Charge density wave in low dimensional materials

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Abstract—Charge density wave (CDW) is an important physical phenomenon and has always been one of the significant research contents in condensed matter physics. The study of CDW helps people to have a deeper understanding of the interactions between various particles in low-dimensional systems. At the same time, the control of CDW in the material can effectively control the physical properties such as superconductivity. The study of CDW originated from one-dimensional and quasi-one-dimensional materials. This paper introduces the origin of CDW and the main formation mechanism of CDW at this stage. Discuss the common regulation methods of CDW and the competitive relationship with other physical properties. Finally, the possible research directions in related fields and the potential applications of CDW are prospected.

1. Introduction

The concept of charge density wave (CDW) originated from Peierls’ early theory that the structure of one-dimensional metallic systems is unstable at low temperatures. At low temperature, when the external environment is disturbed, the crystal structure will be distorted and the period of the charge density will be modulated, eventually forming a charge density wave. When the modulation wavevector q of the charge density is equal to twice the Fermi wavevector (2K_F), the Fermi surface coincides with the boundary of the Brillouin zone, opening an energy gap at the coincidence. Because the energy of the energy gap reduction is greater than the elastic energy of the lattice distortion, the whole system is favorable to the reaction direction of the reduction of the energy of the system, resulting in the transformation of the system from a conductor to an insulator, which is usually called the Peierls transition.
In one-dimensional metal atomic chain, in figure 1(a), the atoms are arranged in a long chain with lattice constant (a) and the electrons are arranged according to the energy level from low to high. Therefore, in figure 1(c), the Brillouin zone boundary is located at ±π/a, the system is half full and the Fermi level is at K_F = ±π/2a. The system remains in the metallic ground state. Since the structure of the one-dimensional metal system is unstable at low temperature, when the external conditions change, the system is disturbed and the lattice is then distorted at low temperature. When dimerization occurs, in figure 1(b), the distortion causes the two adjacent lattice points to form new primitive cell, the atomic spacing becomes 2a and the Brillouin zone boundary is located at ±π/2a (figure 1(d)). The Brillouin zone becomes half of the original and a band gap is formed at the boundary between Fermi level with Brillouin zone. According to the energy band theory, the system undergoes a transition from conductor to insulator at this time. The lattice distortion increases the elastic energy of the system, and the elastic energy is proportional to the square of the atomic displacement, so the moving distance after dimerization is shorter and finally an equilibrium dimerization state is formed. The electron density rearranges in a new periodic potential, known as a charge density wave. Consider that in practical cases, the band filling may not be half-filled, with any Fermi wave vector K_F. When Brillouin zone boundary overlaps Fermi surface, the energy decreases, so the lattice constant of the distortion is related to the Fermi wave vector, not the lattice constant of the chain. After lattice distortion, the lattice constant a′ can be different from 2a, a′/a can be any value, when the value of a′/a is irrational numbers, the resulting charge density wave is called incommensurate CDW. In addition, when the value of the distorted lattice a′/a is a rational number, the resulting charge density wave is called commensurate CDW.

In a perfect lattice, the lattice is periodically distorted due to the interaction of electrons with other collective excitations, resulting in charge density waves. Typically, the formation of charge density wave may arise from electron Fermi surface nesting, electron-phonon coupling, or other as yet unexplored factors. However, the origin of CDW is still controversial is still a hot issue in condensed matter physics and is closely related to quantum phenomena such as superconductivity. In this review, several major mechanisms of CDW formation will be introduced and then the regulation of CDW in low-dimensional systems will be discussed. the existing regulation methods provide a more complete picture of the properties of CDW and describe its competitive relationship with superconductivity. Finally, the research direction and potential application of CDW are prospected.

