Supplementary Information

Interactions between crystalline nanospheres: comparisons between molecular dynamics simulations and continuum models

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1. Effect of temperature on interparticle LJ potentials and mechanical contact forces

Fig. S1-a shows that the LJ potential results obtained at different temperatures from 100 to 400 K are almost identical so that the effect of temperature can be ignored. Likewise, the mechanical force results in the same temperature range are almost identical as shown in Fig. S1-b indicating that they can also be considered independent of temperature.

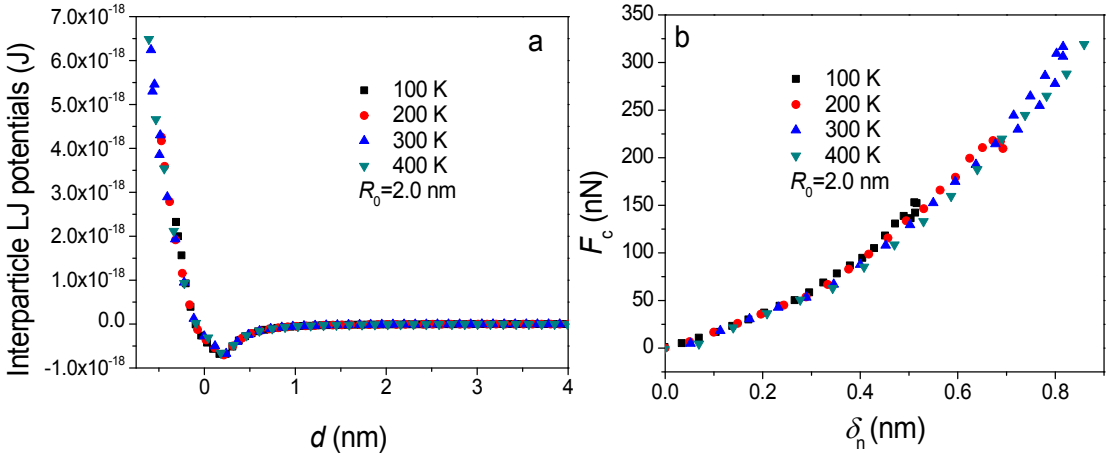

Figure S1. (a) Interparticle LJ potentials as a function of surface separation d and (b) mechanical contact forces F_c as a function of normal displacement δ_n between two silicon carbide nanospheres 2.0 nm radius obtained in the approach process at an initial relative velocity of 500 m/s under different temperatures using a NVT ensemble and Berendsen thermostat method.

2. Supplementary nomenclature

Table S1 Nomenclature for symbols used in this work

Symbol	
A	Hamaker constant
C	vdW attraction interaction parameter
ε	potential well depth
σ	collision diameter of atom
E_{LJ}	interparticle Lennard-Jones potential
R_0	cut-off radius
R	defined particle radius $R = \overline{R}$
$\overline{R}$	averaged radial distance of surface atoms from particle centre
R^{core}	radius of particle core
rms	surface roughness
δ	effective surface thickness
δ_{Max}	maximum surface thickness
δ_n	normal displacement
Δd	part beyond defined particle radius
rms/R	relative surface roughness
d	shortest surface separation of two particles
d_{min}	minimum surface separation

v	velocity or volume of atom
Y	yield strength
C_0	characteristic velocity of a material
ρ	material density or number density of atoms
λ	ratio of particle radii of two particles
ρ_H	number density of atoms determined in the Hamaker approach
ρ_T	true number density of atoms
k_ρ	$k_\rho = \rho_T/\rho_H$
$\mathbf{F}_n$	total normal force
$\mathbf{F}_{vdW}$	van der Waals attraction force
$\mathbf{F}_{Born}$	short range Born repulsion force
$\mathbf{F}_c$	mechanical contact force
$\mathbf{F}_t$	tangential force
$\mathbf{F}_Y$	force along the Y-axis
$\mathbf{F}_Z$	force along the Z-axis
v	Poisson ratio
Z_0	equilibrium separation
m	mass
δ_n^*	maximum normal displacement