

# Simulating the Dynamics of Bimetallic Clusters Deposited onto a Surface Using Molecular Dynamics

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## Abstract

This paper examines the interface development between a single crystalline Ag matrix and core-shell Ag<sub>n</sub>Co<sub>m</sub> nanoclusters that have been deposited with energies varying between 0.25 eV and 1.5 eV per atom using computer modeling techniques. Clusters undergo deformation as a result of the slowing down; they may also become epitaxial with the substrate and maintain their core-shell structure. A detailed analysis of the effects of the cluster-surface interaction is conducted over a realistic size and energy range, and a model is created to show how clusters accumulate. It is discovered that both the silver shells and the cobalt cluster cores exhibit limited epitaxy with the substrate, and that the contact produced is only a few atomic layers thick. The effect is higher for Ag shells than for Co cores, and it is not very energy dependent.

## Keywords

Cluster, Slowing Down, Low-Energy, Molecular Dynamics, Metropolis Monte Carlo, Bi-Metallic

## 1. Introduction

Progress is reported in understanding the features of bimetallic nanoparticles, their surface contact following low-energy deceleration, and the properties of nanostructured materials fabricated with these particles. The average composition of a nanoparticle ranges from a few hundred for the tiniest ones to several thousand for the larger ones that are described here. Quantization gives rise to the properties of an atom, and the molecules they make up are no different. This means that it also applies to the tiniest nanoparticles. Conversely, many macro-

scopic material properties can be well explained by a classical approach, and nanoparticles appear as entities that exist on the border between classical and quantum behaviors. In examining their characteristics, atomic-scale techniques appear to be a natural fit, whether using a quantum or classical approach. Atoms are thought of as distinct entities that only interact with each other through the electrons in their outer shell. However, even with this approximation, the computing burden of calculating the Schrödinger equation increases with the number of participating atoms. Relativistic effects exacerbate the problem for the biggest constituents. Currently, the only workable solution in such situations is the conventional technique. It is common practice to use *ab initio* simulations to predict the configurations of tiny particles as well as their electrical and magnetic properties. In theory, the method is precise. Nevertheless, concerns about the origin of correlation exchange and the difficulty of developing effective numerical methods suggest that experimental validation is often required. When it comes to atomic interactions, the classical technique uses semi-empirical models that are calibrated according to solid-state properties at low energies (about cohesive energies or lower) and atomic collision properties at high energies (approximately matching core electron binding energies or higher). The interactions covered in this paper, such as those between atoms within a nanoparticle and those between nanoparticles and surfaces, belong to the latter group. Potential functions for these interactions are defined using a variety of microscopic and macroscopic bulk material parameters, and are parameterized by means of the local electron density or hopping integrals. It is clear, though, that there is no guarantee of correct prediction of other qualities, and that experimental data must be compared.

The alignment of experimental data with *ab initio*, classical methodologies has not been thoroughly studied in systematic ways, probably because measuring particles that are not interacting with their environment is difficult. Experimental, classical, and *ab initio* modeling investigations are conducted in [1] to ascertain the geometry and stability of small bimetallic silver-clusters that include at least a few ten atoms. In experiments, laser vaporization and inert gas condensation are used to form the clusters. Photo-fragmentation tests offer a way to evaluate a cluster's stability. Some shapes obtained from classical modeling were compared with first-principles results. When clusters contain more than three atoms, the traditional method predicts 3D configurations. On the other hand, 2D configurations are anticipated *ab initio* for relatively bigger clusters. According to *ab initio* calculations and experiments, classical simulations predict that clusters larger than ten atoms will take on icosahedral forms, with silver atoms located on the cluster's edges.

There is more opportunity to compare experimental data with classical modeling since systems with more particles are easier to handle experimentally. For systems with millions of atoms, it is feasible to represent classically the deposition and accumulation of particles on a surface, or the compression of particle assemblies. Measurements of experimental positions throughout life. The mod-

eling work presented here was combined with quantum mechanical predictions [2], high resolution transmission electron microscopy [3]-[6], microscope microscopy [7] [8], surface tunneling or acoustic force microscopy [9]-[11], and Mössbauer microscopy [7] [8].

The focus of this report is on non-structured materials and bimetallic particles. Their optical and magnetic properties are of technological relevance. Magnesium particles exhibit a single domain at the nanoscale and are frequently superparamagnetic.