2. The formation mechanism of CDW

Regarding the formation mechanism of CDW, there are currently three main formation mechanisms,[4] one is the Fermi surface nesting mechanism, which causes the interaction between phonons and
electrons at the Fermi surface, making the phonon unstable; the second type is the electron phonon coupling mechanism, which is related to the inelastic scattering between electrons at the non-Fermi surface; The third mechanism is exciton condensation, where electron-electron (electron-hole) interaction is the main driving force[5]; in addition, there are some special systems, banded Jahn Teller effect, in some transition metal chalcogenides (TMTDs), the transition is driven by structural distortions that break the degeneracy of the ground state energy[6]. In the formation mechanism of CDW in 2D materials, the Fermi surface nesting is not enough to drive the lattice distortion, so the electro-phonon coupling has a certain effect on the formation of CDW.

The Peierls instability has an important relationship with the shape of the Fermi surface of the one-dimensional system. The Fermi plane of a one-dimensional system is two points in K space (±K_F), and the Fermi plane at -K_F is translated by a vector of 2K_F. Then it can nest with the Fermi surface at +K_F. The phenomenon that the Fermi surface coincides with another Fermi surface after the translation of a specific wave vector is called Fermi surface nesting and the translation vector is called the nesting vector, which is the intrinsic driving force of the Peierls mechanism[7]. Previously, we described the formation of charge density waves from the energy band diagram. In addition, we can also intuitively see the relationship between the frequency of lattice vibration (phonon) with the q vector (figure 2). The red line represents phonons. the phonon is in the positive semi-axis under normal circumstances, when the vibration frequency is in the negative semi-axis, Kohn anomaly[8,9] makes the Fermi surface nested vector q=2 K_F. There is the appearance of imaginary frequency. Imaginary frequency generally means the occurrence of phase transition. Fermi surface nesting leads to the instability of phonons. At this time, the frequency of phonon vibration decreases rapidly and is discontinuous, and the lattice is also distorted, which eventually causes the redistribution of periodic atoms and electron density.

Figure 2. For a one-dimensional metallic system, the vibrational frequency of the phonon decreases significantly and ceases to be continuous at q equal to 2K_F.

Therefore, we can qualitatively identify the possibility of the occurrence of charge density wave by relying on the degree of nesting of Fermi surfaces and the difficulty of nesting[10]. The Fermi surface structure of the one-dimensional metal system is shown in figure 3. From the perspective of the nesting degree of the Fermi surface, in the one-dimensional metal system, the Fermi surface -K_F is translated by 2K_F vector When reaching K_F, a complete nesting is formed, resulting in the destabilization of phonons and the distortion of the lattice. while in the actual quasi-one-dimensional material system, due to the existence of metal chains have the interaction force, the geometry of the Fermi surface has certain three-dimensional characteristics and the geometric structure of the Fermi surface is a curve or a curved surface[11]. After the Fermi surface on the left is partially translated by the q vector to the right, only partial nesting can occur with the Fermi surface on the right. From the perspective of the degree of
nesting, the possibility of occurrence of CDW is smaller than that of an ideal one-dimensional system. In two-dimensional system, the shape of the Fermi surface is a circle. After the translation of the \( q \) vector, it cannot form a complete nesting with the other half of the Fermi surface, but only intersects or is tangent to the other half of the Fermi surface. CDW transition seems less likely to occur. For systems that are not prone to Fermi surface nesting, the Fermi surface nesting mechanism is not enough to explain the occurrence of CDW and other mechanisms, such as the electrophonon coupling mechanism, need to be considered. When the Fermi surface is poorly nested, a larger \( g_q \) (electro-phonon coupling strength) is required for the CDW transition to occur.

The third type of CDW usually occurs in the region of electron-electron interactions and a common way to estimate whether this type of interaction is important is to define an interaction parameter \( r_s \). This parameter reflects the contribution of Coulomb energy \( (E_C) \) and Fermi energy \( (E_F) \) to the total energy, which we can express as the ratio of the average interparticle distance \( (a) \) to the effective Bohr radius \( (a_B) \)[12].

\[
r_s = \frac{E_C}{E_F} = \frac{a}{a_B}
\]

Because the distance \( (a) \) is inversely proportional to the carrier concentration, the strength of the electron-electron interaction is greater in the dispersed system. When electron-electron interactions dominate, the system has many possible ground states, some of which are thought to be related to the CDW. For example, the Overhauser effect[13] with wave vector \( 2K_F \) spin density wave and charge density wave, \( 4K_F \) wave vector CDW related to Wigner crystals[12]. A third class of CDW has been found in cuprates and manganates[14], which are known for their charge-order-related complexity and distinct phases. In addition, the charge order in CDW consists of delocalized electrons, while the conventional charge order consists of localized electrons[15-18].

