Phys. Lett.*, 76(17), pp. 2466-2468 (2000).
- Maeng, I.S. and Park, J.W. "Patterning on selfassembled monolayers by low-energy electron-beam irradiation and its vertical amplification with atom transfer radical polymerization", *Langmuir*, 19(10), pp. 4519-4522 (2003).
- Sun, S. and Leggett, G.J. "Generation of nanostructures by scanning nearfield photolithography of self-assembled monolayers and wet chemical etching", *Nano Lett.*, 2(11), pp. 1223-1227 (2002).
- Smith, R.K., Lewis, P.A. and Weiss, P.S. "Patterning self-assembled monolayers", *Prog. Surf. Sci.*, 75(1-2), pp. 1-68 (2004).
- Gao, Y.F. and Suo, Z. "Guided self-assembly of molecular dipoles on a substrate surface", J. Appl. Phys., 93(7), pp. 4276-4282 (2003).

- Plass, R., Last, J.A., Bartelt, N.C. and Kellog, G.L. "Selfassembled domain patterns", *Nature*, 412(6850) p. 875 (2001).
- Li, G., Xi, N., Chen, H., Pomeroy, C. and Prokos, M. "Videolized atomic force microscopy for interactive nanomanipulation and nanoassembly", *IEEE T Nanotech.*, 4(5), pp. 605-615 (2004).
- Sitti, M. and Hashimoto, H. "Controlled pushing of nanoparticles: modeling and experiments", *IEEE/ASME Transactions on Mechatronics*, 5(2), pp. 199-211 (2000).
- Sitti, M. "Atomic force microscope probe based controlled pushing for nanotribological characterization", *IEEE/ASME Trans. Mechatronics*, 9(2), pp. 343-349 (2004).
- Hla, S.W., Braun, K.F., Iancu, V. and Deshpande, A. "Single atom extraction by scanning tunneling microscope tip-crash and nanoscale surface engineering", *Nano Lett.*, 4(10), pp. 1997-2001 (2004).
- Lagoute, J., Kanisawa, K. and Fölsch, S. "Manipulation and adsorption-site mapping of single pentacene molecules on Cu(111)", *Phys. Rev. B.*, **70**(24), pp. 245415 (1-6) (2004).
- Rollot, Y., Regnier, S. and Guinot, J.C. "Simulation of micro-manipulations: adhesion forces and specific dynamic models", *Int. J. Adhesion & Adhesives*, 19(1), pp. 35-48 (1999).
- Mokaberi, B. and Requicha, A.G. "Drift compensation for automatic nanomanipulation with scanning probe microscope", *IEEE Transaction on Automation Sci*ence and Engineering, 3(3), pp. 199-207 (2006).
- Murray, C.B., Bawendi, M.G. and Kagan, C.R. "Synthesis and characterization of monodisperse nanocrystals and close-packed nanocrystal assemblies", Annu. Rev. Mater. Sci., 30, pp. 545-610 (2000).
- Li, G., Xi, N. and Yu, M. "Development of augmented reality system for AFM based nanomanipulation", *IEEE/ASME T Mechatronics*, 9(2), pp. 199-211 (2004).
- Decossas, S., Mazen, F., Baron, T., Bremond, G. and Souifi, A. "Atomic force microscopy nanomanipulation of silicon nanocrystals for nanodevice fabrication", *Nanotechnology*, 14(12), pp. 1272-1278 (2003).
- 22. Garcia-Santamaria, F., Miyazaki, H.T., Urquia, A., Ibisate, M., Belmonte, M., Shinya, N., Meseguer, F. and Lopez, C. "Nanorobotic manipulation of microspheres for on-chip diamond architectures", Advanced Materials, 14(16), pp. 1144-1147 (2002).
- Bhushan, B., Israelachvili, J.N. and Landman, U. "Nanotribology: Friction, wear and lubrication at the atomic scale", *Nature*, **374**(6523), pp. 607-616 (1995).
- Landman, U., Luedtke, W.D., Burnham, N.A. and Colton, R.J. "Atomistic mechanisms and dynamics of adhesion, nanoindentation, and fracture", *Science*, 248(4954), pp. 454-461 (1990).

