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Research Article

Shell Thickness-Dependent Strain Distributions of Confined Au/Ag and Ag/Au Core-Shell Nanoparticles

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The shell thickness-dependent strain distributions of the Au/Ag and Ag/Au core-shell nanoparticles embedded in Al_2O_3 matrix have been investigated by finite element method (FEM) calculations, respectively. The simulation results clearly indicate that there is a substantial strain applied on both the Au/Ag and Ag/Au core-shell nanoparticles by the Al_2O_3 matrix. For the Au/Ag nanoparticles, it can be found that the compressive strain existing in the shell is stronger than that on the center of core and reaches the maximum at the interface between the shell and core. In contrast, for the Ag/Au nanoparticles, the compressive strain applied on the core is much stronger than that at the interface and that in the shell. With the shell thickness increasing, both of the strains in the Au/Ag and Ag/Au nanoparticles increase as well. However, the strain gradient in the shell decreases gradually with the increasing of the shell thickness for both of Ag/Au ad Au/Ag nanoparticles. These results provide an effective method to manipulate the strain distributions of the Au/Ag and Ag/Au nanoparticles by tuning the thickness of the shell, which can further have significant influences on the microstructures and physical properties of Au/Ag and Ag/Au nanoparticles.

1. Introduction

Nanoparticles with core-shell structure have attracted intensive scientific and technical interests due to their potential applications in catalysis, drug delivery, microelectronics, sensor, and many other emerging nanotechnologies [1–5]. Particularly, the bimetallic nanoparticles with core-shell structure have constantly been the subject of these studies because of their improved electronic, optical, and catalytic performances compared with those of monometallic nanoparticles [6, 7]. Moreover, it has been demonstrated that the composition, size, shape, and surface modification of these bimetallic nanoparticles can be tailed for the targeted applications [8, 9]. Among them, Au/Ag and Ag/Au core-shell nanoparticles have currently captured exponential attention due to their unique optical and photonic properties. It has been illustrated that Au and Ag present a broad absorption band in the visible region of the electromagnetic spectrum [10–12], which can be due to the collective oscillation of the free conduction electrons induced by an interacting electromagnetic field [13]. Moreover, Au is a suitable candidate for biomedical applications because of its excellent performances on biocompatibility, chemical stability and easy surface modification, and so forth. Therefore, the Au/Ag and Ag/Au core-shell nanoparticles with surface plasmon enhancement and high levels of sensitivity have tremendous applications for optical, chemical, and bimolecular devices. For example, the generation of detectable Fano-resonance has been demonstrated in Au/Ag core-shell structure [14], which has a great potential in the subwavelength waveguides, and low-loss metamaterials sensors [15–18].

On the other hand, strain engineering provides a general strategy to control the morphology and microstructure of the nanostructures, leading to an enhancement of their device

