低维高温超导的启示: 键收缩与电子双重极化

孙长庆^{1,2}

1. 吉林大学材料科学与工程学院, 长春 130012;

2. School of Electrical and Electronic Engineering, Nanyang Technological University, Singapore 639798, Singapore

E-mail: ecqsun@gmail.com

经典的Bardeen-Cooper-Schrieffer(BCS)理论^[1-3]认为, 费米面附近的电子通过电声耦合作用形成具有玻色子特征的库珀对, 即玻色-爱因斯坦凝聚。库珀对在低温条件下相互协调, 实现在晶格内无阻运输。虽然BCS理论能够很好地描述临界温度 T_c 低于30 K的金属或合金的常规超导行为, 但是却不足以解释于1986年发现且持续发展的以铜氧掺杂为代表的新一代高温超导现象。在30多年的高温超导研究中, 学者们坚持不懈地努力探讨新的物理机制^[2,4], 如电声作用、载流子的输运特性, 以及铜氧面和载流子的本征起源和属性等。2021年5月, 美国Science杂志携手上海交通大学发布了新的125个重要科学问题, 其中包括高温超导的微观机理以及界面现象的微观测量。最近报道的准一维铜氧链的电子间超强吸引作用^[5]、双层铜氧面具有与体相全同的超导行为^[6], 以及铁砷/铜铁氧界面超导现象^[7], 称为降维超导, 尤其令人鼓舞。这些发现进一步激发了人们对探求电声作用机理以及以铜氧面和铜氧链为代表的超导通道的物理本质和起因的研究兴趣。

本文从低配位原子键收缩^[8]、冰水溶液^[9,10]以及氧吸附中耦合氢键^[11]的协同弛豫与电子极化角度出发, 探讨铜氧偶极子单链和铜氧偶极面的属性以及低配位体系电声作用的本质。实验观测表明^[8,11], 铜氧面低配位原子间的键收缩可增强氧的孤对电子的极化效应, 从而弱化氧与偶极子之间的相互作用并降低偶极子的振动频率, 导致极化载流子的有效质量降低、群速度提高, 利于其在铜氧偶极面间的超导通道内输运。

第一, 铜氧链和铜氧面的构型和属性——孤对电子极化。如图1(a)所示^[11], 客体氧与主体原子反应, 生成以氧为中心的稳定的准四面体结构基本单元。黄色小球代表主体离子 M^+ , 绿色大球代表由氧的孤对电子“:”极化的偶极子 M^p 。离子键间夹角小于 102° , 偶极子间非键夹角远大于 104° 且随配位环境改变。由孤对电子作用主导的O:M非键远比O-M离子键长且弱。以水的氢键为例, O:H作用强度仅是H-O共价键的3%~5%。H-O和O:H段的振动频率分别为 3200 和 200 cm^{-1} , 结合能分别为 $4.0\sim 5.0$ 和 $0.1\sim 0.2\text{ eV}$ 。O:M与O:H的振动能量相当, 在 $0.05\sim 0.2\text{ eV}$ 范围或低于 1000 波数^[11]。如图1(b)所示, 氧化调

孙长庆 吉林大学唐敖庆讲座教授。主攻超常配位键工程和非键电子学, 发展了配位键受激弛豫、氢键耦合振子对以及水合反应电荷注入等理论, 拥有多项计量谱学专利。

制主体的价带结构使之呈现成键、非键、反键和空穴(谷)4个态密度特征。反键态位于费米能级之上。氧原子在吸附过程中嵌入主体的表层和次层之间, 与上下两侧近邻M原子形成稳定的四配位结构, 并通过孤对电子极化外侧原子形成表面偶极层。氧的镶嵌扩展最外两原子层的间距~10%。由于O-O的排斥耦合, 相邻的四面体之间形成O:M-O三体准氢键。O:M-O服从水的O:H-O耦合氢键的受激极化和分段协同弛豫规则(hydrogen bond cooperativity and polarizability, HBCP)^[9,11,12]。如果在形成以氧原子为中心的四配位结构时表面存在过剩原子, 这些过剩原子将会逃逸表面而留下空位; 反之, 氧原子将从偶极子获取电子而成键。后者正是某些金属可以通过氧化钝化防止表面继续氧化的原因。大量观测表明^[11], 由于氧化成键的方向性, 一个客体氧原子不能与某一个主体原子形成双键。氧化的动态过程和以氧为中心的四面体的排列取向与主体原子的电负性、晶体取向和晶格常数有关。虽然表面氧化的晶体结构和形貌千变万化, 但每个氧原子的孤对电子数目及孤对电子对近邻主体原子的极化属性不变。