3. Controlling charge density wave state

3.1. Pressure control charge density wave

Applying high pressure or stress to the material can change the microstructure of the system, but does not introduce impurities and defects, so this method is a commonly means to control the properties of materials. As in the family of transition-metal trichalcogenides (TMTCs), ZrTe\(_3\) materials exhibit metallic behavior at room temperature and possess both charge density wave (CDW) and superconducting transition (SC) states. The competitive interaction between CDW and SC is sensitive to applied pressure. ZrTe\(_3\) provides CDW and SC can coexist without any chemical modification or
structural modification, so ZrTe₃ becomes an ideal research platform for interaction between CDW with SC[19-22]. In an earlier study, it was found that CDW transition temperature T_{CDW} of ZrTe₃ is around 63 K, and it exhibits superconductivity below T_c=2 K. Initial pressure studies show that the T_{CDW} is enhanced with a gradual increase in pressure, reaching a maximum value of around 105 K at 1.1 GPa. In figure 4, we can see that the T_{CDW} exhibits a dome-like form at high pressures up to 5 GPa, and when the pressure is higher than 5 GPa, the CDW suddenly disappears; while the superconducting temperature T_c drops at 0.5 GPa Below 1.2 K, SC disappears with increasing pressure. When the pressure reaches 5 GPa, the disappearing SC reappears at a superconducting temperature of 2.5 K. As the pressure continues to increase to 11 GPa, the TC increases to 5K[20]. It can be seen that applying pressure to the material can effectively control the CDW transition temperature, and the disappearance and reentry superconductivity can be explained by Fermi surface dynamics. The CDW driving force is confined to the quasi-1D flakes of the Fermi surface, while the superconducting dynamics are confined to the remaining Fermi fraction. The pressure deforms the shape of the Fermi surface. The area of the Fermi surface decreases with increasing pressure and the formation of CDW is suppressed. The remainder after the CDW transition will be modulated, thereby affecting the density of states participating in the superconducting transition.

In a recent study on ZrTe₃ CDW and SC, as shown in figure 4(b), the pressure was increased to 33 GPa. As the pressure increases, the T_c is elevated, rising from 4 K to a maximum of 7.1 K at 28 GPa and remains relatively constant at this stage from 28 GPa to 33 GPa when the pressure reaches 33 GPa. The superconductivity temperature increases with increasing pressure and at the highest measured pressure of 33 GPa, there is no sign of superconductivity being suppressed[23]. According to first-principles calculations, the increase in superconducting temperature is mainly due to the increase of the Fermi level density of states and the decrease of the characteristic phonon frequency.

3.2. Element doping

Element doping is also one of the powerful means to control the CDW, which is common in one-dimensional or two-dimensional systems. For example, in the two-dimensional system 1T-TaS₂ doped with iron element, 1T-TaS₂ has abundant charge density wave (CDW) transition phase, so it is widely used in the study of CDW. 1T-TaS₂ has three CDW transitions, namely the transition from metallic phase to incommensurate charge density wave (ICCDW); incommensurate to nearcommensurate CDW (NCCDW); and finally nearcommensurate CDW to commensurate (CCDW)[24-27]. From the phase diagram in figure 5(a), we can find that the CDW is gradually suppressed with the doping of Fe element,
and the Mott phase is melted at the same time. For samples at moderate doping levels (0.01 to 0.04), the superconducting (SC) state appears at low temperature, below the CDW state. SC strongly depends on “x” in a narrow doping range, the maximum superconducting transition temperature is 2.8 K and the doping ratio is x=0.02. With further doping (x>0.04), disorder is introduced, superconductivity and NCCDW disappear at the same time, and the material enters the Anderson localized state, the appearance of which leads to a large increase in resistivity\cite{27}. Doping is not only inserting a single element into a system, but also inter-doping between systems, such as inter-doping between 1T-TaS2 and 1T-TaSe2 systems\cite{28}.