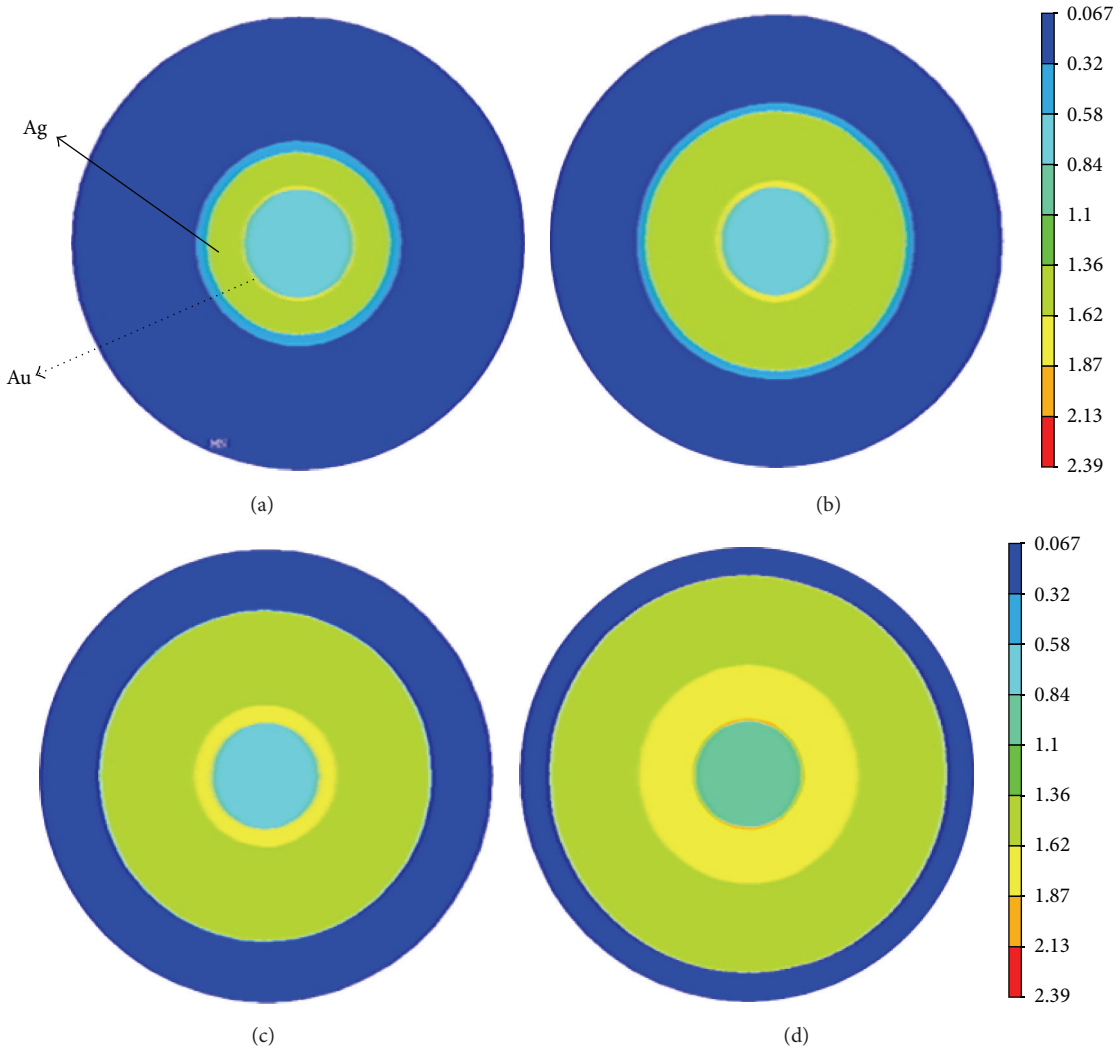

Figure 1: Morphological cross-sectional strain distribution of embedded core-shell Au/Ag nanoparticles with the shell thickness of (a) 2.5 nm, (b) 5 nm, (c) 7.5 nm, and (d) 10 nm, respectively.

performance. For example, quantum dots, a kind of nanostructures for making high performance nanodevices, can be realized by using self-assembled growth technique, which is based on a process of strain accumulation and relaxation in the system [19, 20]. For the core-shell nanoparticles confined in a host matrix, a substantial strain is induced [21–25], which can be used to tune the interplay between the core and shell layers, the morphology [26, 27], and optical properties [28]. Therefore, for the Au/Ag and Ag/Au core-shell nanoparticles, along with the enhanced light absorption, spectral tuning of the surface plasmon resonance by strain can provide another dimension besides the usual size and composition manipulation. Here, the shell thickness-dependent strain distributions of the Au/Ag and Ag/Au core-shell nanoparticles embedded in Al_2O_3 matrix have been investigated, respectively. The simulation results offer an effective method to manipulate the strain distributions of the Au/Ag and Ag/Au nanoparticles by tuning the thickness of the shell, which can further have significant influences on the surface states and surface plasmon resonance of Au/Ag and Ag/Au nanoparticles.

