COMPUTER CALCULATION OF COLLISION CASCADES BY ENERGETIC PARTICLES PENETRATING DUST GRAINS

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ABSTRACT. The penetration of energetic particles from stellar winds, cosmic rays and fast moving gas clouds in interstellar dust grains induces a variety of physical and chemical changes. Detailed information on penetration ranges, number of secondary projectiles produced by knock-on and their energy distribution is obtained from computer simulation of collision cascades with the program MARLOWE. Model targets are polycrystalline H_2O-ice, NH_4Cl, and SiO_2, projectiles are 10^2-10^4 eV H, He, and C. Depending on the energy and the projectile/target mass ratio up to 10^2 secondary projectiles are created per primary impact with energies ranging from a few to some 10^3 eV. In composite grains, condensed gases and ice mixtures the energetic secondaries can undergo hot chemical reactions leading to a series of precursors for larger organic and biomolecules.

1. INTRODUCTION

Interplanetary and interstellar dust grains are bombarded by energetic particles such as electrons, protons, alphas and heavier ions from local radiation belts, solar (stellar) wind, cosmic rays and fast moving gas clouds. These impacts induce a variety of physical and chemical changes. Among them is the build-up of organic material, especially in composite grains with ice layers or frozen mixtures of gases, cf. e.g. (1,2). A new type of interactions has recently be introduced to cosmic chemistry, high energetic (hot) reactions of biogenic implants such as carbon or nitrogen (3). Hot atom chemistry (4,5) is characterized by the fact that endothermic reactions and those with high energies of activation are possible, among them atom molecule interactions. Primary implants and secondary particles knocked on inside the grain material may undergo these reactions. In homogeneous ice mixtures, e.g. H_2O-NH_3-CH_4, the products of the secondaries may be more important than those of the primaries. The hot reactions are accompagnied by radiolytic and photolytic processes which may change the initial products, cf. (6).

The physical consequences of particle impact into the grains are

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not well known. Penetration depths and stopping powers are listed in table works for particles with energies $\geq$ 1oo keV/amu and for monoelemental solids only. The lower energy regime of some 1o to some $1o^4$ eV, typical for accelerated particles in space, can be treated by computer simulation of collision cascades with simple codes such as TRIM (9). Detailed information on ranges, displacements and replacements, defect profiles, recombination of defects, and backscattering or sputtering from surfaces in well defined polyelemental solids can be obtained from the code MARLOWE in the binary collision approximation (1o). This code had been successfully used for studies of collision dynamics in many insulators (11-17). It is now applied to simulate cascades of light and heavier projectiles in substances representative for cosmic dust particles. Some results are presented here: mean penetration of primary and number of secondary projectiles and their energy distribution. A more detailed report will be given elsewhere (18).

2. COMPUTER CODE AND INPUT DATA

MARLOWE was used in a slightly modified version (14), however, with the standard procedure provided by the default option. Projectiles studied were ^1H, ^4He and ^{12}C with the primary energies $1o^2$, $1o^3$, and $1o^4$ eV. Solid H_2O, SiO_2 and NH_4Cl were chosen as model substances for ice, silicate materials and compounds composed out of light, medium and heavier elements. For H_2O and SiO_2 simplified model lattices were selected (cf. TAB. I), since their real structures under cosmic conditions are unknown. The lattice constants preserve the real densities of $\rho(H_2O,77K)$ = o.87 and $\rho(SiO_2)$ = 2.635 gcm^{-3}. For NH_4Cl the real bcc lattice with ρ = 1.527 gcm^{-3} was taken.

TABLE I. Parameters of model substances for MARLOWE calculations

	lattice type	a_o,nm	energies, eV		
			displacement threshold	binding loss	projectile cutoff
H_2O	antifluorite	51.6	4(H), 5(O)	2(H), 3(O)	2(H,O)
NH_4Cl	bcc	38.7	7(N),4(H),5(Cl)	3(N),2(H,Cl)	3(N,H,Cl)
SiO_2	fluorite	53.3	8(Si),6(O)	4(Si),3(O)	3(Si,O)

The displacement threshold energies for the individual atoms in TAB. I were estimated on the base of sublimation and chemical bond energies. They do not represent the classical Wigner energies for creation of stable defects, e.g. Frenkel pairs. The displacement thresholds in TAB. I represent the energy necessary for an individual displacement event, irrespective of spontaneous recombination processes of close by Frenkel pairs. Binding loss energies are substracted from the

kinetic energy, a secondary atom obtains by the knock-on. The projectile cutoff energy represents the value at which a projectile is stopped by the calculation. The sum of the latter two energies should not exceed the displacement threshold energy. They are chosen empirically to about one half of the threshold value.

The projectiles were started inside the crystals. The crystal orientation was slightly changed from collision to collision by a random number generator program in order to simulate a very polycrystalline solid. No thermal vibrations were included. Only the primaries were followed to the cutoff energy. The secondaries and their energies were registered, however, their collisions were not followed for reasons of limited computation time. For 10^2 and 10^3 eV projectiles for each system 10^3 cascades were calculated, for 10^4 eV particles about 10^2 cascades.