以图1(c)所示的 $\text{Cu}(001) - (\sqrt{2} \times \sqrt{2})R45^\circ - 2\text{O}^{2-}$ 表面为例, 超低能($6\sim 12\text{ eV}$ 范围)电子衍射和扫描隧道显微/谱(scanning tunnelling microscopy/spectroscopy, STM/S)(图1(d)^[13])观测分析揭示了氧的四步反应过程: 即由 O^- 到 O^{2-} 的价态转换实现稳定的孪生 Cu_3O_2 四面体结构单元^[11]。首先, 一个氧分子与一个表面铜原子反应形成两条 $\text{Cu}^{2+}-\text{O}^-$ 键。然后, O^- 再分别

图1 氧化耦合氢键的孤对电子极化。氧化物的类水分子结构^[11](a)和价态四密度特征(b)。氧铜(001)面的 Cu_3O_2 四面体单元(c)和反向耦合偶极子对的0.035 nm高度的STM形貌亮斑^[13](d)。沿 $\langle 11 \rangle$ 方向, 第一列为 Cu^{2+} , 第二和第四列为偶极子横跨第三列空位。Reprinted with permission from Ref. [13]. Copyright (1990) by the American Physical Society. (e) 氧铜(110)面的隔列空位和铜偶极子单链的STM形貌。偶极子沿表面法向平行排列, 呈现高度为0.085 nm的亮斑。黄色球为金属离子, 绿色为金属偶极子。Reprinted with permission from Ref. [14]. Copyright (1989) by the American Physical Society

Figure 1 Lone-pair electron polarization of the coupled hydrogen bond formed during oxidation. Water-like tetrahedral bond structure^[11] (a) and four valence band characteristics (b) of oxide. The Cu_3O_2 structure on the O-Cu(001) surface (c) and its STM images showing 0.035 nm bright protrusions of the oppositely coupled Cu dipoles^[13] (d). Along the $\langle 11 \rangle$ direction, the first row is formed by Cu^{2+} , the second and fourth rows are the coupled dipoles cross over the third missing row vacancies. Reprinted with permission from Ref. [13]. Copyright (1990) by the American Physical Society. (e) The STM image of the alternative rows of copper dipoles of Cu-O chains and atomic vacancies on the Cu(110) surface. The dipoles show 0.085 nm height of bright protrusions lined along the surface normal direction. Yellow spheres are metallic ions and green ones are dipoles. Reprinted with permission from Ref. [14]. Copyright (1989) by the American Physical Society

与相邻的次层铜原子形成 $\text{Cu}^+-\text{O}^{2-}$ 键。紧接着, 进行 sp^3 电子轨道杂化, 产生孤对电子并极化近邻铜原子使其形成偶极子 Cu^p 。最后, $\text{Cu}-\text{O}$ 键收缩, $\text{O}:\text{Cu}$ 非键伸长。在此过程中, 两对首首相连的反向偶极子挤出被近邻原子孤立的铜原子而产生一系列空位。表层在氧/铜原子数比例为1/2时饱和。这样, 沿表面 $\langle 11 \rangle$ 方向, 第一列为 Cu^{2+} , 第二和第四列为哑铃状、横跨第三列铜原子空位的反键偶极子对。O-Cu(001)面包括氧的上下两个子层, 表层由 Cu^{2+} 、空位和偶极子对间歇构成, 底层中Cu和 Cu^+ 各占一半。在成键过程中, 键长和键角发生弛豫。表层 $\text{Cu}^{2+}-\text{O}^{2-}$ 键的长度相对体相0.185 nm收缩12%, 为0.162 nm; 氧与次层的 $\text{Cu}^+-\text{O}^{2-}$ 键长为0.176 nm; $\text{O}^{2-}:\text{Cu}^p$ 长度则伸长至0.194~2.00 nm, 此即为HBCP效应。图1(e)为Cu(110)-(2×1)- O^{2-} 面的STM图像^[14]和由四面体构成的 $\text{Cu}^p:\text{O}^{2-}:\text{Cu}^p$ 铜偶极子单链^[11]。O-Cu(110)表层由偶极子单链和铜的空位列间歇构成。所有偶极子都沿表面法线朝外平行排列, 表观高度0.085 nm。每个氧与次层铜原子形成一对 $\text{Cu}^+-\text{O}^{2-}$ 键, 所以次层全部为 Cu^+ 离子。铜氧面和铜氧链的结构与晶体取向密切相关且差异较大。譬如, 在氧的覆盖率为2/3时, 氧在Cu(110)面呈现更为复杂的Cu(110)-(6×2)- 8O^{2-} 表面结构。不过, 它们的电子能谱特征相同, 丰度略有差异。STM/S揭示, $\text{Cu}^p:\text{O}^{2-}:\text{Cu}^p$ 偶极子链的孤对电子态位于-2.0 eV, 而偶极子态位于0.5~2.0 eV。X射线光电子能谱(X-ray photoelectron spectroscopy, XPS)探测到成键态位于-(6~8) eV^[15]。所以, 铜氧面的结构和偶极子取向以及原子空位数目并非唯一, 而铜氧链是由氧和底层原子成键而形成锯齿状且具有低频振动频率的偶极子链。

