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One approximate generic equation for calculating inter-nanoparticle forces

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ABSTRACT

In this work, interaction forces between two identical silicon or dissimilar silicon-diamond nanospheres are calculated using molecular dynamics simulation. Modified formulas for van der Waals (vdW) attraction and Born repulsion forces have been proposed, respectively. Two different function forms are taken after particle's contact deformation, depending on the atomic discrete structure and mechanical properties of the materials. A second-order Fourier expansion is applied to two interacting identical silicon nanospheres, and a simplified linear functional form is used for two interacting dissimilar silicon-diamond nanospheres. Moreover, the constant asymptotic ratios of both vdW attraction and Born repulsion have been correlated to the additional material properties including the ratio k_ρ of the true number density of atoms to that determined from Hamaker approach and refractive index n_0. Upon the analysis of four different nanospheres (*i.e.*, silica, amorphous carbon, diamond, and silicon), one approximate but generic equation is put forward for inter-nanosphere vdW attraction and Born repulsion forces, respectively.

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1. Introduction

With the development of precision processing techniques, the components of electro-mechanical systems devices gradually decrease from microscale to the nanoscale. However, most components (*i.e.*, nanoparticles) do not 'self-assembly' into structures or systems of their thermodynamically lowest energy state. They require an external force to 'direct' them into particular structures or assemblies [1]. To achieve better self- and directed-assembly of nanoparticles through interparticle and/or externally applied forces, understanding the inter-nanoparticle forces, *i.e.*, van der Waals (vdW) attraction and Born repulsion, is becoming crucial for device design, materials selection, and fundamental studies [2,3]. However, the continuum models developed at the macro/μ scale, such as Hamaker approach [4,5], do not generally apply to nanoparticles due to the neglect of atomic discrete structure and surface effects [6–9]. In previous work, interparticle forces between nanospheres of identical materials, such as α-quartz silica [10–12], amorphous carbon, crystalline diamond [13], silicon nanoellipsoids [14], and contact deformation of nanoparticles [15,16] have been theoretically calculated using molecular dynamics (MD) simulations or mathematical methods. These computer simulations or theoretical calculations can overcome some experimental challenges and provide more accurate results than those from atomic force microscopy (AFM) measurement. The accuracy of AFM results, especially in the lateral direction, is critically dependent on factors such as sensitive spring constant, precision calibration of the cantilever, *etc.* The MD simulations have generated a series of modified formulas to calculate vdW attraction and Born repulsion forces between the nanospheres. However, these formulas are usually unique to specific materials since the fitted parameters in formulas vary with materials. This work is to derive one approximate but generic equation for inter-nanosphere forces between arbitrary nano-materials. Apart from the above-mentioned three materials, two more nanosphere cases (*i.e.*, identical crystalline silicon and dissimilar diamond-silicon) will be considered. This paper is organized as follows. Section 2 presents the simulation method and conditions. Section 3 describes the initial characterization of silicon nanospheres, followed by the calculations of interaction forces between two silicon nanospheres, and between silicon and diamond nanospheres. Finally, one approximate but generic equation is established. The main conclusions are summarized in the last section.

2. Simulation method and conditions

The MD simulations are performed using COMPASS forcefield [17] available in Material Studio software package. The simulation procedure is similar to the reports before [11,12]. Briefly, either silicon or diamond nanospheres are carved out of their bulk counterparts by specifying the

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shape and size. Then, the two nanospheres (either two identical silicon nanospheres or two interacting silicon and diamond dissimilar nanospheres) are fully relaxed using the NVT (*i.e.*, constant number of atoms, constant volume and constant temperature) ensemble at 300.0 K, following geometry optimization. Subsequently, the two nanospheres are allowed to move towards each other at an equal but opposite initial atomic velocity using the NVE (*i.e.*, constant number of atoms, constant volume and constant energy) ensemble. And the typical sequence snapshots are displayed in Fig. 1. Numerical integration is performed using the velocity Verlet integration algorithm with time step $\Delta t = 1.0 \times 10^{-15}$ s (1 fs) and frames are output every 100 steps. The cut-off distance used in the MD simulations is set to be as large as 100 nm to completely avoid the errors introduced by the cutoff distance. The values of σ_i and σ_j for silicon and carbon atoms are 4.45 and 3.854 Å, respectively [17,18] and the values of ε_i and ε_j for silicon and carbon are 0.198 and 0.062 Kcal/mol, respectively. Thus the Hamaker constant of silicon can be estimated to be 1.4848×10^{-19} J, which is close to the experimental one of 1.9×10^{-19} J [19] ($A = \pi C^2/\nu^2$, where $C = 3\varepsilon_{Si-Si}\sigma_{Si-Si}{}^6$ is the vdW attraction interaction parameter, $\nu = 4\pi(\sigma_{Si-Si}/2)^3/3$ is the atom volume of about 46.14 Å^3) and the estimated Hamaker constant for diamond is about 4.65×10^{-20} J. Therefore, the Hamaker constant for silicon-diamond interacting across air/vacuum is about $A \approx (A_{Si}A_{Diamond})^{0.5} \approx 8.3 \times 10^{-20}$ J. For a pair of dissimilar atoms, σ_{ij} is governed by the Waldman-Hagler combination rule [20] and the σ_i and σ_j values of the individual atoms as used in previous work [11], thus giving rise to $\sigma_{Si\text{-}C} = 4.204$ Å that will be used in the following Eq. (2).

