§ 14. Neutralization and Re-Ionization of He Ion Colliding with Oxygen Atom


The problem of helium neutrals for plasma fusion is one of critical issues, which should be overcome for realization of plasma fusion reactor. Helium ions, exhaust of fusion reaction, are neutralized by plasma-wall interaction. The neutrals cannot be controlled electromagnetically, and thus, fast He neutrals, which are converted from high energy He+ by charge exchange collision in the core plasma, cause damages to the plasma facing materials. One possible solution of this issue is to reduce the neutralization probability of He ion at the wall. The purpose of the present study is exploring of materials, which can significantly reduce helium neutrals. Promising materials would be oxide insulator materials.

From our preliminary experiments about He ion scattering with O2 gas, we have obtained a useful hint in the present context. He neutrals are re-ionized during collision with O2 at an appreciable probability. Our qualitative interpretation of this experimental fact is as follows. During close collision between He+ and O atom of O2, He+ is transiently neutralized in the incoming way by resonant neutralization between He+ 1s state and O 2s state, and while He collides with O more closely, the transient He neutral promotes He 1s electron to O 2p state, i.e., re-ionization of He neutral. Of course, however, it is possible to occur that the promoted electron is re-captured by He+ when He+ recedes from O atom. Therefore, the re-ionization probability is not very large for He-O2 gas collision.

If this interpretation is correct, an interesting scenario about neutralization and re-ionization of He colliding with oxide insulator materials can be described as follows: in the oxides, the O 2p state is modified to O2 conduction band (empty band), so that the promoted electron will dissipate into the bulk through this band before recapture by He+, yielding much larger re-ionization probability (electron de-localization effect). It is noted that this scenario has been recently confirmed as a primary mechanism for enhancement of re-ionization probability in the system of H+ scattered by rare gas solids.1),2)

For a more quantitative assignment to elementary process, we performed molecular orbital calculations of He-O2 triatomic linear molecule as a function of He-O distance (fig.1). In addition to He 1s state, the energy level of the molecular orbitals having σ and π symmetry is shown by solid and dotted lines, respectively. At adiabatic limit, the highest occupied molecular orbital (HOMO) of He-O2 molecule is 2σ state, which is partially occupied by electron, and no electron occupies the molecular orbitals energetically above 2σ state. For the distance of ≤3 a.u., because of the Demkov-type coupling, the 4σ state is constructed mainly from He 1s and O 2s atomic state, and the 5σ is mainly from He 1s and O 2p atomic state. The 6σ state is mainly from O 2p state, but at a short distance (≤1.5 a.u.), it is constructed from O 2p and He 1s state, because of level crossing interaction (Landau-Zener) between O 5σ and O 6σ state.

We can summarize the mutual interaction among orbitals: the 4σ and 5σ states interact strongly via He 1s state at distance of ≤3 a.u., in which He+ ion is neutralized. When He comes closer to O, the 5σ state is significantly promoted at the distance of ≤1.5 a.u. As a result of level promotion of 5σ state, the 5σ and 6σ strongly interact through Landau-Zener level crossing coupling, in which re-ionization of He neutral takes place. Therefore, we can conclude that the qualitative interpretation about re-ionization process of He-O2 collision is valid from quantum-chemistry point of view.

The threshold energy for re-ionization can be estimated by using known interatomic scattering potentials and the level crossing point. We estimated the threshold energy as low as 0.0529 eV.

In this article, we clarified re-ionization mechanism for He-O2 collision. Thus, our further study will focus on the re-ionization mechanism for oxide materials, in which the electron de-localization in the O 2p conduction band will play an important role on re-ionization process, similarly to the case of H+-rare gas solids.

Fig.1. The energy level of molecular orbitals of He-O2 as a function of He-O distance. The notation such as 5σ state, etc., means the orbital to which the molecular orbital of He-O2 asymptotically converges at an isolation limit of He and O2. Atomic units are used for the distance (1 a.u.= 0.0529 nm).

References: