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Charge states of helium ions after grazing collisions on SnTe surfaces

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Abstract

Emerging charge states for ions impinging grazingly on a SnTe surface are calculated at high impact velocities. The charge state distribution is obtained as result of the interplay of two atomic processes. Electron capture from bound states of the topmost atoms of the surface, and electron loss from bound states of the projectile due to collisions with the surface atoms. We find that at high energies, the projectile comes out of the surface with a charge state larger than the quasi-equilibrium charge state reached in the vicinity of the surface. We explain this behavior in terms of the different ranges of capture and loss mechanisms. As the projectile escapes from the surface, the balance between these two processes is broken: capture is no longer effective, and loss survives ionizing the projectile. Comparisons with the experiments are presented and discussed.

1 INTRODUCTION

The theoretical description of charge state distribution for ions impinging grazingly on a solid surface has recently received considerable attention [1, 2, 3, 4]. At high impact velocities, the emerging charge state of the ion can be considered as a consequence of the interplay of two atomic processes. Electron capture from bound states of the topmost atoms of the surface, and electron loss from the bound states of the projectile due to collisions with the surface atoms. This is the standard approach to deal with the problem, and it is employed in this work.

In grazing collisions at intermediate energies it is observed that the ion reaches an equilibrium charge state close to the surface, which persists until exit[2, 4]. Instead, at high impact velocities, we find that the charge state gets a quasi equilibrium value in the immediate vicinities of the surface, but it tends to another value far from the surface.

We concentrate on collisions of He ions with a SnTe(100) surface, which have been experimentally studied [1, 2, 3, 10, 11]. Atomic units are used.

2 THEORY

Let us consider a heavy projectile (of charge Z_P, mass M_P and initial velocity v) impinging grazingly on a solid surface with an incident angle θ_i. The charge state of the impinging ion during the collision is determined by capture and loss processes. For a given charge state j $(0 \leq j \leq Z_P)$ of the projectile, the time-dependent evolution of the charge state fraction F_j is governed by a system of coupled equations satisfying

$$\frac{dF_j}{dt} = v \sum_k \left[F_k P_{kj}(z) - F_j P_{jk}(z) \right], \qquad (1)$$

where v is the impact velocity nearly parallel to the surface and t is the time. The first term of the summatory represents the processes populating the charge state j and the second term takes account of the processes depopulating j. For the ion charge changing $k \to j$, the transition probability per unit path length $P_{kj}(z)$, corresponding to a trajectory parallel to the surface at a distance z of the topmost atomic layer, is given by

$$P_{kj}(z) = \delta_S \int_{-\infty}^{\infty} \left| A_{kj}(\rho = \sqrt{y^2 + z^2}) \right|^2 dy, \qquad (2)$$

where y is the coordinate directed parallel to the surface and perpendicular to the velocity, and δ_S is the density of target atoms per unit area in the first atomic layer. $|A_{kj}(\rho)|^2$ is the impact-parameter-dependent transition probability for the charge changing $k \to j$, produced by a single collision of the projectile with a target atom.

For a transition of the projectile charge $k \to j$, we estimate the range $\langle z \rangle_{kj}$ of the probability P_{kj} as

$$\langle z \rangle_{kj} = \frac{2 \int_0^\infty z \, P_{kj}(z) \, dz}{\int_0^\infty P_{kj}(z) \, dz}. \qquad (3)$$

As we shall see, this parameter allows us to explain the emerging charge state, since it depends on the comparative values of capture and loss ranges. Next we resume the approximations followed in this article.

As usual it is assumed that the projectile undergoes an elastic collision with the surface via a Moliere potential. Therefore, the projectile trajectory is derived from the conservation of the projectile energy in the direction perpendicular to the surface. The critical angle θ_c is defined as the angle of maximum approach to the surface. For larger incident angles the projectile penetrates the solid.

We calculate the capture probabilities for collisions of He ions with neutral Sn and Te atoms by using the prior version of the eikonal impulse approximation [5]. This theoretical approximation has already proved to be successful in dealing with a wide variety of atomic collisions in the intermediate and high energy range[6]. Despite of the similar nuclear charges of Sn and Te atoms, the capture probabilities from both atoms are quite different. The capture probabilities are obtained by averaging Sn and Te results. For He projectiles with high velocity, the most important contribution to the total capture probabilities comes from the capture process from 4*d* subshell. Contributions of 4p and 4s subshells are less important.