第二, 低配位原子间键收缩——端态极化。铜氧面和铜

氧链的特征是原子低配位 $z(z<12$, 参考面心立方结构)。低配位导致局域键长自发收缩, 强度刚化, 且服从如图2(a)所示的键序-键长-键强关联和非键电子极化(bond order-length-strength correlation and nonbonding electron polarization, BOLS-NEP)的标度关系^[8]。键收缩使局域电荷致密; 键刚化使局域势阱变深, 单键振动频率 ω_m 正比于振子能量的平方根 $E^{1/2}$ 与振子长度 d 的商($\omega_m \propto E^{1/2}/d$), 因而升高; 集体振动模式 ω_c 显含振子的配位数($\omega_c \propto zE^{1/2}/d$), 故频率降低。处于芯能级的电子和成键电子发生致密自陷钉扎, 高密度电子通过极化反作用于边缘原子的外壳层非键电子, 在表面形成包括最外三层原子的电偶极层^[16]。单原子链和单层原子边界的键长收缩程度可达30%, 块体表面最外层原子间距可降低至体相值的12%。局域势阱深度的变化正比于单键能 E , 且与键长 d 的 m 次方成反比, 即 $E \propto d^{-m}$ 。对于金属、碳和硅, m 值分别为1.0、2.56和4.88。另外, 边缘原子的极化具有选择性。极化仅在原子的最外层轨道未满的情况下发生, 如金、银、铜, 而在外层轨道全空和全满条件下, 其价态电子保持自陷特征, 如钴和铂等。极化电子的态密度向高能级移动, 靠近甚至跨越费米能级。电子的局域极化将导致在表面、缺陷、台阶、楞角、吸附原子等位点显示诸如单原子催化、高反应活性等新奇的物理化学特性^[17-19]; 固态和液态表面偶极层内的键收缩主导块体材料中诸如杨氏模量、相变温度、介电常数、禁带宽度等物理常量的尺度效应^[8]。文献[5]中报道的准一维铜氧链的电子间“超强吸引”作用, 或与链内原子间的键收缩有关。

图2(b)和(c)所示的STM/S^[20]和XPS差谱^[15]测量结果揭示

图 2 低配位体系的BOLS-NEP标度规则与端态极化。(a) 局域键长与原子配位数的标度关系和芯能级的致密自陷与端态极化^[8]。STM/S测量的石墨(0001)表面和缺陷的显微形貌和狄拉克-费米共振峰^[20](b)以及XPS差谱态密度演变^[15](c)。(d, e) 密度泛函理论计算的单层石墨烯锯齿状边界自旋分辨电子极化共振端态。Reprinted with permission from Refs. [8,15,20]. Copyright (2007) by Elsevier; Copyright (2015) by the American Chemical Society; Copyright (2010) by the American Physical Society

Figure 2 BOLS-NEP scaling relation and the ending states polarization for the undercoordinated systems. (a) Atomic coordination number dependence of the local bond length and the associated core electron entrapment and nonbonding electron polarization^[8]. Surface morphology and electron resonance at the E_F level revealed using STM/S^[20] (b) and the C 1s energy shift uncovered using XPS differential spectroscopy^[15] (c) of graphite (0001) surface with point defects. (d, e) Density functional theory derived spin-resolved zigzag-edge and defect resonant states of a monolayer graphene ribbon. Reprinted with permission from Refs. [8,15,20]. Copyright (2007) by Elsevier; Copyright (2015) by the American Chemical Society; Copyright (2010) by the American Physical Society