## 2. Computer Simulation Method

The used Molecular dynamics (MD) model will only be briefly described here as it has already been covered in length in another source [12]. Using the algorithm described in [13], the equations regulating the mobility of the atoms within the system are successively integrated over time. An Embedded Atom Model potential (EAM) that was presented in [14] [15] [16] is used to calculate forces. It also takes electron-phonon interaction into account. Assuming a constant electronic temperature, this is achieved by a friction term that controls the energy flow between the ionic and electronic systems. An approximate model that can be established to evaluate the coupling strength without the need for adjustable parameters is demonstrated in [12]. The experimental quantities required for pure elements are known, and it is assumed that the electron density at the Fermi level is one electron per atom. The electron-phonon coupling improves the local cooling of the system and helps to disperse the energy that the cluster in the impact produced. When compared to elementary systems, the current scenario is more complex since it involves two distinct mathematical elements that are not uniformly distributed. The electron-photon coupling model that is now in use is not appropriate for accurately characterizing the transfer of heat by the electronic system over an interface between two fundamental subsystems, as in a core-shell organized cluster. Here, it is thought that since the substrate is pure silver, converting the electron-photon coupling to pure silver and ignoring the variation in copper will be adequate.

The potential is, of course, the primary parameter that controls the interatomic interactions within the system. Its evaluation for the Co-Ag system is covered in detail, and we won't reiterate it here. The equilibrium characteristics of Co clusters embedded in Ag and Co-Ag free clusters were discussed using this potential. The impact of the clusters on a surface, which can include energy of up to 1.5 eV per atom—much higher than those involved at thermal equilibrium—is what makes the current situation different. However, at this energy, the shortest Ag-Ag separation distance involved in the simulations presented below is 2.124 Å at 1.5 eV/at. For Ag-Co and Co-Co couples with the same energy, it is comparable. The EAM potential is developed for first neighbor distances, which is still the case for such distances. A series of characterisation functions are employed to assess the alteration of the clusters resulting from their impact on an

Ag substrate surface. The epitaxial accommodation of the clusters with the substrate is quantified by a structural factor. It provides information about the periodicity in one direction and is measured within the cluster.

$$S = \frac{1}{N} \sum_{j=1}^N e^{ikr_j} \quad (1)$$

In this expression,  $k$  is the wave vector,  $r_j$  is the position of the atom  $j$  and  $N$  is the total number of atoms in the cluster. If the periodicity in the direction of  $k$  corresponds to the inverse of  $|k|$ , then the value of  $|S|^2$  is unity. If there is no such periodicity in this direction,  $|S|^2$  is zero. In order to measure the epitaxial accommodation of the deposited cluster with the substrate, substrate lattice wave vectors are used

$$k = \frac{4\pi}{a_0}(h, k, l) \quad (2)$$

where  $h$ ,  $k$ , and  $l$  are the Miller indices of the lattice directions, and  $a_0$  is the substrate lattice parameter. The short-range order in the clusters is characterized using a pair correlation function,

$$g(r) = \frac{1}{2(N-1)} \sum_{i=1}^{N-1} \sum_{j=i+1}^N \delta(r_{ij} - r) \quad (3)$$

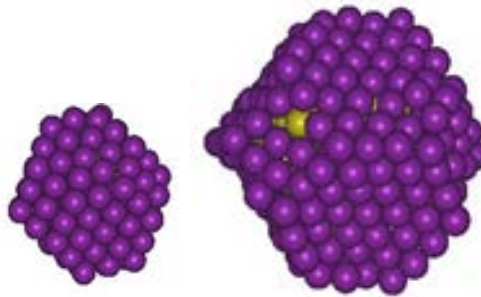
where  $\delta$  is the Dirac function,  $N$  is the number of atoms in the cluster and  $r_{ij}$  the distance between atoms  $i$  and  $j$  in the cluster. The number of atomic pairs divided by a given distance,  $r$ , is provided by the pair correlation function. Separate calculations are made for the three main types of pairs: Ag-Ag, Ag-Co, and Co-Co. It is characteristic of the lattice structure.

### 3. Results and Discussion

The graphene clusters with  $n = m$  ( $n = 100, 250, 500, 750, 1000, 1250, \text{ and } 1500$ ) have been deposited on a Ag(100) surface at energies of 0.5 eV per atom for the purpose of examining thin film growth processes by low energy cluster beam deposition (LECBD) using parallel programming with MPI. In this instance, the VCOM clusters with the following numbers of attributes: 200, 500, 1000, 1500, 2000, 2500, and 3000 are sorted in order of preference by selecting the subsequent cluster from the list of clusters. Every cluster slows down for 150 ps, after which comes the following one. The substrate has a size  $148.2 \text{ \AA} \times 148.2 \text{ \AA} \times 98.8 \text{ \AA}$  which consists of 124,416 atoms. The computation has been carried out at room temperature, accounting for the periodic boundary condition on two dimensions and the electron-phonon coupling [17].

Non-miscible clusters are characterized by their distinct morphologies in bulk materials and their distinct sequences at the nanoscale that are investigated. Metropolis Monte Carlo studies  $\text{Co}_x\text{Ag}_{201-x}$  clusters with 201 atoms in the first stage. Using means of Metropolis Monte Carlo sampling in the (NPT) canonical ensemble at zero pressure and at temperatures ranging from 100 K to 1000 K, the ideal truncated octahedral configurations at thermodynamic equilibrium are re-

vealed for  $0 < x < 201$ . We anticipate reusable configurations in this temperature range. As a result of a competition between protein and CO binding at low temperatures, CO is dispersed just below the cluster surface layer into groups of no more than five organisms, each with clearly defined positions, and the cluster central area is occupied for  $x < 20$ . To enhance the temperature preferences, these small groups cluster together. It is anticipated that they will dissolve at temperatures greater than the cluster's melting point. At  $x > 50$ , CO regrows at the cluster center and crosses  $\{111\}$  faces when  $\backslash g$  atoms are not sufficiently numerous to form a complete surface shell. Even above the melting point, the temperature is insufficient in these geometries to combine Ag and CO. Though still smaller than sig centers, the sig atoms are dispersed at the lowest coordination sites, around the cluster's margins, providing both inner and cluster faces. In intermediate geometries ( $20 < x < 50$ ), it is possible to have either a compact group at the cluster's center or a plate Co group below the surface [18].

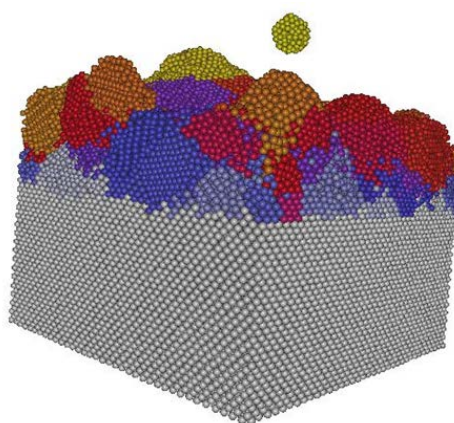


**Figure 1.** Configuration of a  $\text{Co}_{10}\text{Ag}_{191}$  (small) and  $\text{Co}_{285}\text{Ag}_{301}$  (big) cluster.

Even more ambitious is the second stage, which is presently in progress. The range of sizes experimentally achievable for low-energy cluster beam deposition is covered by expanding the analysis to include clusters with sizes up to 3000 atoms (see **Figure 1**). Both Metropolis Monte Carlo and Molecular Dynamics are used in atomic scale modeling. This involves a large-scale set of simulations (175 examples), with further computations added when necessary for more precise parameter tuning. An important task that is still in progress is the analysis of the findings. This method guarantees coverage over the whole spectrum of compositions and pertinent temperature ranges for both the liquid and solid states, in addition to a realistic variety of sizes. The requirements for achieving core-shell structures, cluster morphology, short- and long-range order in the clusters as a whole as well as within the silver and cobalt subsystems, melting conditions and the order of the solid-liquid phase transition in the clusters, and cobalt dissolution conditions in the silver-cobalt clusters are of particular interest. In order to capture all conceivable thermodynamic states of Co-Ag clusters and their transitions, a thorough analysis is presently being conducted. Some phenomena have already been explained in part: the energetic and stoichiometric conditions for clusters to precipitate into a core-shell structure; the wetting of cobalt cores by silver in cobalt-dominated clusters; the stoichiometric

conditions for a roughening transition of spherical clusters (and vice versa); the disordering of silver shells; the role of the internal Co/Ag interface and the cluster surface in the dynamics of melting; the occurrence of a solid-liquid coexistence temperature; and the condition for cobalt dissolution in clusters mainly composed of silver [19].

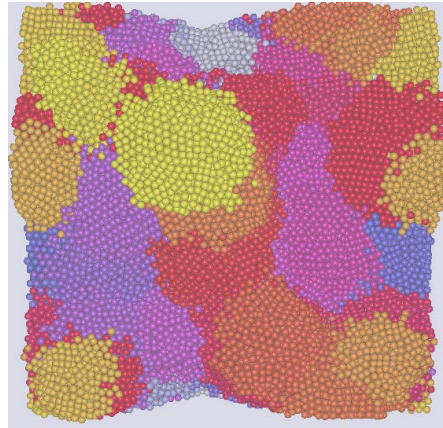
Clusters with similar size ranges are utilized to moderate their drooping on surfaces. Using classical molecular dynamics simulations, the slowing down of  $\text{Co}_{10}\text{Ag}_{191}$  and  $\text{Co}_{285}\text{Ag}_{301}$  nanoclusters on a  $\text{Ag}(100)$  surface is examined at the atomic scale. After 65 clusters, the film grown by 0.5 eV/atom  $\text{Ag}_n\text{Co}_m$  clusters with numbers of atoms 200, 500, 1000, 1500, 2000, 2500, and 3000 is shown in **Figure 2**. The decreasing beam energy, ranging from 0.25 to 1.5 eV/atom, is typical of low energy cluster beam deposition and aerosol focused beam methods. The two clusters differ from one another in terms of size, shape, and structure. Whereas in  $\text{Co}_{10}\text{Ag}_{191}$ , Co forms one or more groups just beneath the cluster surface,  $\text{Co}_{285}\text{Ag}_{301}$  shows a shell structure in which Ag forms a single complete layer surrounding the Co core. Following the impact, the smallest cluster undergoes profound restructuring and becomes completely epitaxial with the substrate.



