Lunar Dust Particle Simulation in the (12-6) Lennard-Jones Potential Approximation

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Introduction

We model lunar dust particles as interacting ellipsoidal dipoles by means of Lennard-Jones potentials (L-J). Lunar surface dust particles are continuously bombarded by plasma charge particles coming from the solar wind. It has been recognized that solar wind bombardment leads to strong intergrain interactions between dust particulates leading to collective effects such as attraction of charged dust particles. Formation of electrostatically ordered dust structures is believed to be due to strong attractive van der Waals-like potentials at distances in the order of interparticle separation. Dust-dust electrostatic interactions and collisions may lead to particle coalescence or dust-lumps kept together due to Coulomb forces. On the other hand, dust ionization occurs after solar wind electrons collide with grains in the plasma sheath formed on the lunar surface. Particle coalescence and to an extent condensation is feasible when an attractive potential is present. Ellipsoidal dipole condensation is possible in the presence of a Lennard-Jones (L-J) potential.

Specifically, two neighboring dust dipoles are considered as two harmonic oscillators near each other, and their Hamiltonian H_o is just the sum of their kinetic and potential energies. The Hamiltonian is then corrected by adding the electrostatic term H_1 representing Coulomb interaction. It can be shown that the correction term H_1 is inversely proportional to cube of the distance R between the two dipoles (~R^{-3}).

The total Hamiltonian H_o+H_1 is expressed in symmetric and antisymmetric modes. The dominating term in the finalized energy of the dipole-dipole system is found to be inversely proportional to the 6th power of the dipole separation distance R and is usually written as -A/R^6, where A is a constant factor. As it is typically recognized in the L-J context, the cohesion in the dipole-dipole coalescence can happen only when a strong repulsive potential is present as well, namely some U(r) =B/r^{12}, that keeps the electron clouds in the individual atoms from overlapping. Note that B is a constant, and the exponent is empirically found (from the condensation of inert gas atoms into crystalline fcc structures). Typically, the L-J cohesion energy is formed from the sum of the attractive and the repulsive terms and in the following form:

$$U(r) = 4\epsilon\left\{\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right\},$$

where the two parameters s and e are $\sigma = \left(\frac{B}{A}\right)^{\frac{1}{6}}$ and $\epsilon = \frac{A^2}{4B}$ respectively.

Intermolecular Potential Energy

The Lennard-Jones potential approximates the true intermolecular potential energy curves. It models the attractive component by a contribution that is proportional to 1/r^6, and the repulsive component by a contribution that is proportional to 1/r^{12}. Specifically, these choices result in the Lennard-Jones (12,6)-potential.

Although there are good theoretical reasons for these choices, there is plenty of evidence to show that 1/r^{12} is only a very poor approximation to the repulsive part of the curve.

The formula is

$$E_p = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]$$

Where ε (kJ·mol-1) is the depth of the well, σ (pm) the separation at which E_p = 0, and r is the separation in picometers.

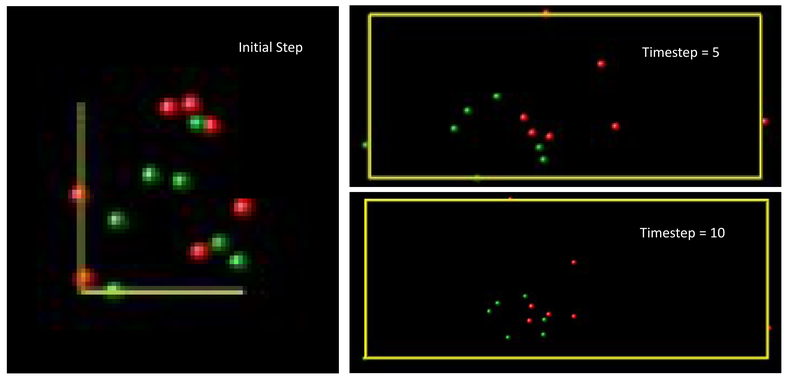
Molecular Dynamics Simulation

Molecular dynamics is a computing simulation technique that models the physical movement of atoms and molecules. In our case, we will model the physical movement of dust particles on solar cells and other optical devices on the lunar surface. For our analysis, we will employ LAMMPS which is developed in Sandia National Laboratory and is a free, open-source simulator. LAMMPS is extensively used by the research community, especially in molecular dynamic modeling.

Data and Analysis

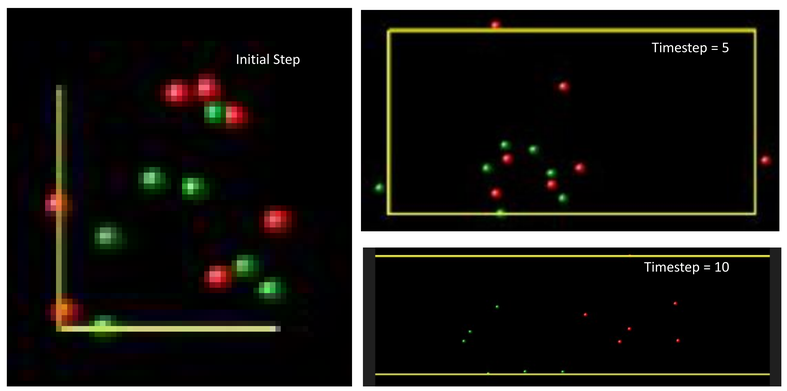
We present two case studies to optimize the modeling of lunar dust using LAMMPS. In both case studies, we start with 14 charged atoms, 7 negatively charged, and 7 positively charged. We introduced an electric field and modeled the results of the atoms in various timesteps.

Case Study #1: Fourteen Charge Particles, Electric Field of 10 V/Å



Progression of atoms over timesteps. Note that half the atoms are positively charged, and half are negatively charged.

Case Study #2: Fourteen Charge Particles, Electric Field of 50 V/Å



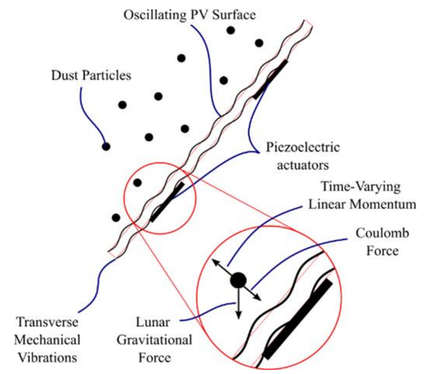
Progression of atoms over timesteps. Note that half the atoms are positively charged, and half are negatively charged.

Ultrasonic Excitation

Our preliminary MATLAB simulations of PV devices harmonically excited with ultrasonic PZT actuators with a frequency of about 20 kHz have exhibited the potential of the high-frequency transverse vibration to prevent the lunar dust accumulation of PV devices that are not oriented horizontally relative to the Moon's surface.

The transverse mechanical excitation offers a linear momentum for the attached dust particles to overcome the adhesive forces and separate dust particles from the surface. This dust separation period will allow the dust particles to travel down about multiples (10 times the particle size) of the surface of PV structures by the lunar gravity through consistent mechanical oscillations.

The preliminary results showed removing the dust with mechanical vibrations in the presence of weak gravity could be a prospective surface-cleaning strategy on the Moon [6]. Further investigations need to be carried out by consideration of different particle sizes and charges and simulations. Besides the excitation intensity (i.e. the relative ultrasonic amplitude excitation) compared with particle sizes are being studied to determine an optimized excitation frequency and the relative amplitude as a function of the lunar dust particles.



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