

Shallow level muonium center in TiO₂K. Shimomura¹, R. Kadono¹, M. Mihra², and K. Nishiyama¹¹*Muon Science Laboratory, Institute of Material Structure Science, High Energy Accelerator Research Organization, Tsukuba, Ibaraki 305-0801*²*Department of Physics, Osaka University, Machikaneyama 1-1 Toyonaka, Osaka Japan*

Hydrogen is a ubiquitous impurity in most of the basic semiconductors, including elemental (e.g., Si) and compound (e.g., GaAs) ones. In these systems, hydrogen is known to be amphoteric, forming an acceptor level in *n*-type and a donor level in *p*-type materials. While these amphoteric levels are situated relatively deep in the band gap, it is theoretically predicted that hydrogen might serve as shallow level center in some wide gap semiconductors such as ZnO, which triggered studies on hydrogen centers in ZnO.

Here, the primary issue is to pin down the factors that control the electronic structure of H centers; is it possible to make a systematic prediction on the electronic conductivity associated with the incorporation of H in various semiconducting materials? Experimentally, μ SR studies on muonium (Mu) centers have played a key role on this subject, as demonstrated in the case of Mu studies in ZnO. While the dynamical aspects (e.g., diffusion) may be considerably different between Mu and H due to the light mass of Mu, the local electronic structure of Mu is virtually equivalent to that of H after a small correction due to the difference in the reduced mass ($\sim 0.4\%$). Recently, novel Mu states having extremely small hyperfine parameters and low ionization energy (~ 10 meV) were reported in several compound semiconductors including CdS, InN and GaN, implying that Mu (and hence H) may act as a donor in these materials. Along with these experimental revelations, significant progress has been made on theoretical studies, where one of the most interesting predictions is that H would serve as a donor in titanium dioxide (TiO₂).

In this contribution, we will report our μ SR study on rutile TiO₂. Mu centers with extremely small hyperfine parameters have been observed below 10 K. The electric structure of Mu has been clearly determined using a single-crystalline sample; it has a four-fold symmetry along with the *c*-axis, indicating that they are located at the channel center site. It is inferred from their small ionization energy (~ 1.2 meV) and hyperfine parameters ($\sim 10^{-4}$ times the vacuum value) that these centers behave as shallow donors, strongly suggesting that hydrogen is one of the primary origins of *n*type conductivity in as-grown TiO₂.