3. RESULTS

The mean penetration of H, He and C projectiles is plotted in Fig. 1-3 versus the primary energy. The ranges decrease with increasing mass number of the projectile and with increasing density of the target. From the rather linear behaviour of the curves it seems to be possible to extrapolate to projectile energies exceeding 10^4 eV, at least for the heavier projectiles which perform an appreciable amount of elastic (nuclear) collisions.

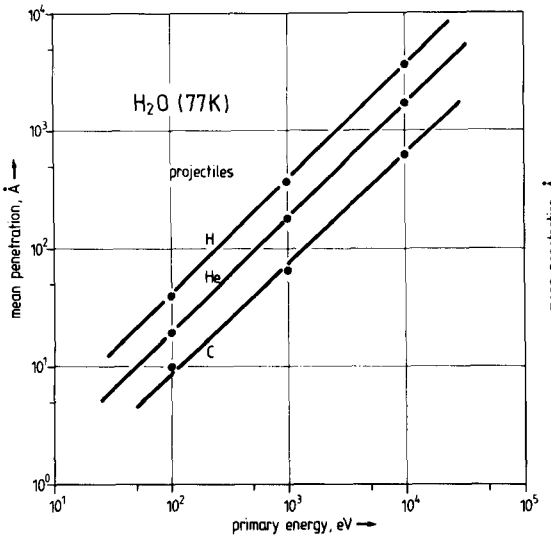

Figure 1. Mean penetration of some projectiles in H_2O-ice (77K)

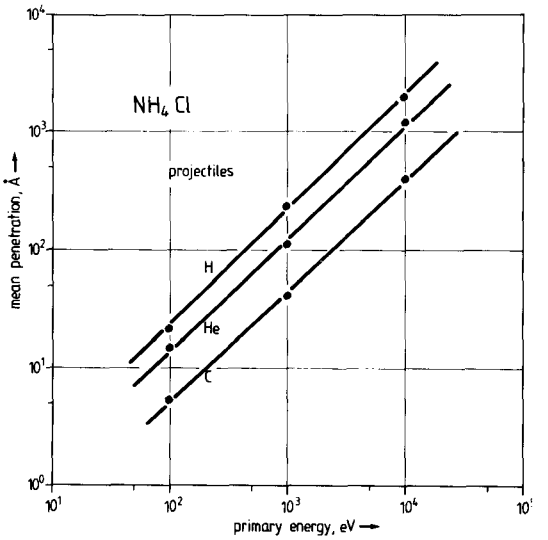

Fig. 2. Mean penetration of some projectiles in NH_4Cl

The numbers of secondary projectiles produced by knock-on processes within the solids are reported in TAB. II. The number increases with the primary energy, more steadily in the case of the

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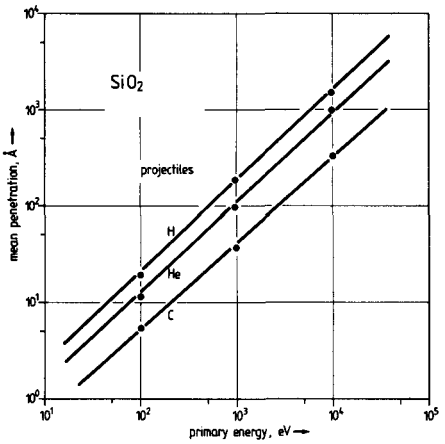

heavier projectiles than for hydrogen. It depends also on the projectile-target mass ratios. At 10^4 eV up to 100 secondaries are ejected. More information can be obtained from Figs. 4-7 which describe in more detail kind and energy distribution of the secondaries. The numbers are plotted for the individual kind of secondary ordered according to the primary energies. The distribution is given for groups ranging from 1 to 10, 10 to 10^2, 10^2 to 10^3 and 10^3 to 10^4.

Figure 3. Mean penetration of some projectiles in SiO_2 (ρ=2.635 gcm^{-3}).

TABLE II. Number of secondary projectiles per cascade

prim. projectiles and energy, eV		targets H_2O	NH_4Cl	SiO_2
H	10^2	4 ± 1	3 ± 1	1 ± 1
	10^3	13 ± 3	14 ± 4	8 ± 2
	10^4	16 ± 4	27 ± 5	20 ± 5
He	10^2	5 ± 1	5 ± 2	3 ± 1
	10^3	21 ± 5	24 ± 5	15 ± 3
	10^4	76 ± 10	69 ± 10	49 ± 8
C	10^2	5 ± 2	6 ± 2	3 ± 1
	10^3	28 ± 10	24 ± 6	16 ± 5
	10^4	92 ± 21	101 ± 19	45 ± 12

4. DISCUSSION.

The calculations prove that energetic primary particles can produce an appreciable amount of secondaries, many of them with energies > 10 and even > 100 eV. Slight changes of the energetic parameters in TAB. I might somewhat affect the number of secondaries. However, the number of particles with energies > 10 eV, which are important for hot atom chemistry, will not be diminished. The higher energetic secondaries may induce displacement and, thus, create tertiary projectiles and so on. The amount of hot chemical reactions by biogenic projectiles is magnified by the creation of secondary, tertiary etc. atoms by particles which themselves do not directly form organic material such as protons, helium ions, heavier ions up to uranium, and electrons. Another possibility for the formation of