Electron loss processes by binary collisions of He ions with neutral Sn and Te atoms are calculated with the first Born approximation, normalizing the probabilities with the method of Kaneko [7]. No appreciable differences were found by describing the interaction between the surface atom and the electron bounded to the projectile with a Moliere or Hartree-Fock potential. We have also investigated the description of the valence electrons as a free electron gas, and no substantial changes were observed in the total electron loss probability. Our electron loss probabilities were compared with those calculated with the multipole expansion defined on one center (MEDOC) [8, 9] and with the Classical Trajectory Montecarlo (CTMC) method [4]. For the cases here considered differences do not exceeds ten percent.

3 RESULTS AND DISCUSSIONS

In Fig. 1 we show the values obtained for the emerging charge fraction F_1 for He^+ ions impinging on a SnTe surface with the incident angle θ_c. From the figure, it is possible to observe that as the projectile gets very close to the surface, the fraction remains around a constant, which happens to be

$$\frac{F_1}{F_2} \simeq \frac{P_{21}(z=0)}{P_{12}(z=0)}.$$

However, when the ion comes out of this region its charge state increases. This behavior can be explained in terms of the different capture and electron loss ranges. Close to the surface topmost layer, both charge exchange mechanisms are present, but at a certain distance capture turns off, and only electron loss survives. Thus, the emerging charge state of the projectile is

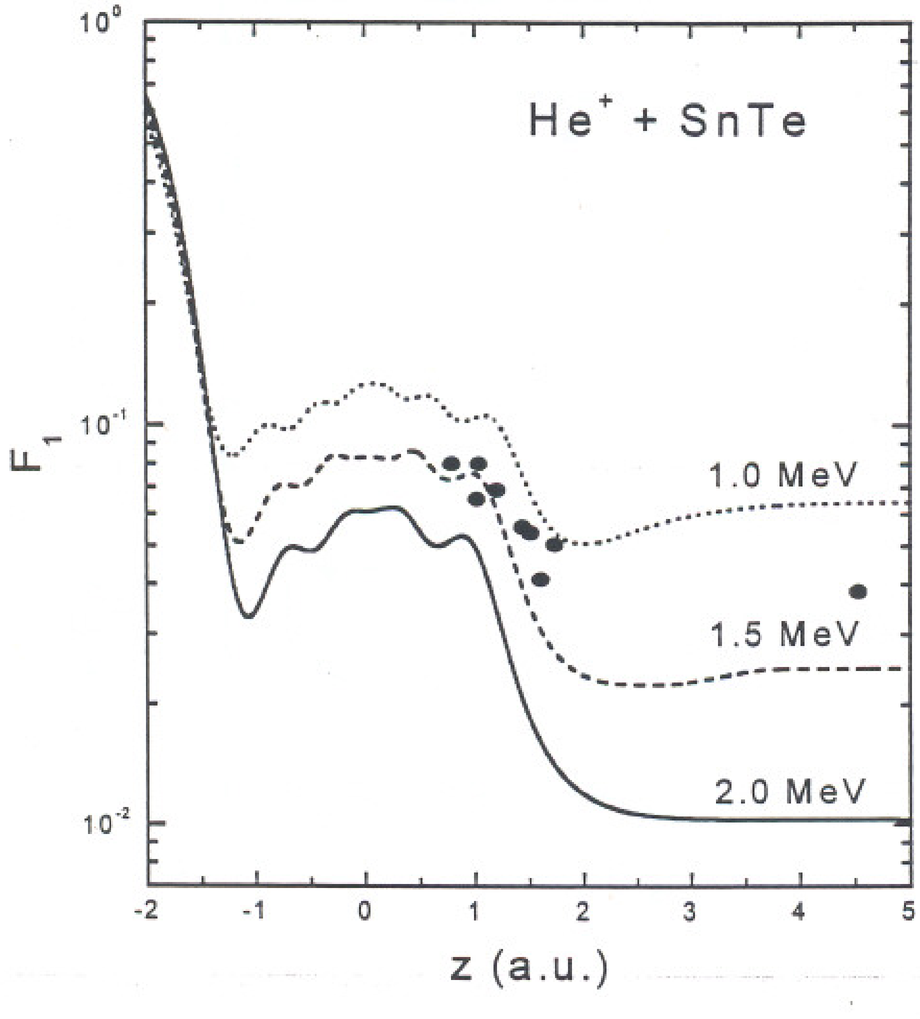

Figure 1: Fraction of He$^+$ for He$^+$ projectiles impinging grazingly on a SnTe surface.The entrance channel is denoted with negative values of z. Simbols: dots, experimental results of Fujii *et al.* [1].

