Energy structure of hollow atomic ions in the bulk of metallic materials

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The interaction of high charged ions (HCI) with surface is a subject of increasing interest [1, 2, 3]. Basically, three steps are involved in the interaction of HCI with surfaces: (1) formation of the hollow atom above the surface; (2) decay of the hollow atom at or below the surface and (3) total neutralized in the bulk of materials [1]. The formation of the hollow atom is strongly related to the HCI's impact velocity, incident angle and other dynamic processes. In the final neutralization process, the hollow atomic ions emit Auger electrons or X-rays [4, 5]. The emitted x-ray can provide some static information of the hollow atomic ions in the bulk of materials from the energy positions and the dynamic information from the spectra intensity. Arnau *et al.* [6], has used the local density functional method to study the energy structure of hollow atomic ions in the bulk of metallic materials. The advantage of this method is that the total energy of the N-electron system can be characterized by the total electron density. Similar to the traditional local density functional theory, such method contains self-interaction energy which should be removed in the exact calculations. To remove the self-interaction energy, we use the local spin density functional method with the optimized effective method and self interaction correction method [7] to study the energy structure of hollow atomic ions in a metallic material. Such method has already successfully applied to study the atomic energy structure both in the non-relativistic [7] case. Different from atomic ions in the vacuum, hollow atomic ions in the bulk of metallic materials also involve free electrons in the conduct band. The free electron in the conduct band is treated by the jellium model at present. The advantages of our method over ref. [6] are that (1) we use local spin-density approximation, which allow us to study the spin polarized hollow atomic ions in the bulk of metallic materials; (2) we use the optimized effective potential with the self-interaction correction for bound electron, which can remove the self-interaction energy completely. In the numerical side, we use a square grid ($r = r_{max}(i/N)^2, i = 1, N/2$) in the inner region, which is optimized for the bound electron and an equal space grid ($r = r_{max}/4 + 3r_{max}(i - N/2)/(2N), i = N/2 + 1, N$) in the out region, which is optimized for the free electron in the conduct band. Therefore, we can describe both bound electron and free electron more accurately with limited computer efforts.

Based on this method, we have calculated the free electron density changes (as shown in Fig. 1), the emitted x-ray energy levels (as shown in Fig. 2) from $K^1L^yM^x$ to $K^2L^{y-1}M^x$ for Ar^{q+} in the bulk of Ag. Our calculated x-ray spectra are in reasonable agreement with the

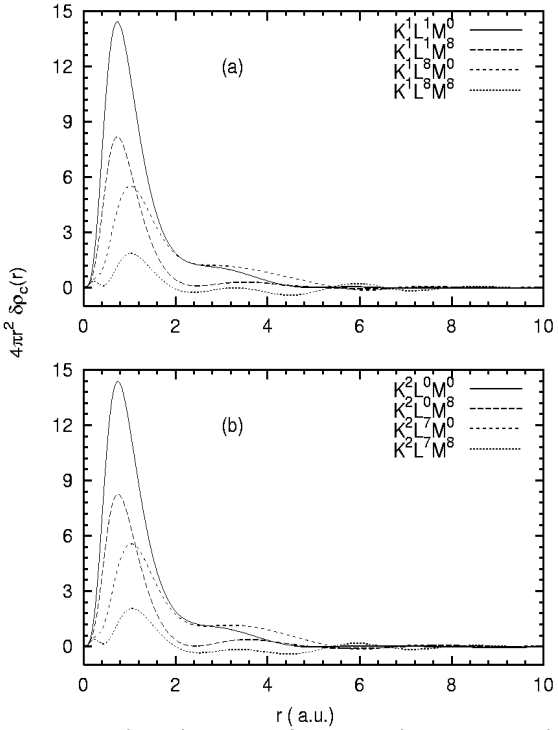

Fig. 1. The electron density changes in the (a) initial and (b) final states for Ar^{q+} in the bulk of Ag.

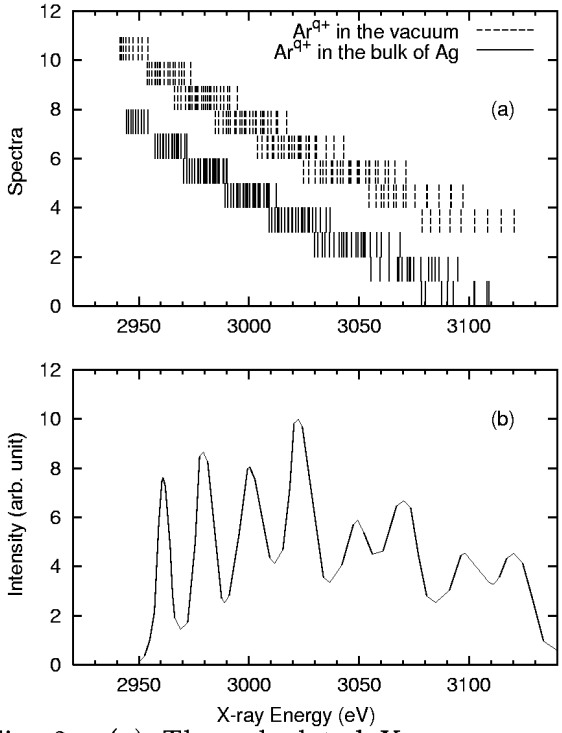

Fig. 2. (a) The calculated X-ray energy levels and (b) experimental spectra from Ref. [4].

experimental measurement [4]. Furthermore, we have also discussed the screening effect of the conducting electrons and phase shifts in details.

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