2. Methods

In this paper, a FE calculation is performed to simulate the strain distribution of embedded Au/Ag and Ag/Au core/shell nanoparticles with different shell thickness. The interplay between the strain and the structure of confined Au/Ag and Ag/Au nanoparticles has been investigated. FE calculation has been applied successfully to continuum modeling of deformation [29] of materials. Recently, simulation on the strain distribution of nanoparticles by FE method has been widely studied [30, 31]. For materials at nanoscale, the simulations by the continuum elastic FE method and the atomistic strain calculations have reached a general qualitative agreement [32, 33]. Many physical properties of nanomaterials, including elastic anisotropy, thermal expansion, and three-dimensional morphology, can be understood well by the FE simulation results. In our simulation, the FE model for the strain distribution is based upon the following assumptions. A spherical, linear-elastic core-shell Au/Ag or Ag/Au nanoparticle is confined in an isotropic and linear-elastic

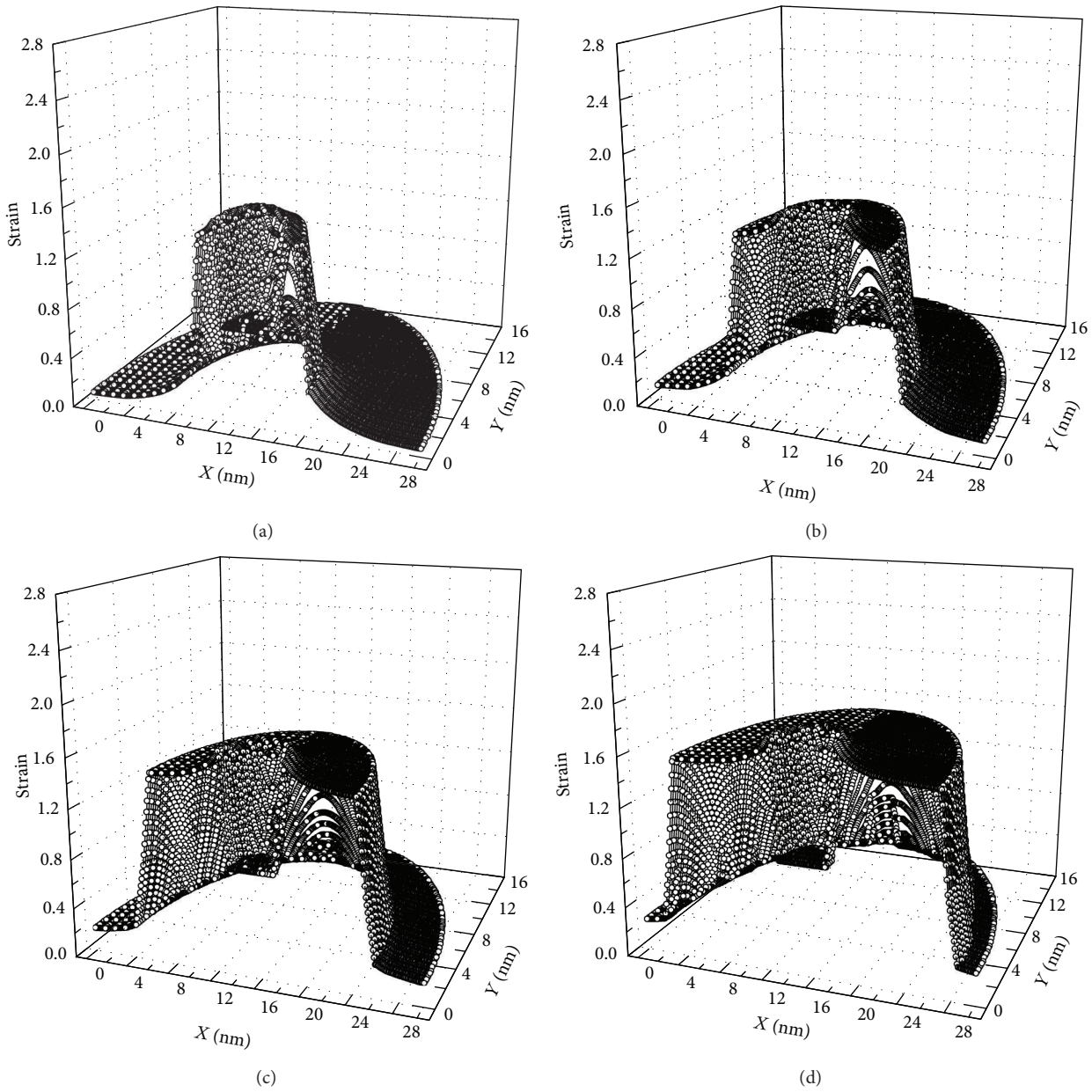

Figure 2: *X-Y* plane strain profiles for Au/Ag nanoparticles with the shell thickness of (a) 2.5 nm, (b) 5 nm, (c) 7.5 nm, and (d) 10 nm, respectively.

matrix. The Au/Ag or Ag/Au nanoparticle surface is welded to the Al_2O_3 matrix. The core size is 2.5 nm and the shell thickness is 2.5 nm, 5 nm, 7.5 nm, and 10 nm for each nanoparticle, respectively. The thermal expansion mismatch between the nanoparticles and Al_2O_3 matrix leads to a substantial strain in the confined Au/Ag or Ag/Au nanoparticles. Young's modulus is taken to be 170 GPa, 76 GPa, and 360 GPa for Au, Ag, and Al_2O_3, while Poisson's ratio is taken to be 0.42, 0.38, and 0.24 for Au, Ag, and Al_2O_3, respectively.

3. Results and Discussion

The morphological cross-sectional strain distributions for the core-shell Au/Ag nanoparticles embedded in Al_2O_3 thin film with the shell thickness of 2.5 nm, 5 nm, 7.5 nm, and 10 nm are presented in Figures 1(a)–1(d), respectively. It can be found that the strain distributes inhomogeneously, which can be tuned by the shell thickness. Correspondingly, the *X-Y* plane strain profiles for embedded Au/Ag nanoparticle with the shell thickness of 2.5 nm, 5 nm, 7.5 nm, and 10 nm are shown in Figures 2(a)–2(d), respectively. Figures 2(a)–2(d) illustrate quantitatively that there is a large compressive strain applied on the Au/Ag nanoparticle by the Al_2O_3 matrix. The strain is weaker in the core than that in the shell. It reaches the maximum at the interface and decreases with the layer away from the interface. With the shell thickness increasing, it can be seen that the strain existing in the core-shell Au/Ag nanoparticles becomes stronger. The strain distribution in

