

## Departure from velocity proportionality in low-energy electronic stopping

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A recent paper by Golser and Semrad [Phys. Rev. Lett. **66**, 1831 (1991)] showed a departure from velocity proportionality in their energy-loss measurement of a hydrogen projectile in the gas below 20 keV. We point out that their result is a consequence of complex collision dynamics that is common in the molecular regime and has been known for some time among atomic physicists. The observation is well reproduced by a compilation of published stopping cross sections.

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On their recent energy-loss measurement of a hydrogen projectile in He gas, Golser and Semrad [1] reported a significant deviation below 20 keV of the electronic stopping cross section from the projectile velocity  $v$  proportionality. The common argument of the  $v$  proportionality of the electronic stopping cross section at low energy is based on the constant-density electron-gas model of Lindhard and Scharff [2]. The purpose of this Brief Report is to point out two considerations. First, inelastic processes in ionic collisions at low to intermediate energies (below  $\sim 25$  keV/amu) are now well recognized [3–5] by atomic physicists as complex events. Although charge transfer becomes dominant among those processes, many channels (charge transfer, excitation, and ionization) simultaneously interplay as a sensitive function of a combination of collision energy, coupling strengths, and energy defects among relevant channels and hence collision dynamics significantly vary from one system to another. Therefore a simple model such as an electron-gas model would not be expected to provide universally accurate results for inelastic cross sections or stopping cross sections in this energy regime. Consequently, the  $v$ -proportionality is no longer always valid. Second, the general trend found by Golser and Semrad [1] can be reasonably well reproduced by reconstructing stopping cross sections of He and H<sub>2</sub> for protons from compiled cross section data and supplemental calculations that account for an energy-loss effect due to charge transfer.

Figure 1 shows stopping cross sections for He and H<sub>2</sub> reconstructed from available data [6–9] and present calculations. In the stopping cross sections shown, He(2<sup>1</sup>S), He(2<sup>1</sup>P), He(3<sup>1</sup>S), He(3<sup>1</sup>P) and ionization channels and H<sub>2</sub>(1s,  $n=2$ ), H<sub>2</sub>(1s, 3s) and ionization channels are included for each case as the primary energy-loss processes, with respective mean energy-loss values of 20.6, 21.2, 22.9, 23.1, 24.6, 12, 14, and 15.4 eV. In reconstructing these cross sections, He(2<sup>1</sup>S) and He(3<sup>1</sup>S) and He(2<sup>1</sup>P) and He(3<sup>1</sup>P) data are taken from Refs. [6] and [8], respectively, while H<sub>2</sub>(1s,  $n=2$ ) data and ionization are from Ref. [7]. Furthermore, we carried out molecular representation calculations [3] for the H<sup>+</sup> + He system; He(2<sup>1</sup>S), He(2<sup>1</sup>P), He(3<sup>1</sup>S), and He(3<sup>1</sup>P) excitations and H(1s) and H( $n=2$ ) charge transfer are included. Ioniza-

tion is also accounted for through discretized continuum states (15 states). For the calculation of the H<sup>+</sup> + H<sub>2</sub> system, H<sub>2</sub>(1s,  $n=2$ ) and H<sub>2</sub>(1s, 3s) excitations and H(1s) and H( $n=2$ ) charge-transfer channels are included, while ionization is neglected. Using these theoretical results as a guideline, we critically reexamined the published cross-section data to assess their accuracy. For some cases [for example, He(2<sup>1</sup>S) and He(3<sup>1</sup>S)], we felt that previous results may be somewhat underestimated and we slightly shifted values of these data accordingly (at most 25%). These slight changes in the cross section do not affect overall energy dependence of the stopping cross sections in Fig. 1. Dominant charge-transfer states, i.e., H(1s) + He<sup>+</sup> and H + H<sub>2</sub><sup>+</sup>(1 $\sigma_g$ ) channels, lie energetically next to the initial H<sup>+</sup> + He and H<sup>+</sup> + H<sub>2</sub> channels, respectively. The corresponding charge-transfer cross sections are known to be the largest by several orders of magnitude of all the inelastic processes in this energy region [6–9] and the effect of charge transfer to energy loss is

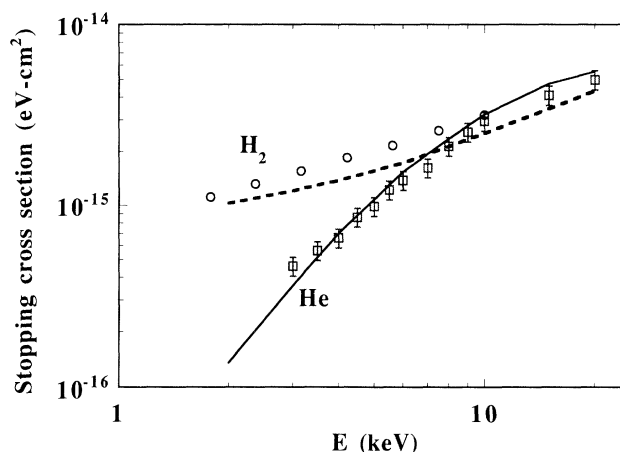


FIG. 1. Stopping cross sections of He and H<sub>2</sub> for protons. Lines are the present results reconstructed by compiled data and supplemental calculations. Solid line, He; dashed line, H<sub>2</sub>. □, experimental data of Golser and Semrad [1] for He; ○, compiled data by Phelps [9] for H<sub>2</sub>. Note the data are per atom.

properly included in the present result. Cross sections to other highly excited states are known to be smaller by several orders of magnitude, although the corresponding mean energy losses are somewhat larger than those included. These highly excited states are excluded from the present evaluations. The present result for He is in very good accord with the measurement of Gloser and Semrad [1], while that for H<sub>2</sub> appears to nearly follow the  $\nu$ -proportionality reasonably and is in qualitative agreement with those by Phelps [9]. The remaining discrepancy seen in H<sub>2</sub> may be attributable to our neglect of other major contributors such as dissociation and vibrational

excitation channels. Nevertheless, important aspects of the energy dependence of the stopping cross sections are well reproduced; from our point of view, the departure from the  $\nu$ -proportionality is *not* striking, but is rather expected.

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