Announcing the Final Examination of ABRAR H. QUADERY for the Degree of Doctor of Philosophy in Physics

Date: Wednesday, November 1, 2017
Time: 3:00 pm
Room: PS 161 (4111 Libra Dr)

Dissertation Title:
COMPUTATIONAL MODELING OF PHYSICAL AND CHEMICAL PROCESSES DURING SPACE WEATHERING AND PLANET FORMATION

Abstract:
We investigate the mechanisms of space weathering and dust grain collisions, two topics of interests from planetary sciences, using atomic-scale simulations. Space weathering is the change in chemical and physical properties of minerals exposed to solar radiation and micrometeorite bombardment on surfaces of airless planetary bodies like the Moon and asteroids. An understanding of the connection between the surface evolution of the minerals to the underlying thermodynamic and kinetic factors is still missing. We address this issue and determine the time evolution of Frenkel defects in the silicate minerals olivine ((Mg,Fe)$_2$SiO$_4$) and orthopyroxene ((Mg,Fe)SiO$_3$) using molecular dynamics with a pair potential. Defect diffusion and clustering are observed in both the minerals. Cation diffusion occurs more readily in olivine than in orthopyroxene and leads to faster annealing in the former. In orthopyroxene, diffusion of anion defects, especially oxygen interstitials, occurs more rapidly and also exhibits anisotropy, which hinders the annealing process. This difference in defect evolution may explain the experimental observation that surface modifications due to irradiation is more pronounced in orthopyroxene than in olivine. Dust grain collision is the dominant process in the initial stage of planet formation, however, the mechanisms by which dust grains grow to larger aggregates and eventually to kilometer sized planetesimal is still not understood. We explore the role of surface chemistry in energy dissipation and grain adhesion during collision of amorphous silica (SiO$_2$) nanograins using molecular dynamics using a reactive potential, namely ReaxFF. We found nonhydroxylated amorphous silica nanoparticles stick with higher probability than their hydroxylated counterpart. This difference is attributed to the preponderance of unsatisfied dangling bonds on the dry silicate surface which facilitate bond formation during collision, and thereby provide a mechanism for energy dissipation. The speed below which sticking occurs in the dry nanograins is much higher than that found in Earth-based experiments, which suggests any experimental study of dust grain collision should take into account of the chemical environment. We probe into the nanograin collisions further and carry out atomistic simulatons of collisions of molten silica nanograins. We observed in the molten state, amorphous silica is more sticky than it is in the solid phase. This happens due to increased viscoelastic energy dissipation. The result may explain how rocky planets originated from the inner rings of the protoplanetay disks where temperatures were as high as $\sim$ 2000 K. In order to increase the range of materials that could be simulated with ReaxFF potential, and also to examine the different oxidation states of iron associated with nanophase iron formation during space weathering, we made attempt to develop ReaxFF potential for fayalite (Fe$_2$SiO$_4$). We found out fundamental limitation of the ReaxFF model to describe three-component minerals. However, during the fitting process we developed models for iron silicide (FeSi) and also silica, and with the latter we simulate dust grain collision to see how the models affect the collision outcome.

Outline of studies:
Major: Physics

Educational Career:
B.Sc. (Honors) Physics, University of Delhi, 1995
M.Sc. Physics, University of Delhi, 1997

Committee In Charge:
Dr. Patrick K. Schelling, Chair
Dr. Daniel T. Britt, Committee Member
Dr. Robert E. Peale, Committee Member
Dr. Abdelkader Kara, Committee Member
Dr. Yongho Sohn, External Committee Member

Approved for distribution by Dr. Patrick K. Schelling, Committee Chair, on October 25, 2017.

The public is welcome to attend.