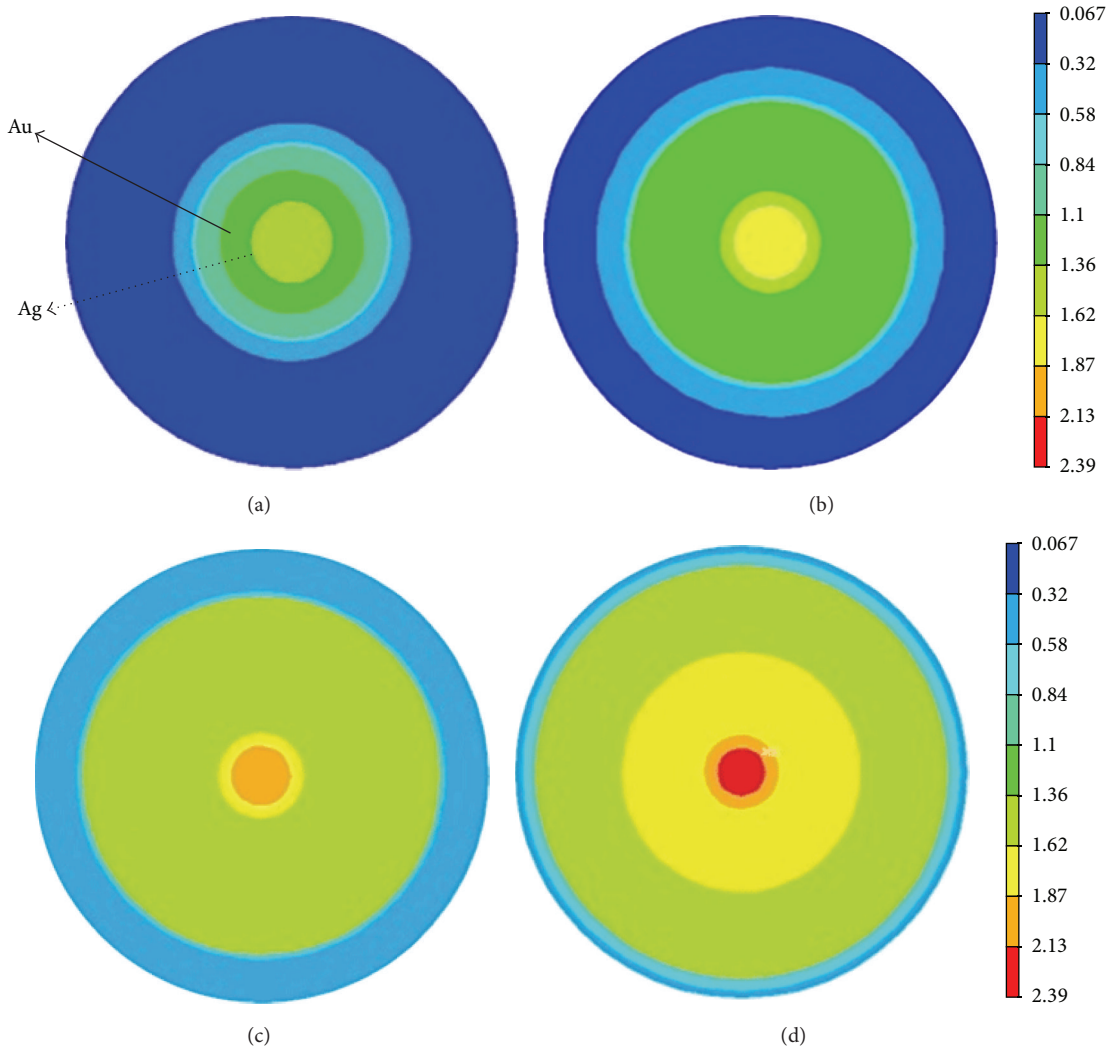

FIGURE 3: Morphological cross-sectional strain distribution of confined Ag/Au nanoparticles with the shell thickness of (a) 2.5 nm, (b) 5 nm, (c) 7.5 nm, and (d) 10 nm, respectively.

the core keeps homogenous. However, the inhomogeneousity of strain distribution existing in the shell is enhanced.

Similarly, the morphological cross-sectional strain distributions for Ag/Au nanoparticles embedded in Al_2O_3 thin films with the shell thickness of 2.5 nm, 5 nm, 7.5 nm, and 10 nm are presented in Figures 3(a)–3(d), respectively. The X-Y plane strain profiles for embedded Ag/Au nanoparticle with the shell thickness of 2.5 nm, 5 nm, 7.5 nm, and 10 nm are illustrated in Figures 4(a)–4(d), respectively. It also can be seen that there is a compressive strain applied on the Ag/Au nanoparticles by the Al_2O_3 matrix. However, the strain distributes quite differently from that in the Au/Ag nanoparticle, which reaches the maximum in the core and decreases monotonously from the core to the shell in the Ag/Au nanoparticles. With the shell thickness increasing, the strain increases as well. The strain distribution in the core keeps homogenous, and the inhomogeneousity of strain distribution existing in the shell is enhanced.

