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## Deformation and fracture of nano-sized metal-coated polymer particles: A molecular dynamics study



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### ABSTRACT

The mechanical behavior of Ni-coated polyethylene (PE) nanoparticles subjected to compression loading is systemically investigated by classical molecular dynamics simulation. Results show that the Ni coatings on PE nanoparticles lead to a densification of particle surface and remarkably enhance the compression strength. The particle size-effect and the coating thickness effect on the compression responses in terms of compressive strength and particle burst are observed. Burst of Ni-coated PE nanoparticles initiates at the high stress-concentrated grain-boundaries zone of polycrystalline Ni-shell, and propagates along the compression direction to the flattened contact surface, resulting in release of core PE molecules.

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## 1. Introduction

Polymer nanoparticles are fascinating materials that have potential applications in a wide spectrum of areas such as optoelectronics, photonics, bioimaging, biosensing, nanomedicine, molecular recognition and cosmetics [1–7]. Driven by their applicability in modern material science and by their technological importance, much effort has been devoted to the fabrication of polymer nanoparticles with tailored properties over the last decades. However, single-component polymer particle with well-controlled molecular composition and architecture, in some aspects, is still unable to meet rigorous requirement of certain emerging applications. Accordingly, nanoengineering of particles surface has been employed to better improve the functions and performances, as well as further broaden their applications [8,9]. Depending on the properties of the coating materials, various functions, such as physical (electronic, magnetic, optical), chemical (catalytic) and biological functions can be readily imparted to monodispersed polymer particles. For instance, reversible addition–fragmentation chain transfer end groups of poly((2-acetoacetoxy)ethyl methacrylate) on the surface of polystyrene particles are not only able to control the molecular weight, block-copolymer formation, and particle morphology, but also facilitate the selective binding to Hg<sup>II</sup> over Co<sup>II</sup> at low concentrations [10].

Specifically, metalized polymer particles composing of a variety of metallic shell coating and dielectric core materials exhibit improved physical properties over their single-component counterparts. Lee et al. [11] showed that Ag-coated polymer particles were the most effective surface-enhanced Raman scattering substrates, exhibiting highly enhanced Raman signals of polyvinyl pyrrolidone capping molecules. Siiman and Burshteyn [12] demonstrated that polystyrene particles

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## Nomenclature

PE	is the polyethylene polymer
Ni	is the nickel material
Hg <sup>II</sup>	is the heavy metal ion mercury
Co <sup>II</sup>	is the heavy metal ion cobalt
Au	is the gold material
Ag	is the silver material
Cu	is the copper material
ACAs	is anisotropic conductive adhesives
MD	is molecular dynamics
C(sp <sup>3</sup> )	is the carbon atom with sp <sup>3</sup> hybridization
CH <sub>2</sub>	is the middle methine group of polyethylene polymer
CH <sub>3</sub>	is the terminal methyl group of polyethylene polymer
EAM	is the embedded atom method
NVT	is constant mole, volume, and temperature ensemble
$r_{\text{particle}}$	is the initial average radius of simulated particle
$P_{\text{plate}}$	is the total reactive force of beads onto the plate
$D$	is the displacement of the plate
$d_0$	is the gap distance between plate and simulated particle prior to compression
MSD	is the mean square displacement

coated by Au or Ag layer can enhance 2- to 10-fold side scatter over metal-free polystyrene particles. Narkis et al. [13] reported that polystyrene particles coated by less than one volume percent Cu, Ni or Cu/Ni exhibit very high conductivities. The resistivity, dielectric constant, and dissipation factor of these metal-coated particles strongly depend on the metal concentration, coating adhesion, and temperature. One renewed interest in conductive polymer particles by metal-coating for anisotropic conductive adhesives (ACAs) has been focused on their utilization in liquid crystal display (LCD) and Microsystems [14–17]. Advantages for their use in ACAs include reduction of package sizes, assembly temperatures, manufacturing costs and enhancement of the interconnection compliance [18].

Typically, a large deformation of exceeding 20% is imposed to metal-coated particles during both manufacture process and in-serve operation in ACAs [19]. This suggests that high mechanical performance of individual metal-coated polymer particles is required to ensure good process yield and reliable products. Because of many characteristics of these particles such as small dimension and spherical geometry, only very rare attempts have been devoted to investigate their mechanical properties hitherto. Zhang et al. [19–23] developed a nano-indentation based flat punch method to determine the compressive response of both metal-free and metal-coated polymer particles. They reported that the mechanical responses are sensitive to different factors such as chemical composition, cross-linking density, load rate, and particle size. The relatively high cost and inaccessible from the molecular level to link the mechanical properties by experiments led to computational studies of mechanical properties of polymer particles. Both united-atom and coarse-grained simulation models predicted a size-dependent compressive response of polyethylene (PE) particles, which was in agree with the experimental measurements [21]. Zhao et al. [24] concluded that relative surface energy for decreasing particle sizes is the main source of the increases in modulus. Wu et al. [25] showed that, via molecular dynamics (MD) simulation, the molecular architecture has an impact on compressive behavior of PE nanoparticles.

Despite of above important investigations, there are still many perplexing questions concerning the deformation responses of core-shell polymer composites, particularly for atomistic failure mechanism of metallization polymer particles, remain unanswered. The deformation properties of metal-coated polymer particles are strongly associated with the properties of metal nanoshell, and core polymeric structures, as well as metal-polymer adhesion (van der Waal interaction). This study focuses on the compressive flat-punch behaviors of Ni-coated PE particle by employing classic MD simulations. Our efforts on metallized polymer particle modeling aim to understand the origin of the deformation and fracture from atomistic point of view.

## 2. Methods

### 2.1. Atomistic model

There have been reported several methods in preparation of modeling polymer particles in literature [24–26]. In this study, a semi-crystalline lattice method has been adopted to generate core PE spheres [27,28]. Linear PE molecule with a specific molecular length of 1000 carbons per chain is chosen as a unit for the PE particle. Fig. 1 shows the main procedure of construction of polymeric structures. Initially, a spherical diamond lattice in which the lattice spacing equals to the length

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