- Landman, U., Luedtke, W.D. and Nitzan, A. "Dynamics of tip-substrate interactions in atomic force microscopy", Surface Science, 210(3), pp. L177-L184 (1989).
- Mahboobi, S.H., Meghdari, A., Jalili, N. and Amiri, F. "Molecular dynamics simulation of manipulation of metallic nanoclusters on double-layer substrates Robbins", *Physica E*, 42(9), pp. 2364-2374 (2010).
- Mahboobi, S.H., Meghdari, A., Jalili, N. and Amiri, F. "Planar molecular dynamics simulation of Au clusters in pushing process", *Int. J. Nanomanufacturing*, 5(3/4), pp. 288-296 (2010).
- Mahboobi, S.H., Meghdari, A., Jalili, N. and Amiri, F. "Qualitative study of nanocluster positioning process: Planar molecular dynamics simulations", *Current Applied Physics*, 9(5), pp. 997-1004 (2009).
- Mahboobi, S.H., Meghdari, A., Jalili, N. and Amiri, F. "Two-dimensional atomistic simulation of metallic nanoparticles pushing", *Modern Physics Letters B*, 23(22), pp. 2695-2702 (2009).
- Rafii-Tabar, H. "Modelling the nano-scale phenomena in condensed matter physics via computer-based numerical simulations", *Physics Reports*, **325**(6), pp. 240-310 (2000).
- Sutton, A.P. and Chen, J. "Long-range Finnis-Sinclair potentials", *Philosophical Magazine Letters*, 61(3), pp. 139-146 (1990).
- Rafii-Tabar, H., Shodja, H.M., Darabi, M. and Dahi, A. "Molecular dynamics simulation of crack propagation in fcc materials containing clusters of impurities", *Mechanics of Materials*, 38(3), pp. 243-252 (2006).
- Nayak, S.K., Khanna, S.N. and Jena, P. "Thermodynamics of small nickel clusters", J. Phys.: Condensed Matter, 10(48), pp. 10853-10862 (1998).
- Todd, B.D. and Lynden-Bell, R.M. "Surface and bulk properties of metals modelled with Sutton-Chen potentials", Surface Science, 281(1-2), pp. 191-206 (1993).
- Doye, J.P.K. and Wales, D.J. "Global minima for transition metal clusters described by Sutton-Chen potentials", New J. Chem., 22(7), pp. 733-744 (1998).
- Rafii-Tabar, H. and Sutton, A.P. "Long-range Finnis-Sinclair potentials for fcc metallic alloys", *Philosophi*cal Magazine Letters, 63(4), pp. 217-224 (1990).
- Yaghmaee, M.S. and Shokri, B. "Effect of size on bulk and surface cohesion energy of metallic nanoparticles", *Smart Mater. Struct.*, 16(2), pp. 349-354 (2007).
- Shandiz, M.A. "Effective coordination number model for the size dependency of physical properties of nanocrystals", J. Phys.: Condens. Matter, 20(32), pp. 325237 (1-9) (2008).
- Nose, S.A. "A unified formulation of the constant temperature molecular dynamics methods", *Journal of Chemical Physics*, 81(1), pp. 511-519 (1984).
- Hoover, W.G. "Canonical dynamics: equilibrium phase-space distributions", *Physical Review A*, **31**(3), pp. 1695-1697 (1985).

- Mahboobi, S.H., Meghdari, A., Jalili, N. and Amiri, F. "Precise positioning and assembly of metallic nanoclusters as building blocks of nanostructures: A molecular dynamics study", *Physica E*, 42(2), pp. 182-192 (2009).
- Samela, J., Kotakoski, J., Nordlund, K. and Keinonen, J. "A quantitative and comparative study of sputtering yields in Au", Nuclear Instruments and Methods in Physics Research B, 239(4), pp. 331-346 (2005).
- Postawa, Z., Czerwinski, B., Szewczyk, M., Smiley, E.J., Winograd, N. and Garrison, B.J. "Enhancement of sputtering yields due to C-60 versus Ga bombardment of Ag{111} as explored by molecular dynamics simulations", Anal. Chem., 75(17), pp. 4402-4407 (2003).
- Henery, R.J. "The generalized Langevin equation and the fluctuation-dissipation theorems", J. Phys. -A: Gen. Phys., 4(5), pp. 685-694 (1971).
- Garrison, B.J., Kodali, P.B.S. and Srivastava, D. "Modeling of surface processes as exemplified by hydrocarbon reactions", *Chem. Rev.*, 96(4), pp. 1327-1342 (1996).
- Schafer, C., Urbassek, H.M., Zhigilei, L.V. and Garrison, B.J. "Pressure-transmitting boundary conditions for molecular-dynamics simulations", *Computational Materials Science*, 24(4), pp. 421-429 (2002).

#### BIOGRAPHIES

Seyed Hanif Mahboobi received his B.S., M.S. and Ph.D. degrees in Mechanical Engineering from Sharif University of Technology in 2002, 2004 and 2009, respectively. He is currently a postdoctoral researcher at Institute for Nanoscience and Nanotechnology (INST) and a member of Center of Excellence in Design, Robotics and Automation (CEDRA) at Sharif University of Technology. His research interests include Robotics, Nanomanipulation, Computational Nanoscience, Nonlinear Dynamics and Control.

Ali Meghdari received his Ph.D. in Mechanical Engineering from the University of New Mexico in 1987. In 1988, he joined the Sharif University of Technology in Tehran as an Assistant Professor of Mechanical Engineering. In 1997, he was granted the rank of Full-Professor of Mechanical Engineering at Sharif University of Technology. Dr Meghdari has performed extensive research in the areas of Robotics Dynamics, Flexible Manipulators Kinematics/Dynamics, and Dynamic Modeling of Biomechanical Systems. He has published over 140 technical papers in refereed international journals and conferences, and has been the recipient of various scholarships and awards, the latest being the 2001 Mechanical Engineering Distinguished. He was also nominated and elected as a Fellow of the ASME (American Society of Mechanical Engineers) in 2001. He is currently a Professor and the Vice-President of Academic Affairs and the Director of the Center of Excellence in Design, Robotics and Automation (CEDRA) at the Sharif University of Technology.

Nader Jalili joined the faculty of Northeastern University in September 2009 from Clemson University (Clemson, South Carolina) where he was a tenured Associate Professor and Assistant Professor since 2000. Dr. Jalili is currently an Associate Editor of ASME Journal of Dynamic Systems, Measurement and Control, and founding Chair of ASME Dynamic Systems and Control Division (DSCD) Technical Committee on Vibration and Control of Smart Structures. As a past Technical Editor of IEEE/ASME Transactions on Mechatronics, he is the author/co-author of more than 250 peer-refereed technical publications including over 90 journal papers. His research interests include Piezoelectric-Based Actuators and Sensors, Dynamic Modeling and Vibration Control of Distributed-Parameters Systems, Dynamics and Control of Microelectromechanical and Nanoelectromechanical Sensors and Actuators, and Control and Manipulation at the Nanoscale.

**Farshid Amiri** received his B.S. and M.S. degrees in Mechanical Engineering from Sharif University of Technology in 2003 and 2006. He also holds B.S. in Electrical Engineering from Sharif University of Technology. His research interests include Robotics, Computational Nanoscience, Machine Design, Automation and Control.