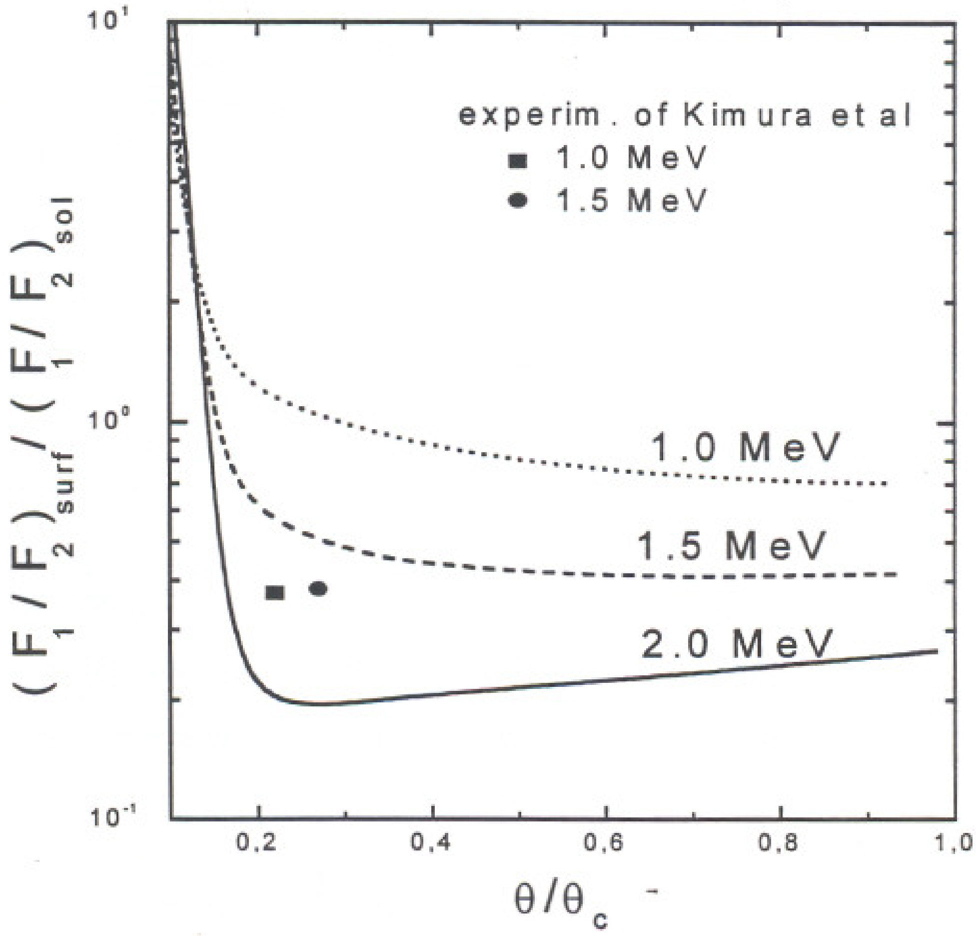

Figure 2: Ratio of charge fractions for He^+ ions impinging grazingly on a SnTe surface, as a function of the incident angle normalized to that of maximum approach to the surface θ_c. Simbols: square and dot, experimental results of Kimura *et al.* [11].

bigger than that obtained in the surface vicinity. This effect becomes more remarkable when the velocity increases. Our conclusion is in qualitative agreement with the theoretical calculations of Fujii *et al.* [10], and with the experimental results of Fritz *et al.* [3].

With the aim of normalizing our results with a measurable magnitude, we introduce the equilibrium charge fractions for ions passing through the solid. In Fig. 2 the ratio of charge fractions emerging from the surface, normalized to that in the solid is shown as a function of the incident angle. Note that as experimentally observed[10], the results change very little for $0.4\theta_c \leq \theta_i \leq \theta_c$.

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