了石墨(0001)表层原子和点缺陷的BOLS-NEP特征。与点缺陷空位相邻的偶极子呈现凸起的STM亮斑,且在费米能级处出现偏压为零的扫描隧道谱共振峰,即为有效质量非常小且群速度非常高的狄拉克-费米极化子。XPS差谱的C 1s谱谷位置对应体相中的C 1s电子能量,而谱峰分别对应表面单层或点缺陷周围的处于C 1s能级的电子能量相对于体相值的变化。XPS特征能级的移动正比于单键能 E 的变化。结果表明,石墨表层的有效配位数为3.1,表层碳键比体内的碳键短18%且强30%,点缺陷处的键更短更强,对应有效配位数2.2~2.4。由于缺陷处偶极子对局域势场的屏蔽,C 1s能带发生劈裂而呈现缺陷电子极化P峰。令人震惊的是,引入不足一个配位数的差异,3.1-(2.2~2.4),竟使碳原子的C 1s电子由表面的完全自陷态部分过渡为极化态。由此可见原子低配位的重要性。图2(d)和(e)所示的密度泛函理论计算的极化谱学特征与STS测量结果全同。自旋分辨极化仅发生在石墨烯的点缺陷处和锯齿形边缘,而扶手椅型边缘因其近邻原子间准键的形成,

并未发生极化。这也是前者显示类金属属性而后者显示类半导体属性的原因。有兴趣的读者可以从文献[15]中查阅更多原子配位分辨的电子声子谱学实例。

第三,电声作用与超导通道——极化载流子的有效质量与群速度。铜氧链和铜氧面受制于耦合氢键的HBCP和低配位原子的BOLS-NEP两项规则。铜氧面内原子配位数降低不仅强化O-Cu键,而且通过进一步极化弱化O:Cu^p的作用并调制各自的声子频率。因此,电声作用的本质是通过强化偶极子的极化程度以降低其振动频率,从而提升载流子的群速度和减小其有效质量。单层掺杂铜氧超导^[6]和铁砷/铜铁氧界面超导^[7]的发现直接证明了原子低配位和氧合砷的孤对电子极化的重要性。Bi-2212铜氧超导体的临界温度与其块体的相同,皆为105 K^[21]。两者的相干共振峰距费米能级30 meV。 T_C 和相干峰的间隙均与样品厚度无关这一事实足以证明原子低配位的重要性。Bi-2212单层超导体包括由范德瓦耳斯作用分开具有镜像对称的两个铜氧面: $\text{Cu}^+ - \text{O}^{2-} : \text{Cu}^p \leftrightarrow \text{Cu}^p : \text{O}^{2-}$

$-\text{Cu}^+$, 且 Cu^p 子层内含有原子空位. 由于偶极子间的排斥作用“ $\Leftrightarrow$ ”, 每个侧面等效于一个断面, 故BOLS-NEP规则适用. 超导通道两侧之间的范德瓦耳斯作用通过一侧的 Cu^+ 与另一侧的 $\text{Cu}^p\text{:O}^{2-}$ 吸引和两侧之间的“ $\Leftrightarrow$ ”排斥的平衡来实现. 超导载流子是两个铜氧面上偶极层的极化反键态电子, 其有效质量 $m^*(k)$ 正比于 (∞) 色散关系的曲率的倒数, $m^*(k) \propto [\nabla_k^2 E(k)]^{-1}$, 而其群速度 $v(k)$ 正比于色散关系的梯度, $v(k) \propto \nabla_k E(k)$ ^[22]. 其中, k 是波矢, $E(k)$ 为电子能量的色散关系. 在外场激发下, 这些极化反键态电子(Dirac-Fermion polariton)在两铜氧面间隙的超导通道中相干共振运行. 至于掺杂调制效应和载流子在低温和外场作用下诸如自旋取向、自旋耦合以及相干共振等动力学行为, 暂不在本文讨论范围之内.

综上所述, 铜氧面和铜氧链原子低配位导致的成键收缩

刚化和非键伸长弱化以及电子的双重极化对铜氧高温超导的贡献不可忽略, 而且它们服从低配位原子的BOLS-NEP和耦合氢键的HBCP标度关系. 铜氧偶极子单链和铜氧偶极面是由以氧为中心的四配位结构单元连接而成, 并非理想的二维结构, 它们的构型与铜氧面的晶体取向密切相关. 低配位诱导的成键收缩刚化和非键伸长弱化不仅可以改变局域晶格振动声子的频率, 而且还可以通过强化非键电子的极化提高载流子的群速度, 并降低其有效质量. 孤对电子的存在是关键. 孤对电子总是伴随V~VII族元素原子参与的化学反应过程中, 只是 sp^3 电子轨道杂化程度依元素种类略有差异. 上述观测事实也证明了电子声子计量谱学的重要性^[23]. 这些观测和认知对以超低配位共振端态和以 sp^3 电子轨道杂化主导的譬如拓扑绝缘体和砷基超导的理论和实验研究或有参考意义.

