

§17. Study of Hydrogen Negative Ion Production Processes from Metal Surface

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[Introduction] Negative hydrogen isotope ions are used as sources in accelerator laboratories around the world and its application as a heating source in fusion reactions [1] may solve our heavy dependence in fossil fuels. In addition, variety of negative ion beams has been used for surface modification [2]. In these applications, it is known that most of negative ions are produced on the surface of metal electrodes, but details of production mechanism have not been clarified yet. Recently, Bacal and Wada have recalled the importance of the negative hydrogen ion production due to fast and thermal ions and atoms on low work function surface [3], and the surface temperature effect was pointed out. Upon these backgrounds, this research is (1) aiming a more stable and efficient material surface design for negative ion production, and (2) theoretical understanding underlying its formation and interaction, starting from the first principle investigation and (3) its experimental validation.

[Work function variation in alkali metal] In the 2012 NIFS collaboration program, the calculated work functions with varying coverage were reviewed, and compared with experimental results [4]. In general, they are in good agreement with experiments. Among the different alkali metals, Cs / W(110) systems has the lowest work function and is attributed to the large amount of charge that is polarized in the interface region. A good indicator / descriptor for work function is the state that signifies the interaction of the adsorbates. The adsorbate-adsorbate interaction results to the further increase in work function after reaching the minimum possible value. The effect of alkali metal in work function lowering is further established from the local electrostatic energy.

[Dissociation and adsorption of hydrogen molecule on metal surfaces] Theoretical investigation on the molecular orientation dependence of the dissociation probability of neutral molecular hydrogen scattered from metal surfaces were reviewed [5, 6]. The probability distributions are calculated in the cases when positive and negative hydrogen ions (ion pair) are formed and when two neutral hydrogen atoms are formed. On the basis of numerical results, it is found that a parallel orientation preference of probability distributions shows a tendency to

be suppressed in the case when an ion pair is formed as compared with the case when two neutral hydrogen atoms are formed. Recent studies of the theoretical group focused on the behaviors of different molecules and atoms on different systems [6-9, and others]. For instance, the dissociation and adsorption of hydrogen molecule on metal surfaces were analyzed with reference to the electronic and geometric structures of the system [10-12, and others].

[Experimental Validation] The apparatus at National Institute for Fusion Science has capability of measuring the angle-resolved energy distribution function of positive/negative ions produced at metal surfaces, and production of neutral particles bombarded by H^+ , H^- , He^+ in keV region [13-15, and others]. The theoretical group's recent works have shown that the scattering of hydrogen molecule on surfaces is greatly affected by its initial orientation, the initial translational energy of the impinging molecule and the released kinetic energy of the scattered atoms. These findings will be compared with experimental observation, and provide experimental insights and information on the dynamics of the impinging molecules on metal surfaces, and the relevant plasma-surface interaction.

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