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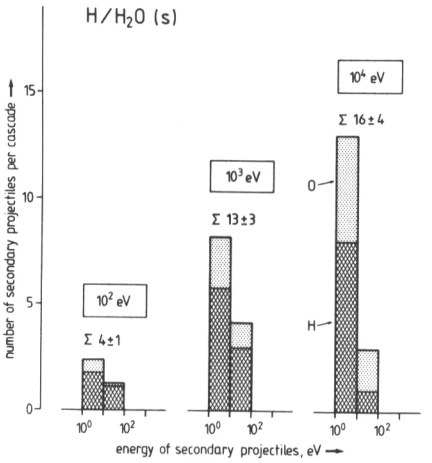

Figure 4. Secondary projetiles by H impact in poly-cryst. H_2O ice (77 K)

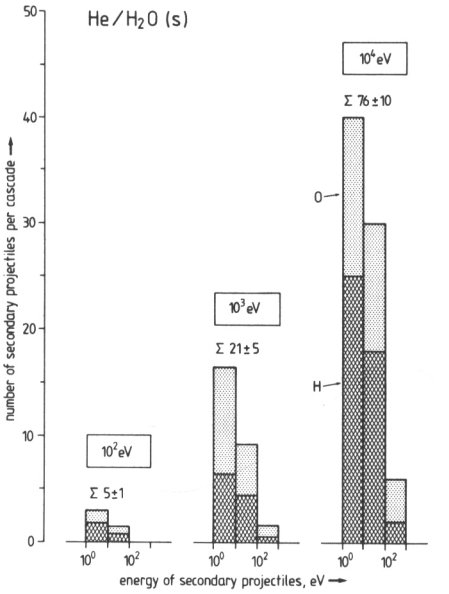

Figure 5. Secondary projectiles by He impact in poly-cryst. H_2O ice (77 K)

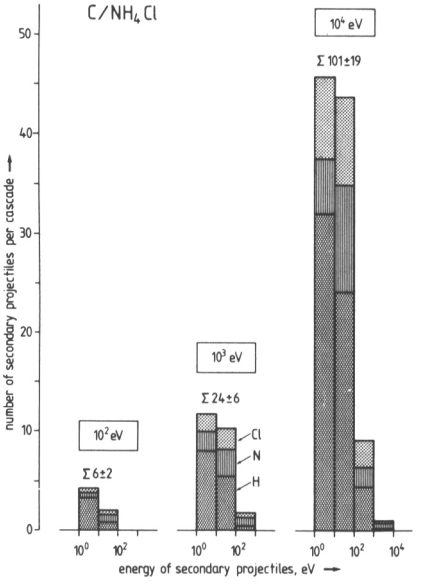

Figure 6. Secondary projectiles by C impact in poly-cryst. NH_4Cl

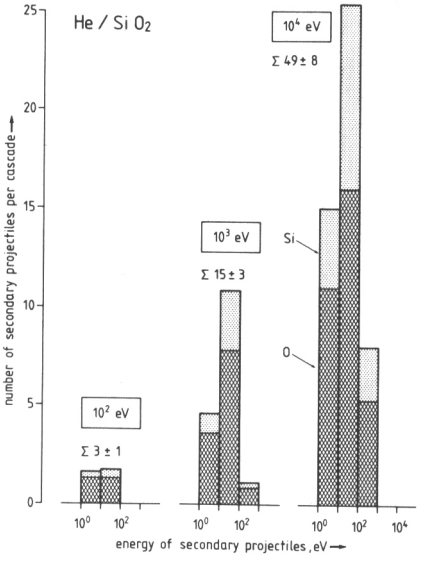

Figure 7. Secondary projectiles by He impact in poly-cryst. SiO_2

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energetic particles in solids may be coulomb repulsion upon the passage of fast, ionizing rays, e.g. from cosmic radiation. The MARLOWE calculations furnish physical data on collison dynamics in dust grains which improve the probability of chemical reactions such as shown schematically in Fig. 8. Together with photolytic or radiolytic processes, hot atom chemistry may play an important role in the formation of organic material on interplanetary and interstellar dust grains, comets and surfaces of some of the moons of outer planets.

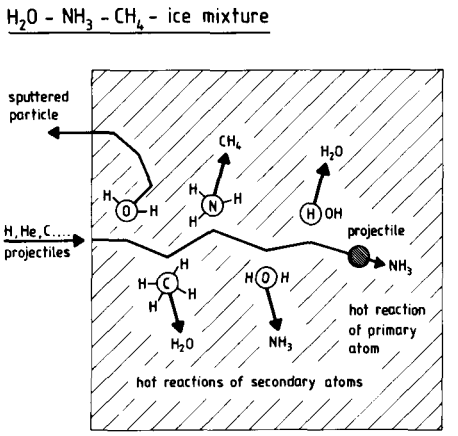

Figure 8. Schematic reactions of primary and secondary particles in an ice mixture.

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