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Impact of energetic cosmic-ray ions on astrophysical ice grains

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ABSTRACT

Using molecular-dynamics simulation with REAX potentials, we study the consequences of cosmic-ray ion impact on ice grains. The grains are composed of a mixture of H_2O, CO_2, NH_3, and CH_3OH molecules. Due to the high energy deposition of the cosmic-ray ion, 5 keV/nm, a strong pressure wave runs through the grain, while the interior of the ion track gasifies. Abundant molecular dissociations occur; reactions of the fragments form a variety of novel molecular product species.

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1. Introduction

Surfaces of moons, dwarf planets and smaller bodies in the outer solar system are covered by ices [1]. Also ice-covered dust grains populate the interplanetary and interstellar medium [2]. Besides H_2O, these ices contain mixtures of NH_3, CO_2, and other molecular species [3].

Ice grains are exposed to particle irradiation stemming from various sources: the solar wind, cosmic-ray ions, and possibly magnetospheric ions and electrons. Cosmic rays are ubiquitous and can induce a variety of changes in the grain: compaction, phase transformation, erosion and chemical transformations [4,5]. The elemental composition of cosmic-ray ions peaks at H and He, but also all other elements are present, albeit in smaller concentrations; for instance, Fe ions are by a factor of 10^4–10^5 less abundant than protons [6, Fig. 1]. While energies have a broad maximum at 10–100 MeV/amu [7], they fall off with a soft power-law decay $\propto E^{-2.7}$ beyond this maximum, and highest energies in the range of 10^{20} eV have been observed [8].

The effects of cosmic-ray impacts on ice surfaces have been studied using laboratory experiments, where energetic ions irradiate ice samples [9]. In addition, molecular dynamics (MD) simulations offer an important theoretical tool to study the processes occurring after energetic-particle impact. Initially such simulations were restricted to simple atomic systems, and Lennard-Jones targets were used in order to identify the generic response of materials to the impact [10–12]. In particular, Bringa and Johnson performed dedicated MD simulations to observe sputtering from spherical grains [13].

The recent invention of the so-called REAX potentials [14–16] allowed to model the breaking and formation of chemical bonds in MD simulations for a wide group of elements; previous so-called 'reactive' potentials, such as REBO and AIREBO [17,18], were essentially restricted to hydrocarbons. REAX potentials were used to study the irradiation of ice surfaces [19], and in particular the effects of cosmic-ray impacts on ice grains [20].

In the present paper, we study the effect of cosmic-ray impact on an ice grain using MD simulation. We choose an event with a high energy deposition, 5 keV/nm, which we can compare with our previous results [20] for a more moderate energy deposition, 1 keV/nm. Focusing on the generation of the pressure wave in the grain and the fragmentation and chemical reactions occurring after the cosmic-ray impact, we can identify the differences between moderate and high energy deposition.

2. Method

We prepare a spherical amorphous ice grain consisting of H_2O, CO_2, NH_3, and CH_3OH with molar ratios of 9.10:8.00:3.75:1.00. Such a mixture has been recommended by Martins et al. [21] to be representative of cometary material, and has been used by us previously [20]. The grain consists of 28,428 H_2O, 24,992 CO_2, 11,715 NH_3, and 3,124 CH_3OH molecules. After relaxation, it has a radius of $R = 93$ Å.

The intra- and intermolecular interactions in this ice mixture are described by the REAX potential developed by van Duin et al.

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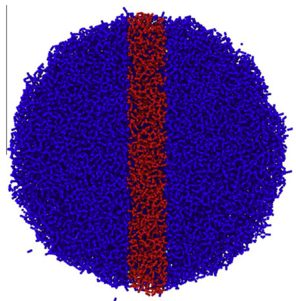

Fig. 1. Meridional cut through the grain immediately after track formation. Color denotes the local temperature. Figure prepared with OVITO [26]. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

[14–16,22]. Towards higher energies we add the Ziegler-Biersack-Littmark (ZBL) [23] potential to model the repulsive short-range interaction. Details of the combination of the REAX and ZBL potentials have been described previously by us [19].

