COMPUTER SIMULATION OF ION RADIATION DAMAGE IN SILICATES: APPLICATION TO PARTICLE RIMS AND FORMATION OF "GEMS" IN IDPs,

R. Christoffersen and D.S. McKay, Code SN, NASA Johnson Space Center, Houston, TX 77058

Introduction. The recent debate about the origin of amorphous rims on lunar regolith grains [1,2,3,4], together with the hypothesized formation of pre-accretionary aggregates (GEMS) in interplanetary dust particles (IDPs) by ion radiation effects [5], have revived the need for new data on solar ion radiation effects in extraterrestrial materials. Although new ion irradiation experiments are an important and necessary approach to obtaining these data, it is possible to leverage the existing experimental results on ion radiation effects in silicates and oxides using computer simulations. These simulations do not replace experiments but allow radiation effects studied for a particular ion at a particular energy to be extrapolated to other ions and energies. Here we review one type of computer simulation algorithm for calculating ion range distributions and atom displacement damage effects, with examples of its applicability to solar (or interstellar) ion radiation effects in IDPs.

Computer simulation methods. At present the most widely used algorithm for simulating ion radiation effects in solids is embodied in the TRIM (*TR*ansport of *I*ons in *M*atter) codes introduced by Ziegler et al. [6]. TRIM is a Monte-Carlo algorithm based on the binary-collision approximation model for atomic collision processes in solids. Its accuracy in calculating ion range distributions in various substances including oxides is well-established, and the code allows for corrections due to spherically-incident radiation and a receding surface due to sputtering.

TRIM calculates target damage in terms of atomic displacements due to nuclear stopping within an "average" collision cascade for a given ion. Recent *in-situ* radiation experiments using a tandem TEM and ion-accelerator [7,8] have suggested that amorphization in certain silicates, including olivine, occurs at a critical value of displacements per target atom (DPA) that is constant irrespective of the energy and type of ion used. Using the constant DPA model, and the results of at least one irradiation-induced amorphization experiment, TRIM calculations can be used to estimate the dose from a given ion at a particular energy that is needed to produce amorphization due to direct atomic collisions. The contribution to the amorphization from atom displacements due to ionization effects (i.e., ion explosion spikes from heavy ions that leave latent tracks) is a separate problem that can be treated assuming all atoms are displaced within a specified track volume. The contribution of such displacements to the total amorphization process will depend on the flux of heavy ions that leave tracks at target depths of less than 300 nm.

Application to Ion Radiation Effects in IDPs. Two problems pertaining to solar/interstellar ion radiation effects in IDPs are: 1) the production of amorphous rims around the outer margins of whole IDP particles, and 2) the possible formation of amorphous grains with enclosed metal and sulfides (GEMS) within IDPs by pre-accretionary ion radiation damage of a crystalline precursor [5]. Bradley [5] has proposed that such radiation effects imply an exotic origin for GEMS either in the interstellar medium, or possibly during a more active phase of the early sun.

While the formation environments that have been postulated to date for GEMS and IDP rims are very different (i.e., interstellar or early solar system versus more recent solar system), the amorphization depth implied by the radius of most GEMS and the width of IDP rims is roughly the same, on the order of 150-250 nm. The two features therefore coincidentally have similar requirements in terms of the atom displacement damage versus depth needed to produce them. TRIM range calculations for H, He and heavier ions in silicate targets show that amorphization depths above 150 nm are larger than can be accounted for using the low ion energies (0.3-3 keV/nucleon) that characterize the contemporary solar wind. Instead both GEMS and IDP rims require damage contributions from ions with energies no lower than 10-20 keV/nucleon if no sputtering occurs, or 10-80 keV/nucleon assuming a reasonable sputtering rate over a 100,000 year exposure age. Using the constant DPA model for silicate amorphization, the TRIM damage calculations show that, for a 100,000 year particle exposure lifetime, an average

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integrated proton flux of 10^4-10^5 protons/cm^2 sec over the above energy intervals would be required to account for the IDP rim amorphization depths. (Incorporation of additional damage from alpha particles and slow heavy ions in solar wind proportions changes the result by less than an order of magnitude).

For the IDP rims, which received their irradiation in the relatively recent solar system, possible sources for ions with the requisite energies could be: 1) an unusually energetic ancient solar wind, 2) the lowest energy range of particles from transient solar events such as flares and 3) plasmas associated with planetary magnetospheres, particularly those of the outer planets. As there is presently little or no evidence, theoretical or otherwise, for an anomalously more-energetic ancient solar wind, this first source does not appear to be realistic. Solar flare ions of an intermediate (10-100 keV/nucleon) energy type have been thought to exist at significant per-event fluxes based on extrapolations of particle fluxes at higher energies. Unfortunately few direct measurments of such ions have been made outside the earth's magnetosphere, making dose calculations for them speculative at the present time. Our results so far, however, make us suspect that such low-energy solar-energetic particles may make more of a contribution to radiation-induced amorphization in space-exposed silicates than previously considered.

A possible role for outer planet magnetospheric plasmas in irradiating IDPs or their constituents is supported to the extent that direct measurements of these plasmas [9] show a high enough dose of intermediate (10-100 keV/nucleon) energy particles to damage silicates to the required depth in about 100, 000 years. Further support for such a role must await a mechanism for ejecting IDP-sized particles from the outer planets into the inner solar system.

Allowing for the hypothesized formation of GEMs in the interstellar medium or around the proto-sun, there are naturally more options for obtaining the ion dose-depth relationships needed to form them compared to IDP rims. The interstellar option has the advantage of exposure times on the order of 10^8 years [10], but the integrated cosmic ion flux over the narrow 10-80 kev/nucleon energy interval must still average on the order of 10^1-10^2 particles/cm^2 sec. The early solar system option works insofar as the early Sun during its T-tauri phase and at other times probably emitted a considerably higher flux of intermediate-energy particles [11]. However, the net radiation transmission through a dust-shielded ecliptic plane in the nebula is an unresolved problem.

An alternative origin for GEMS that cannot be ruled out on the basis of the observed radiation effects is that they were produced in a solar-system radiation environment that post-dates the proto-sun. This is suggested by the fact that IDPs irradiated in the relatively recent solar system have rim amorphization depths similar to that required to make GEMS from a crystalline precursor grain. Thus, GEMS might not inherently require an exotic radiation environment in order to form. The only thing that supports an exotic origin is the pre-requisite that the irradiation took place before GEMS became incorporated into their host IDP.

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