致谢 感谢国家自然科学基金(21875024)资助.

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Summary for “低维高温超导的启示: 键收缩与电子双重极化”

Enlightening of the low-dimensional high- T_C superconductivity: Bond contraction and electron dual polarization

Chang-Qing Sun^{1,2}

¹ School of Materials Science and Engineering, Jilin University, Changchun 130012, China;

² School of Electrical and Electronic Engineering, Nanyang Technological University, Singapore 639798, Singapore

E-mail: ecqsun@gmail.com

Electron-phonon interaction that couples the carriers for the Bose-Einstein condensation and the nature and configuration of the O–Cu chains and O–Cu planes that accommodate carriers are key issues to the cuprite high- T_C superconductivity discovered in 1986. However, the new kind of high- T_C superconductivity is beyond the description of the conventional Bardeen–Cooper–Schrieffer (BCS) theory. Here we address these two issues based on the bond order-length-strength correlation and nonbonding electron polarization (BOLS-NEP) notion for the effect of atomic undercoordination and the hydrogen bond (O:H–O equivalent of O:Cu–O) cooperativity and polarizability (HBCP) premise for water ice with involvement of electron lone pairs “:” interactions. First, a $\text{Cu}^{\text{p}}\text{:O:Cu}^{\text{p}}$ dipolar chain is formed by connecting a series of tetrahedrons made of two Cu^+ ions and two Cu^{p} dipoles surrounding the center O^{2-} . The O–Cu(110) plane includes three sublayers. The first one is made of alternative rows of Cu^0 vacancies and the $\text{Cu}^{\text{p}}\text{:O:Cu}^{\text{p}}$ dipolar chain with dipoles pointing out the surface; the second sublayer is formed by O^{2-} whose lone pairs polarize the dipoles and squeeze out the missing rows of Cu atoms, and the third sublayer is made of Cu^+ . However, the O–Cu(001) plane shows a different manner of the sublayers. The first sublayer is made of Cu^{p} , Cu^0 , and Cu^{2+} , and the third sublayer of Cu^+ and Cu. The O^{2-} bonds to the Cu^+ and polarizes the Cu to form the oppositely-coupled dipoles on the Cu(001) surface. The O–Cu bonding proceeds in four discrete stages: O^{2-} bonds to one Cu to form the $\text{Cu}^{2+}\text{--}2\text{O}^-$ and then each O^- bonds to its neighboring Cu in the second layer to form the twin tetrahedron with the production of the lone pairs. The introduction of O to Cu host creates valence density features of the O–Cu bonding, lone pair nonbonding, the dipolar antibonding above E_{F} , and electron holes. Second, atomic undercoordination of the O–Cu chains and the O–Cu planes shortens and stiffens the local O–Cu bond and lengthens and weakens the O:Cu^p nonbonding interactions associated with further enhancement of the Cu^{p} dipoles polarization, this process is the same as the O:H–O bond relaxation and polarization occurred to the skins of water and ice. Last, the electron-phonon interaction is realized by the undercoordination-induced bond relaxation and the dual polarization by lone pairs and bond contraction. The dual polarization weakens the O:Cu^p interactions and lowers the vibration frequency of the Cu^{p} , reducing the effective mass of the Cu^{p} electrons with high group velocity for carrier transport between the adjacent O–Cu planes that are made of atomic vacancies and dipoles. The self-entrapment of the core and bonding electrons, and the localized polarization and O:Cu^p weakening may describe the effect of electron-phonon coupling. The discovered “attraction force” between electrons along the Cu–O chain may fingerprint the effect of atomic undercoordination-induced bond contraction. The understandings of the dual polarization by oxidation and atomic undercoordination of carriers and the electron-phonon interaction may extend to devising the low-dimensional high- T_C superconductivity and the edge states polarization for the topological insulator superconductivity. The BOLS-NEP and HBCP regulations could be essential ingredients for the carrier generation and their interactions, which shall play certain substantial roles in the new types of superconductivity.

O–Cu plane, coupled hydrogen bond, polarization, bond contraction, cooperative relaxation, undercoordination

doi: [10.1360/TB-2021-0993](https://doi.org/10.1360/TB-2021-0993)