A cosmic-ray ion is assumed to pass along a straight trajectory through the center of the grain. It is modeled by heating at time $t = 0$ a cylindrical volume – the 'ion track' – of radius $r = 5$ Å around the ion path. We choose a high energy deposition of $dE/dx = 5$ keV/nm; such an (electronic) energy deposition is around the value reached by an Fe ion at maximum energy deposition; in our ice mixture it amounts to 4.4 keV/nm at 55 MeV ion energy according to the SRIM code [24]. We determine the length of the ion trajectory in the grain as $L = 182.3$ Å; hence the total energy deposited in the grain amounts to $E_{dep} = L \cdot dE/dx = 91.15$ keV. The energy is given to each of the $N_{track} = 1101$ atoms in the cylindrical track region as kinetic energy; each atom receives on average a kinetic energy of $E_0 = E_{dep}/N_{track} = 82.8$ eV, but with random direction. Fig. 1 pictures the grain containing the heated track shortly after track initiation. Only a single cosmic-ray event is simulated.

We use the massively parallel open-source code LAMMPS for performing the simulations [25]. The variable time step changes from initially 5 to finally 51 as; this small time step is necessary in order to capture the motion of H atoms reliably. The simulation runs until 9.63 ps after ion-track formation; at this time, chemical reactions appear to have saturated, see Fig. 4 below. Further details of the simulation procedure and of the detection algorithms are described in Ref. [20].

3. Results and discussion

Fig. 2 presents a side view (meridional cut) and a top view of the irradiated grain at 9.63 ps after track formation. Due to the high energy deposition, the track has widened laterally and considerable ejection occurs from the top and bottom ends of the track. Only an equatorial strip of the original grain has stayed intact, and it must be presumed that at later times the grain will eventually disintegrate completely.

The high energy density in the track leads to the formation of a strong pressure pulse traveling outwards in axial direction. Fig. 3 provides details of the density and temperature profiles at various times after track formation. The track center quickly becomes depleted of molecules, while the outer surface of the grain expands. Finally the grain consists only of a narrow shell extending between 70 and 120 Å from the track center, while the entire interior has reached a density of less than 10% of the original density. The temperatures indicated in Fig. 3(d)–(f) must be taken to represent kinetic-energy densities, at least at early times when the system has not yet equilibrated thermally. After around 2 ps the central temperatures reach 4000 K and decline only little (to around 2000 K) at the end of the simulation. Such high temperatures are considerably beyond the critical temperatures of the molecular species present in the ice mixture; the highest value is provided by water with 647 K. In consequence the material inside the track has been heated beyond the critical temperature of the liquid-gas phase transition and can freely flow out of the track volume.

As a consequence of the high energy densities reached in the track volume, abundant molecule dissociation events occur, see Fig. 4. The main part of these dissociations occur quite early, within 1–2 ps after track formation; however, also towards later times these reactions continue but appear to have mostly reached saturation at the end of the simulation. Note that water behaves differently than the other species in that recombination events occur that restore the destroyed H_2O molecules almost completely. The number of water molecules reaches a minimum (1177 dissociations) at a time of around 0.25 ps, and thereafter rises again; finally, only 104 water molecules are dissociated. We note that among the 1073 recombination events, only around 15% of the H_2O molecules are 'restored' in the sense that the prior partners found together to the same molecule; in the remaining cases the atomic content of the H_2O molecules has changed.

The dissociation products may react to form further product molecules. Fig. 5 shows the product molecules in the form of a mass spectrum. The results are compared with those of a reference simulation, where an ion track in the same grain was considered

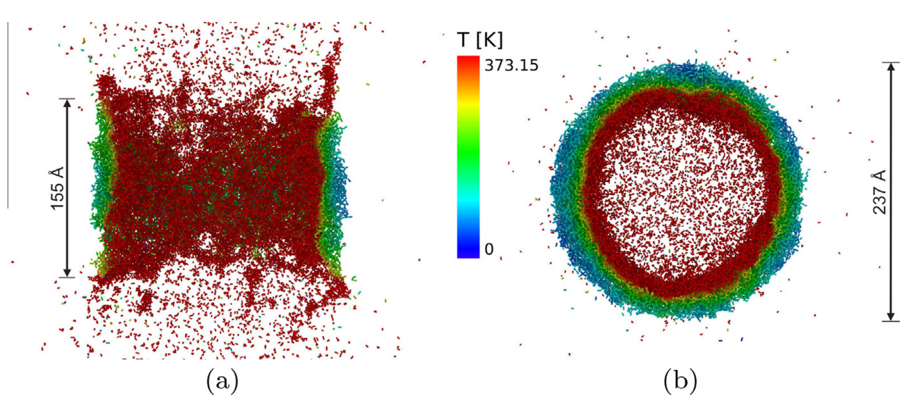

Fig. 2. Meridional cut through the irradiated grain (a) and top view (b) at the end of the simulation, 9.63 ps after track formation. Color denotes the local temperature, see color bar. Figure prepared with OVITO [26]. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

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