

Positronium emission from various semiconductor surfaces

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Positronium is spontaneously emitted from solids, when the formation potential or the work function is negative. So far, positronium emission from solids have been investigated mainly with metals and insulators. The number research on semiconductors is rather limited. It is intriguing to study positronium emission from semiconductors, because semiconductor has intermediate features between metal and insulator, for instance, the band gap and free carrier density. In this presentation, we will report our research about positronium emission from Si [1], SiC [2] and GaN(0001) surfaces mainly through the positronium time-of-flight spectroscopy. The theoretical positronium formation potentials ($\Phi_{\text{Ps}}^{\text{calc}}$) were also obtained by first-principles calculation.

Figure below shows the positronium energy spectra obtained for n-type 4H SiC(0001), n-type Si(111) and also as references for Al(111) and W(001) metal surfaces. The expected maximum positronium energies ($-\Phi_{\text{Ps}}^{\text{calc}}$) are shown in the figure as broken lines. The positronium energy spectra for Al(111) and W(001) rise around $-\Phi_{\text{Ps}}^{\text{calc}}$. This means that positrons pick up electrons from the top of the occupied state (the Fermi level) as assumed in the calculation of formation potential. Contrarily, the positronium energy spectra for SiC(0001) and Si(111) rise significantly above $-\Phi_{\text{Ps}}^{\text{calc}}$. Moreover, the spectrum shapes are different from those for Al(111) and W(001). In the calculation of formation potential, the electrons at the top of the valence band are assumed to be picked up by positrons. Therefore, the above experimental results imply that electrons located sufficiently above the valence band top are picked up by positrons. The maximum energies observed for SiC(0001) and Si(111) are separated from their $-\Phi_{\text{Ps}}^{\text{calc}}$ values approximately by the band gap energies (3.2 eV for SiC, 1.1 eV for Si). Thus, we propose that the conduction electrons also participate in the positronium formation in SiC and Si. In the presentation, we also report the results on GaN and more thorough analyses of positronium energy spectra based on the Monte Carlo simulation.

[1]A. Kawasuso et al., Phys. Rev. B 97(2018)245403.

[2]A. Kawasuso et al., J. Phys. Condens. Matter. 33(2021)035006.