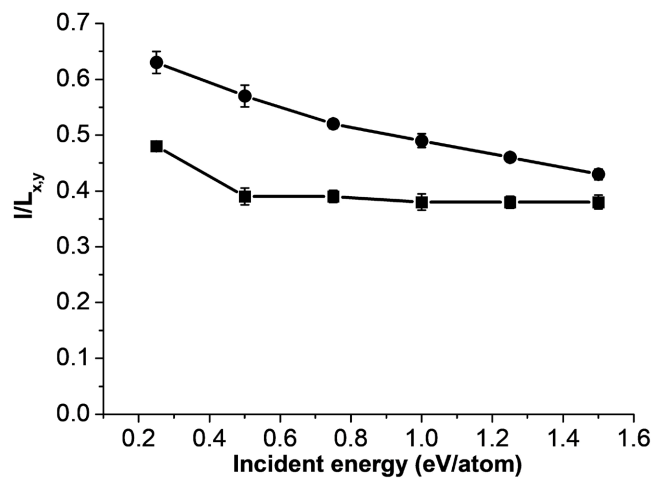
**Figure 2.** Molecular dynamics simulation of the impact of  $\text{CoAg}_m$  clusters on a  $\text{Ag}(100)$ .

The larger one only undergoes partial adaptation and partially retains its original methodology (**Figure 3**). Following the impact, the Co forms one group that Ag covers for both. The effect of the increasing binding energy with more atoms in the cluster is reinforced by the fact that the relative concentration of Co is higher in the large cluster, which has a larger binding energy than the Ag cluster. As a result, the definition of the smallest cluster after the impact is larger and uses less energy per atom. The associated standard deviations are only three times larger than the standard error on the mean shown in **Figure 4** since mean aspect ratios are estimated over ten statistically independent cases. This shows that the results are somewhat widely distributed, indicating that the aspect ratio for both types of clusters only weakly depends on the impact point or the inci-

dence cluster orientation.



**Figure 3.** Thin film growth by low energy cluster deposition.



**Figure 4.** Aspect ratio of the deposited clusters as a function of the slowing down energy. Squares: small cluster, circles: big cluster.

There is significant substrate degradation that changes with the deceleration energy. This results in the cluster being surrounded by a silver step that may reach a height of many atomic layers and contain small monolayer islands or isolated add-atoms separate from the step. While the former originates from the substrate, the latter comes from the cluster. Additional details about the impact's effects are given, emphasizing cluster penetration, deformation, and lattice distortions—paying special emphasis to the size and stoichiometry of the clusters [20].

This represents the art in its current state. Consistent with the pattern for miscible clusters, a comparison with the experiment is shown. Large-scale computational efforts are also made to model nanostructured graphene materials created via cluster deposition and investigate their thermodynamic and mechanical characteristics. Molecular dynamic codes are subsequently developed for use with parallel computers. The preliminary findings are readily available and will be showcased.

Through this succinct overview of our current research methodology, we hope to demonstrate the degree to which traditional modeling at the atomic scale may aid in our understanding of the characteristics of nanoparticles and the nanostructured materials they confirm.

#### 4. Conclusions

Research has demonstrated that  $\text{Ag}_n\text{Co}_m$  cluster deposition on an Ag(100) surface can be effectively studied at slowing down energies (0.25 eV - 1.5 eV per/atom) using the EAM potential that Johnson described.

It was discovered that the slowing down conditions greatly alter the properties of deposited Ag-Co clusters. Compared to the smaller cluster, the  $\text{Ag}_{301}\text{Co}_{285}$  cluster maintains its inner structure better, but the core-shell structure might be compromised. It is possible to track the penetration—and thus, the pinning—of the incident clusters using the energy that is slowing down.

It was shown that either low incident energy ( $\leq 0.25$  eV/atom) or somewhat large clusters (where the number of Co atoms is more than 250) should be employed in order to preserve the initial state of cluster. It is helpful to use relatively high energy to improve the epitaxy. Further exploration of the underlying mechanisms driving the limited epitaxy and the differences between Ag and Co would provide deeper insights.

#### Conflicts of Interest

The authors declare no conflicts of interest regarding the publication of this paper.

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