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Precise positioning and assembly of metallic nanoclusters as building blocks of nanostructures: A molecular dynamics study

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ABSTRACT

Molecular dynamics simulations are used to study the manipulation of metallic nanoclusters. These particles are assumed as potential building blocks for bottom-up manufacturing of nanoscale structures. One of the key factors in the assembly of nanoclusters is the precise positioning of them by a manipulation system. Prediction of the corresponding behavior under the influence of working conditions is of crucial importance for planning of controlled positioning and assembly of nanoclusters. The focus of the present research is on ultra-fine metallic nanoclusters. The effects of material type and manipulation strategy on the success of the process have been investigated by molecular dynamics. Such qualitative simulation studies can evaluate the chance of success of a certain nanopositioning scenario regarding different working conditions before consuming high experimental expenses.

1. Introduction

Metallic clusters are among the best candidates to be utilized as building blocks for construction of nanostructures. Rieth and Schommers [1] have used molecular dynamics to investigate the meta-stable states of clusters. In addition, they have studied the deviation of clusters from bulk properties and their undesirable deformation under different conditions. In addition, they could be vulnerable to the forced movement during controlled development of complex nanostructure namely "nanomanipulation".

Nanomanipulation is a promising tool for creating nanometer scale structures and has been a replacement for lithography approaches in some special cases [2]. One of the first experimented nanomanipulations was done by Eigler and Schweizer [3] using STM. They formed the 'IBM' logo by single atoms. Many researchers have addressed nanomanipulation during the past decade [2–14]. Some of the performed nanomanipulation processes are applied to single atoms [3–5], nanowires [6], nanotubes [7], functional biological structures [8–11] and micro/nanoparticles [2,12–14].

Manipulation of particles with dimensions of a few nanometres has a great impact on nanometer scale technology. Patterns of metallic nanoparticles can be constructed by SPM manipulation [15]. Prototype fabrication of tiny electrodes and metallic contact point are one of their applications. The fabricated structures can be used to store digital information [15] and single-electron devices [16].

Precise manipulation and assembly of nanoparticles is crucial for these aims. Hence, a reliable modeling approach of the underlying phenomena is highly demanded for the prediction of the performance of manipulation routines. Currently, utilized modeling approaches for nanomanipulation assume the bulk properties [17–19]. They are based on continuum contact mechanics and long-rage atomic forces.

Because of the emergence of particle nature of matters at the nanometer scale, continuum mechanics approaches cannot lead to precise modeling of the occurred phenomena. Therefore, molecular dynamics (MD) simulations may compensate for this issue [20–22]. This method has been used comprehensively for modeling of surface interactions [23,24].

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In this paper, the processes of positioning and assembly of metallic nanoparticles are modeled and simulated using molecular dynamics. These processes aim at precise positioning of nanoclusters individually or in the presence of other clusters. The aim of the performed simulation is to study the role of working conditions on the quality and the feasibility of these processes. The involved working conditions are material type and manipulation strategy. General approach of the studied manipulation process is contact-based mechanical pushing to be realized by the scanning probe microscope (SPM).

2. Modeling and simulation methodology

The scope of our study is limited to metals with FCC structure. A multi-body long-range potential proposed by Sutton and Chen (SC) [25] is adopted here. The general form of the SC potential is

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

where ε is a parameter with 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 the positive constants. The use of SC potential has been extended to binary alloys by Rafii-Tabar and Sutton [26], which will be utilized to model the interactions of unlike materials (e.g., between cluster and substrate) in our studies. Four parameters, ε^{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

$$m^{AB} = \tfrac{1}{2}(m^{AA}+m^{BB})$$
$$n^{AB} = \tfrac{1}{2}(n^{AA}+n^{BB})$$
$$a^{AB} = (a^{AA}a^{BB})^{1/2}$$
$$\varepsilon^{AB} = (\varepsilon^{AA}\varepsilon^{BB})^{1/2} \quad (2)$$

where the parameters ε^{AA}, ε^{BB}, c^{AA}, c^{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. Parameter values to be used in the present research are listed in Table 1.

In the simulations, Nose–Hoover dynamics [27,28] is utilized as a heat bath to impose the environmental temperature on the system. Accordingly, the equations of motions in the velocity Verlet form have been used for simulations [29].

Fig. 1 depicts the configuration of the tip/cluster/substrate system during the nanomanipulation process. First, the system passes through the relaxation phase in which atoms of the nanoparticle and substrate take their minimum-energy

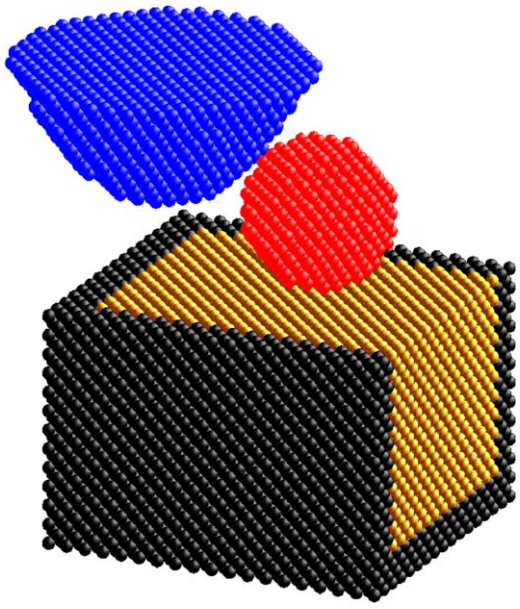

Fig. 1. Configuration of the tip/cluster/substrate system during the nanomanipulation process.

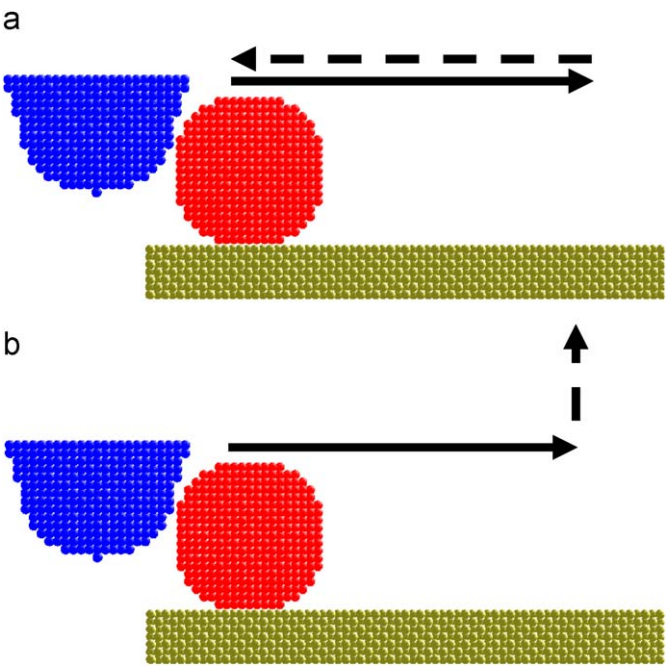

Fig. 2. Different strategies for positioning process (a) push-pull and (b) push-up.

Table 1
Parameters of the Sutton–Chen potentials [14].

Element	m	n	ε(eV)	c
Ni	6	9	1.5707×10^{-2}	39.432
Cu	6	9	1.2382×10^{-2}	39.432
Pd	7	12	4.1790×10^{-3}	108.27
Ag	6	12	2.5415×10^{-3}	144.41
Ir	6	14	2.4489×10^{-3}	334.94
Pt	8	10	1.9833×10^{-2}	34.408
Au	8	10	1.2793×10^{-2}	34.408