For a comparison, Figure 5 illustrates the strain distributions and the strain gradient for the Au/Ag and Ag/Au nanoparticles with the shell thickness of 2.5 nm, 5 nm, 7.5 nm, and 10 nm, respectively. It can be found that, for both of Au/Ag and Ag/Au nanoparticles, the strain is enhanced with the increasing of the shell thickness. Moreover, the strain increases faster for Ag/Au than that for Au/Ag nanoparticles. For these two core-shell nanoparticles with the same shell thickness, the strain on the core is larger for Ag/Au than that for Au/Ag nanoparticles, which can be due to the larger Young's modulus of Au than that of Ag. The strain gradient in the shell decreases gradually with the increasing of the shell thickness for both of Ag/Au ad Au/Ag nanoparticles. However, the strain gradient in the shell decreases faster for Au/Ag than that for Ag/Au nanoparticles. The homogeneous strain distribution in the core and the inhomogeneous strain in the shell can have a significant influence on the microstructure and morphology of Au/Ag and Ag/Au nanoparticles, which

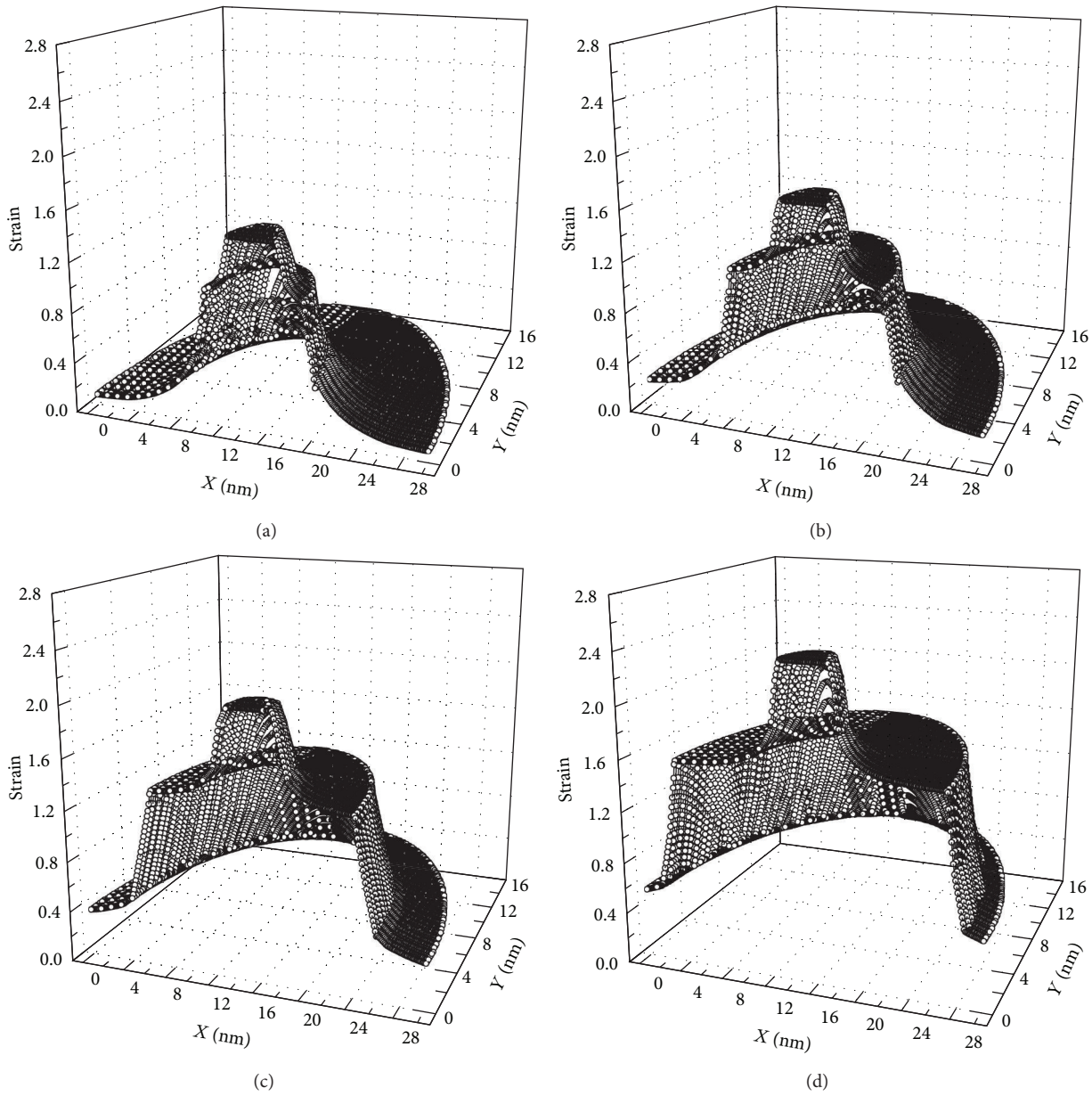

Figure 4: X-Y plane strain profiles of Ag/Au nanoparticles with the shell thickness of (a) 2.5 nm, (b) 5 nm, (c) 7.5 nm, and (d) 10 nm, respectively.

plays an important role in tuning the surface states and surface plasmon resonance of Au/Ag and Ag/Au nanoparticles.

4. Conclusion

