Superconducting ‘hydrogen’ at diamond tips

(iTHES Newsletter vol.121, revised on 2016/04/21)

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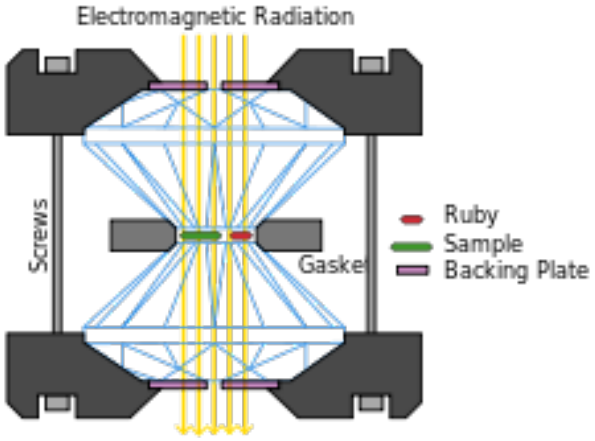

The centers of gas giant planets consist of a rocky core surrounded by a layer of hydrogen and helium. This layer is compressed to an extremely high density, leading to such a high overlap of the hydrogen atom electron wave functions that electrons begin to move freely, i.e., hydrogen metallizes [1]. Following many years of research efforts to experimentally verify metallic hydrogen, it is expected that this goal will be achieved in the next few years [2, 3]. In 1968, N.W. Ashcroft proposed [4] that, based on the standard theory of superconductivity or Bardeen-Cooper-Schrieffer (BCS) theory [5], metallic hydrogen may become superconducting with a high transition temperature (high T_c) because its phonon frequencies and, hence, T_c are very high owing to the hydrogen atom’s small mass. While the efforts to experimentally realize metallic hydrogen were ongoing, in 2004, Ashcroft proposed [6] an alternate route to metallic hydrogen, suggesting that metallization will occur at a much lower external pressure when the hydrogen atoms are pre-compressed by chemical bonds in a hydride. In the decade following this proposal, several research groups, including our group [1], theoretically predicted that a number of hydrides [7], such as SiH_4 [8, 9], GeH_4 [10], SnH_4 [11, 12], PtH [13], and CaH_6 [14], become high-T_c superconductors under pressure according to first-principles electronic-structure calculations and crystal-structure prediction methods [15, 16, 17, 18]. In 2008, tentative evidence for superconductivity was reported in SiH_4 under high pressure [19].

In 2014, it was theoretically predicted that the molecular compound of hydrogen sulfide and hydrogen, $(H_2S)_2H_2$, will dissociate completely above 180 GPa [20] and form crystalline H_3S with a high T_c of 191-204 K [20]. The zero-electric resistivity was confirmed [21] at a record high T_c of 203 K and P=153 GPa in the summer of 2015. The existence of the Meissner effect [22] at T=4.7–140 K and P=153 GPa was also observed [23] in the spring of 2016 according to the nuclear resonant scattering of synchrotron radiation by a Sn foil placed inside a H_2S sample in a diamond anvil cell. Currently [24], the low-T_c-phase H_5S_2 of sulfur hydride at approximately 120 GPa is believed to successively transform into the high-T_c-phase H_3S [20, 25, 26] at approximately 200 GPa via "Magneli" intermediate phases [27].

Advances in hydrogen superconductivity research have been facilitated by new methods for material design based on first-principles calculations and BCS theory. Unfortunately, the extremely high pressure required for hydrogen superconductivity is unfavorable for industrial applications. In the near future, superconductivity at room temperature and atmospheric pressure may be realized with the synthesis of crystal structures specially designed by computational methods [6].

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[1] This is collaboration with Prof. Yanming Ma and Prof. John Sak Tse