Computational Materials Science 152 (2018) 393–407

Contents lists available at ScienceDirect

Computational Materials Science

journal homepage: www.elsevier.com/locate/commatsci

Evolution of nanostructure and mechanical properties of silver nano-particle in the confined region between graphene sheets: An atomistic investigation

Sunil Kumar[a,*], Suchandan K. Das[a], Sudip K Pattanayek[b]

[a] CSIR-National Metallurgical Laboratory, Jamshedpur 831007, India
[b] Department of Chemical Engineering, IIT Delhi, 110016, India

ARTICLE INFO

Keywords:
Silver nano-particle
Graphene substrate
Molecular dynamics simulations
LAMMPS
Dimension-less aspect ratio
Confined region

ABSTRACT

Solidification and organization of silver nano-particle in a confined region between graphene sheets, shows much importance for the various application in the field of biomedical, electrochemical, coating materials, catalyst, metal-matrix nanocomposite etc. To understand the processes involved, we have studied the atomistic behaviour of solidification, organizations and mechanical properties of silver nano-particle in the bulk and as well as in confined region by molecular dynamics simulations. In the bulk, silver nano-particle shows phase transition from liquid to crystalline phase at a temperature, T ≈ 1030 ± 25 K. However, in the confined region, silver nano-particle depicts the same phase transition at a relatively higher temperature. The tensile stress, initiation of cracks and subsequent detachment of silver during tensile deformation depends upon the temperature and interfacial interactions. The tuning of 12–6 Lennard Jones interaction potential energy parameter between graphene and silver (ε_{Ag-C}) drastically influenced the phase transition of silver nano-particle in the confined region. At a high interaction potential energy (ε_{Ag-C}), silver nano-particle shows good wettability over the graphene sheets and depicts the phase transition at a higher temperature compared to lower interaction potential energy.

1. Introduction

Solidification and organization of metallic materials in the confined region has been found to direct impact many desirable properties of metal matrix nano-composite, including mechanical [1,2], thermal [3–5], electrical [6–8], optical [9–10], anti-microbial [11–13], etc. The accountable factors which direct the above properties are the interactions and wettability of metal atoms with interface, stress transfer, the mobility of thermal vibrations, electronic conductions and chemical reactivity. In order to understand, the appropriate reasons behind the above influenced behaviour of properties, it is much needed to study the solidification and organization of metallic material in a confined region between graphene sheets. Reported studies [14–16] suggest that the metal atoms make a sheathing organization over the graphene substrate during the processing of nano-composite systems. The utmost interface area between the metal - matrix and graphene substrate enhance the strength of the metal-matrix graphene composite against during external load applications. Hwang et al. [14] depicted the reduced graphene oxide homogeneously dispersed in the copper matrix, which acquired considerably improved mechanical performance by a molecular-level mixing method. Li et al. [15] have found that the Ni-coated graphene substrate not only prohibited the aggregation, but also improved the interface strength between graphene and the copper matrix. Salam et al. [17], have synthesized silver-graphene nanocomposites by experimental methodology. They have shown that the developed silver graphene nano-composite material has excellent catalytic properties, is inexpensive and can be reused five times without decrease in activity and selectivity. Bhunia and Jana [18] have developed a simple and a large-scale experimental methodology for the synthesis of graphene oxide-silver composite. They have found that the photo catalytic efficiency of graphene oxide-silver nano-composite under visible light is significantly higher. However, some experimental investigations have been reported that the inclusion of graphene in metals matrix decreases its mechanical properties due to poor graphene/metal interface adhesion/bonding and high processing temperatures [19–22].

Despite of a large number of reported experimental studies concerning to metal matrix nanocomposite, there are only a few studies are available using molecular dynamic simulations of metal/graphene nanocomposites [23,24]. Amal et al. [23] have investigated the distribution and evolution of atomic nanoclusters of variety of metallic materials over the graphene substrate using molecular dynamics

* Corresponding author.
E-mail address: sunil@nmlindia.org (S. Kumar).

https://doi.org/10.1016/j.commatsci.2018.06.021
Received 3 March 2018; Received in revised form 5 June 2018; Accepted 11 June 2018