In summary, the shell thickness-dependent strain distributions of the Au/Ag and Ag/Au core-shell nanoparticles embedded in Al_2O_3 matrix have been investigated by FEM calculations, respectively. The simulation results clearly indicate that there is a substantial strain applied on both the Au/Ag and Ag/Au core-shell nanoparticles by the Al_2O_3 matrix, and the strain distributes homogeneously in the core and inhomogeneously in the shell. For the Au/Ag nanoparticle, the strain reaches the maximum at the interface and is weaker in the core than that in the shell. For the Ag/Au nanoparticles, the strain decreases monotonously from the core to the shell. For these two nanoparticles with the same shell thickness, the strain in the core is larger for Ag/Au than that for Au/Ag nanoparticles. With the shell thickness increasing, both of the strains in Au/Ag and Ag/Au nanoparticles are enhanced, and the strain gradient in the shell decreases gradually. These results demonstrate an effective method to manipulate the strain distributions of the Au/Ag and Ag/Au nanoparticles by tuning the thickness of the shell, which plays an important role in optical properties of Au/Ag and Ag/Au nanoparticles.

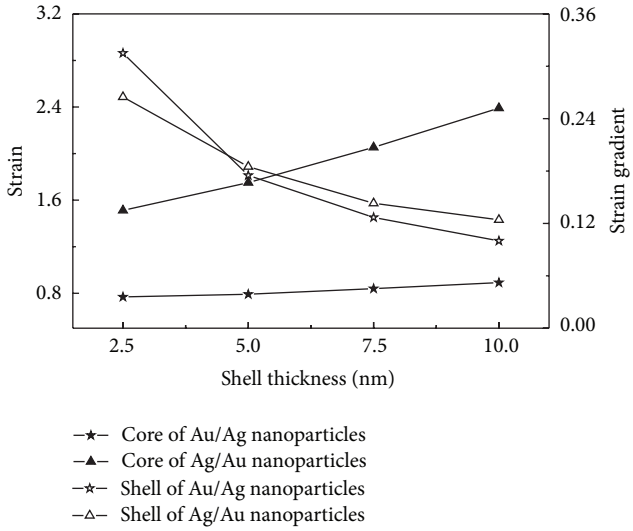

FIGURE 5: Strain on the core, strain gradient in the shell of the Au/Ag and Ag/Au nanoparticles with the shell thickness of 2.5 nm, 5 nm, 7.5 nm, and 10 nm, respectively.

Conflict of Interests

The authors declare that there is no conflict of interests regarding the publication of this paper.

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