The snapshots of a typical simulation process are shown in Fig. 1. The simulation involves two equally-sized silicon nanospheres of 1.876 nm in radius. Initially, the two identical nanospheres move towards each other at an initial relative velocity of $V_{r,0} = 200$ m/s, reach a relative position as depicted in Fig. 1a and b under the influence of external load. And then, the two nanospheres continue moving towards each other as displayed in Fig. 1c and come in close proximity as shown in Fig. 1d and e. Indicated in Fig. 1f–h are the relative positions of the two nanospheres in the departing process.

3. Results and discussion

3.1. Characterization of silicon nanospheres

The thermal vibration may cause surface atoms in nanospheres to fluctuate out of the arbitrary cut-off radius (R_0) and the size of nanospheres becomes vague [21]. Therefore, the structure of silicon nanospheres will be characterized in a similar way as silica nanospheres [11]. All atoms with saturated coordination number are reflected as the "core" of a nanosphere. Atoms with unsaturated coordination are referred to as "surface atoms" while those with saturated coordination are termed as "core atoms". The individual radial distances of surface and core atoms from the nanosphere centre are denoted as R_i^{surf} or R_j^{core}, respectively. By analyzing the equilibrated structure of nanospheres from the MD simulations, the following structural parameters can be defined: core radius (R^{core}, the maximum value of R_j^{core}), surface roughness (rms), particle radius (R, the average value of R_i^{surf} from all surface atoms), relative surface roughness (rms/R), effective surface thickness (δ), maximum surface thickness (δ_{Max}) and the part of the nanoparticle that is beyond the defined particle radius (Δd). The d denotes the corresponding shortest surface-to-surface separation, $d = r\text{-}2R$, where r is the center-to-centrer separation, R the nanoparticle radius. Surface roughness rms, effective surface thickness δ and maximum surface thickness δ_{Max} vary slightly and can be regarded as independent of particle size. The results show that for silicon nanospheres, rms is about 0.62 ± 0.02 Å, δ is about 1.65 ± 0.08 Å, and δ_{Max} is about 2.37 ± 0.37 Å. The defined particle radii corresponding to cut radii R_0 of 1.0, 2.0, 3.0, 4.0 and 5.0 nm are 0.862, 1.876, 2.864, 3.839 and 4.849 nm, respectively. Besides, there is almost no surface atom fluctuating out of R_0 since in most cases it satisfies $R^{core} + \delta_{Max} \le R_0$.

As for the structural parameters for diamond nanospheres, characterizations have been performed before [13]. For diamond nanospheres, the core radii R^{core} of diamond corresponding to $R_0 = 1.0$, 1.5, 2.0, 2.5 and 3.0 nm are 0.875, 1.343, 1.850, 2.343 and 2.852 nm, respectively; and the corresponding defined particle radii $R \equiv \overline{R}$ are 0.935, 1.419, 1.931, 2.423 and 2.928 nm, respectively; rms is about 0.42 ± 0.05 Å, δ about 1.17 ± 0.13 Å, and δ_{Max} about 1.53 ± 0.18 Å.

3.2. Calculation of interaction forces between silicon nanospheres

Fig. 2 shows the evolution of interparticle potentials as a function of surface separation d between two identical silicon nanospheres. It can be observed from the inset that both the vdW attraction and Born repulsion potentials vary with particle size in a regular fashion. For a given particle size, the magnitudes of both vdW attraction and Born repulsion potentials increase with the decrease in surface separation; for a given separation, both the magnitudes of vdW attraction and Born repulsion potentials increase with increase in particle size. With decrease in

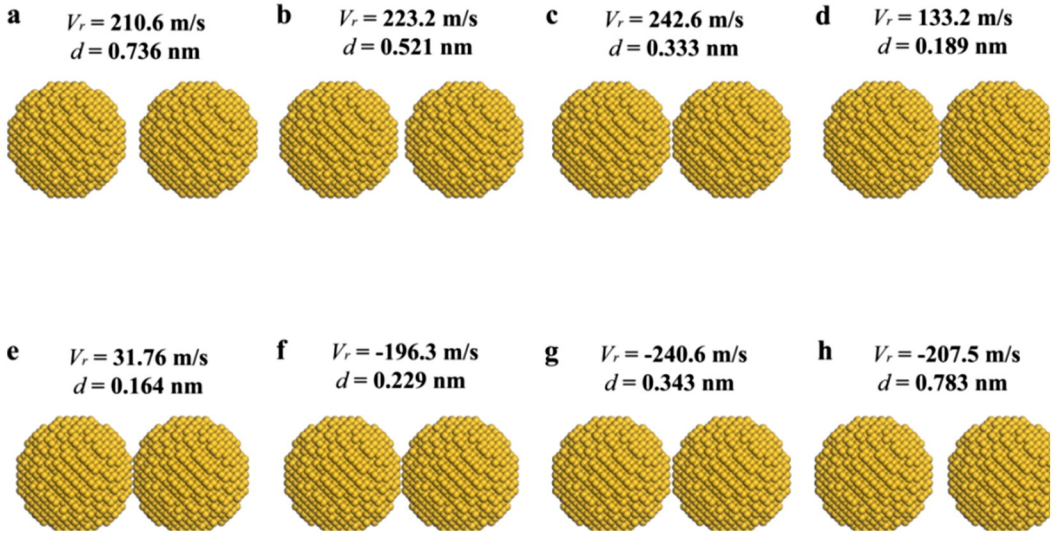

Fig. 1. Sequence snapshots of two silicon nanospheres during the head-on collision at different times of (a) 17.5, (b) 18.5, (c) 19.3, (d) 20.0, (e) 20.3, (f): 21.0, (g): 21.5 and (h): 23.5 ps. The relative velocity, $V_r > 0$, denotes the approaching process while $V_r < 0$ represents the departing process.

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