Road to Room Temperature Superconductivity: Hydrides and Other Systems

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June 18, 2017 (HP126, STH49). The goal of attaining room temperature superconductivity (this dream was born shortly after the discovery of superconductivity in 1911) has become perfectly realistic. There are several directions paths pursuing this search. The most promising family of materials is that of compounds containing hydrogen and heavy ions (hydrides). The record value of $T_c=203$ K (!) has been observed for sulfur hydride under high pressure [1, 2], see the review [3]. The high- T_c state for these hydrides was predicted in [4, 5]. The H-S system can form different structures and the stability of each depends on the external pressure. The highest T_c has been found for the cubic structure (Fig.1a). The superconducting state with such a high T_c is caused by strong electron-phonon coupling enabled by the presence of highfrequency optical H-modes. However, the usual description of the phonon mechanism (see, e.g., [6-8]) is not applicable here because the phonon spectrum is uniquely broad (up to 200 meV) and its structure is quite complicated (Fig. 1b).

It is possible to develop a generalized approach [9], whereby the system is characterized by two characteristic phonon frequencies $\tilde{\Omega}_{opt.}$ and $\tilde{\Omega}_{ac.}$ and, correspondingly, by two coupling constants,

 $\lambda_{opt.}$ and $\lambda_{ac.}$ The following analytical expression can be derived: $\ensuremath{1}$

$$\mathbf{T}_{c} = \left[1 + 2 \frac{\lambda_{ac.}}{\lambda_{opt.} - \mu^{*}} \frac{1}{1 + (\pi T_{c}^{0} / \tilde{\boldsymbol{\Omega}}_{ac.})^{2}} \right] T_{c}^{0}.$$

Here T_c^0 is the value of the critical temperature caused by the interaction with only the optical phonons (it can be described by [8]). The values of the parameters turn out to be as follows: $\tilde{\Omega}_{opt.} = 1700 \text{ K}$, $\tilde{\Omega}_{ac.} = 450 \text{ K}$, $\lambda_{opt.} = 1.5$, and $\lambda_{ac.} = 0.5$. We obtain $T_c \approx 215 \text{ K}$, in quite good agreement with the experimental data [1,2]. Moreover, $T_c^0 \approx 170 \text{ K}$ and $\Delta T_c^{ac} \approx 45 \text{ K}$. It is interesting that for the lower pressure phase (P \approx 100-120 GPa) with a lower $T_c \approx 120 \text{ K}$ the value of the total coupling constant $\lambda_T = \lambda_{opt.} + \lambda_{ac}$ is approximately the same as for the high- T_c phase ($\lambda_T \approx 2$), but $\lambda_{opt.} \approx \lambda_{ac} \approx 1$. Therefore, the drastic increase in T_c from 120K to 200K is caused by a "redistribution" of the interaction strength [9]. The transition into the high- T_c phase is first-order [9, 10].

Hydrides may reach even higher values of T_c , up to room temperature. For example, higher critical temperatures are predicted for CaCl₆, $T_c \approx 240$ K [9,11], for YH₆, $T_c \approx 255$ K [12].

High T_c also can be observed for selected metallic nanoclusters [13]. The effect has been observed for Al₆₆ clusters [14], whose $T_c \approx 120$ K is much higher than that of bulk aluminum's $T_c \approx 1.1$ K. The quest is to build nanocluster-based Josephson tunneling networks, which would be capable of transmitting a macroscopic supercurrent much stronger than in bulk networks [15].

More than fifty years ago, W. A. Little introduced the electronic mechanism of superconductivity [16]. Recently, a manifestation of this mechanism was finally observed experimentally [17] with the use of two

carbon nanotubes. According to [17], future modifications of the system may create the superconducting state at room temperature.

One can fully expect room temperature superconductivity to be observed in the near future.



Fig. 1. (a) The high- T_c (≈ 200 K) phase is cubic [5]. (b) Phonon spectrum for the high- T_c (≈ 200 K) phase. It contains two groups: (1) acoustic modes (up to ~ 70 meV, motion of the S ions) and (2) optical modes (up to ~ 200 meV, dominated by the motion of the H ions.

References

[1] A. Drozdov, M. Eremets, I. Troyan, V. Ksenofontov, S. Shylin. "Conventional superconductivity at 203 Kelvin at high pressures in the sulfur hydride system". *Nature* **525**, 73 (2015).

[2] M. Einaga, M. Sakata, T. Ishikawa, K. Shimizi, M. Eremets, A. Drozdov, I.Tpoyan, N. Hirao, Y. Ohishi, "Crystal structure of 200K-superconducting phase of sulfur hydride system", *Nature Physics* **12**, 835 (2016).

[3] M. Eremets, A. Drozdov, "High temperature conventional superconductivity", Uspechi, 59,1154 (2016).

[4] Y. Li, J. Hao, H. Liu, Y. Li, Y. Ma, 2014, "The metallization and superconductivity of dense hydrogen sulfide", *J. of Chem. Phys.* **140**, 174712 (2014).

[5] D. Duan, Y. Liu, F. Tian, D. Li, X. Huang, Z. Zhao, H. Yu, B. Liu, W. Tian, T. Cui, "Pressure-induced metallization of dense $(H_2S)_2H_2$ with high T_c superconductivity", *Sci.Rep.* **4**, 6968 (2014).

[6] A. Migdal, "Interaction between electrons and lattice vibrations in a normal metal", JETP 7, 996 (1958).

[7] G. Eliashberg, "Interaction between electrons and lattice vibrations in a superconductor", JETP 11, 696 (1960).

[8] W. McMillan, "Transition temperature of strong-coupled superconductors", *Phys. Rev.* 167, 331 (1968).

[9] L. Gor'kov and V.Kresin, "Pressure and high -T_c superconductivity in sulfur hydrides", *Sci. Rep.* **6**, 25608 (2016).

[10] L. Gor'kov and V. Kresin, "Phase diagram of the sulfur hydride: transition into high T_c state", arXiv:1705.03165 (2017).

[11] H. Wang, J. Tse, K. Tanaka, T. Litaka, Y. Ma, "Superconductive sodalite-like clathrate calcium hydride at high pressures". *PNAS* **109**, 6463 (2012).

[12] Y. Li, J. Hao, H. Liu, J. Tse, Y. Wang, Y. Ma, "Pressure-stabilized superconductive yttrium hydrides", *Sci. Rep.* **5**, 9948 (2015).

[13] V. Z. Kresin and Y. Ovchinnikov, "Shell structure and strengthening of superconducting pair correlation in nanoclusters", *Phys. Rev. B* 74, 024514 (2006).

[14] A. Halder and V. V. Kresin, "Spectroscopy of metal "superatom" nanoclusters and high-T_c superconducting pairing", *Phys. Rev. B* **92**,214506 (2015).

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[15] V. Kresin and Y. Ovchinnikov, "Theoretical investigation of Josephson tunneling between nanoclusters", *Phys. Rev. B* 81, 214505 (2010).

[16] W. Little, "Possibility of synthesizing an organic superconductor", Phys. Rev. 134, A1416 (1964).

[17] A. Hano, A. Benyamini, I. Shapir, I. Khivrich, J. Walssman, K. Kaasbjerg, F. von Oppen, S. Llani, "Electron attraction mediated by Coulomb interaction", *Nature* **535**, 395 (2016).