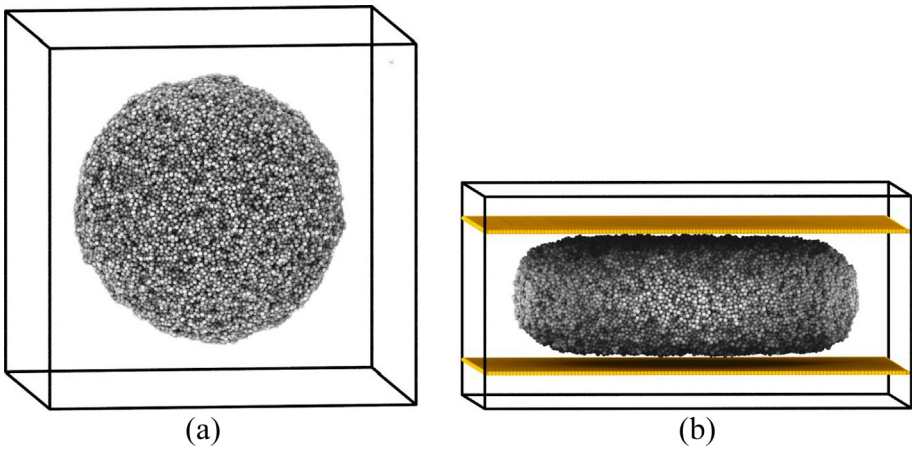

Fig. 1. Snapshots of simulation systems for solidification and structural organization of silver in bulk and in confined region: (a) silver (150,000 atoms) placed in a cubical simulation box of dimension (± 175 Å, ± 175 Å, ± 175 Å) and (b) silver (150000 atoms) placed in a confined region between two square graphene sheets (side length 350 Å). Graphene sheets have been placed along x-y plane and at z = 0 Å and z = 100 Å.

Table 1
Embedded Atoms Method (EAM) due to Finnis-Sinclair (FS) [28] parameters for silver atoms.

m	n	ε(eV)	c	a(Å)
6	12	0.025415	144.41	4.09

simulations. They have found that the silver, gold, and copper formed aggregates or globules of different sizes, which was arbitrarily spread over the graphene substrate. On the contrary, lithium, sodium, and potassium have formed a mono-atomic layer distribution over the graphene substrate. Duan et al. [24] have developed a copper/graphene nanocomposites and investigated it's mechanical properties using molecular dynamics simulation. They found that the fracture strain, Young's modulus and the tensile strength of nanocomposites rises with increase in the number of graphene layers within the copper matrix. Despite these studies, the solidification, structural organization (phase transitions) and mechanical properties of metals in the confined region between graphene sheets still needs to be explored. To the best of our knowledge, the solidification, structural organization (phase transitions) and mechanical properties of metals in the confined region between graphene sheets by molecular dynamics simulation has not been studied till now.

In this study, the solidification, structural organization and its mechanical properties of silver nano-particle in a confined region between graphene sheets have been explored by molecular dynamics simulations. Silver is selected as a metal nanoparticle due to its wide applications in flexible electronics, biomedical devices, catalyst, etc. In the first step, adsorption and organization of silver nano-particle in a confined region between two graphene substrate was simulated. In the second step, the tensile deformation of composite system has been carried out at various temperatures to study the mechanical behaviour. The adaptive common neighbour analysis, radial distribution and potential energy evolution have been used to characterize the organization of silver nano-particle in the confined region.

2. Simulation details

Molecular dynamics simulation [25–27] has been carried out under the constant- number of atoms, volume and temperature (NVT) ensembles to study the solidification, structural organization and mechanical properties of silver nano-particle in bulk and the confined region between graphene sheets as shown in Fig. 1.To execute intra-atomic interactions for silver nano-particle, Finnis and Sinclair[28] form of embedded atom method (EAM) potentials has been employed during molecular dynamics simulation. The total intra-atomic interaction potential energy of silver nano-particle, E_{Ag-Ag} is estimated by

$$E_{Ag-Ag} = \sum_i \varepsilon \left[\frac{1}{2} \sum_{j \neq i} \mathrm{V}(r_{ij}) - c\sqrt{\rho_i} \right] \tag{1}$$

$$V(r_{ij}) = \left(\frac{a}{r_{ij}} \right)^n \tag{2}$$

$$\rho_i = \sum_{j \neq i} \left(\frac{a}{r_{ij}} \right)^m \tag{3}$$

where r_{ij}, a, c, n, m, and ε are depicting the separation between i^{th} and j^{th} silver atom, lattice parameter and other positive constants for silver nano-particle respectively.$V(r_{ij})$ is showing the pair intra-atomic potential energy to account for silver atom, and ρ_i the local charge density. Eqs. (1)–(3) can be written in the generalized form of Hamiltonian pertaining to silver atoms as given by equation (4) below

$$H = \frac{1}{2} \left[\sum_{i \neq j} \sum \hat{p}_i \hat{p}_j V(r_{ij}) \right] - d \sum_i \hat{p}_i \left[\sum_{j \neq i} \hat{p}_j \varnothing(r_{ij}) \right]^{1/2} \tag{4}$$

$$\hat{p}_i = \begin{cases} 1, & \text{if site } i \text{ is occupied by a metal atom,} \\ 0, & \text{otherwise} \end{cases} \tag{5}$$

$$V(r) = \varepsilon \left[\frac{a}{r} \right]^n \tag{6}$$

$$\varnothing(r) = \varepsilon \left[\frac{a}{r} \right]^m \tag{7}$$

$$d = \varepsilon \times c \tag{8}$$

The numerical values ofε, a, c, m and$n$ for the silver atoms have been given in Table 1. The Finnis and Sinclair form of embedded atom method potential is a semi-empirical method for performing molecular dynamics simulation of metallic materials. However, it has some limitations, like no angular dependency on electron density, without consideration of covalency of metal atoms, and excluding Fermi-surface effects [47]. Despite of these limitations, Finnis and Sinclair form of embedded atom method potentials are widely incorporated during