The same doping is also seen in some one-dimensional systems. The kinetics of CDW and superconductivity can be adjusted by chemical doping. When selenium is doped in the one-dimensional system CDW conductor ZrTe3, with the increase of the doping ratio, the lattice structure changes. When the long-range CDW order is gradually suppressed, its superconductivity begins to emerge (figure 5(b)). When the doping ratio is (0.04≤x≤0.07), the superconducting critical temperature Tc in ZrTe3-xSex (0≤x≤0.1) increases to 4 K\cite{29}.

![Figure 5. (a) Electronic phase diagram of 1T-Fe0.7Ta0.3S2 single crystal\cite{27}. (b) Phase diagram of ZrTe3 doped with a small amount of Se\cite{29}.](image)

3.3. Dimension control
Dimensionality has a profound effect on the instability of CDW. Since the layers of TMTDs and TMTCs rely on van der Waals force connections, few-layer and single-layer materials can be prepared by techniques such as liquid phase and mechanical exfoliation, so as to control physical properties such as charge density waves by means of dimensionality reduction. In the study of the two-dimensional material NbSe2, Xi et al used NbSe2 to study the relationship between CDW with dimension. The results are shown in figure 6(a). It can be seen that the superconducting transition temperature decreases with decreasing film thickness, but the observed charge density wave transition temperature increases from 33 K in bulk to around 145 K in monolayer\cite{30}. This anomalous enhancement of charge density waves in atomically thin samples can be understood as a result of the dramatic enhancement of electron-phonon interactions in 2D NbSe2.

Another material in the two-dimensional system, 1T-TaS2, has also been studied in terms of dimensionality. Yoshida et al have prepared many 1T-TaS2 nanometer-thick devices with thicknesses ranging from 7 nm to 100 nm. figure 6(b) is the result of device test. In the previous section, we mentioned that 1T-TaS2 has three CDW transition phases. From the figure, it can be observed that the NCCDW transition has little dependence on the thickness, the temperature has been kept around 350 K. Under cooling, the reduction of dimensionality significantly reduced the TCCDW transition, indicating that dimensionality reduction has an inhibitory effect on the CDW of 1T-TaS2\cite{31}. From the two materials, NbSe2 and 1T-TaS2, it can be seen that the dimensionality reduction enhances the CDW of NbSe2, while inhibition for 1T-TaS2 material. Dimension reduction has different results for different materials, indicating that size effect has different effects on CDW of different systems.
In addition, in the study of CDW regulation, there are also methods such as gate voltage regulation, in-plane current regulation and ion bombardment, which can control the charge density wave order of the system.

![Figure 6. (a) Thickness-temperature phase diagram of NbSe$_2$[30]. (b) Temperature-thickness phase diagram of 1T-TaS$_2$ nanometer-thick crystals[31].](image)

4. Conclusion

The research of CDW originated from one-dimensional materials, but with the development of material preparation and measurement technology, the research of CDW has been extended to two-dimensional materials, especially those based on transition metals (Ta, Nb, V, etc.). The stacking of two-dimensional materials into heterojunctions has also become a research method. The CDW states in low-dimensional materials can be regulated by various means, which provides the possibility for the application of nanodevices. For example, 1T-TaS$_2$ has different CDW transitions and metal-insulator transition at low temperature. It provides a wealth of optional voltage platforms for memory devices[32,33]. The resistivity of CDW materials often changes abruptly at the transition temperature. Devices based on 1T-TaS$_2$ thin layers can effectively control the oscillation of the system by changing the gate voltage and are expected to be applied to electronic devices such as voltage oscillators[34]. While CDW in some materials have been found to be multiband[35] and topological[36], which provides a possible idea for quantum computing.

At present, there is still considerable controversy over the physical nature and origin of CDW generation in low-dimensional materials. In traditional one-dimensional materials, there are still many problems that can not be solved perfectly, such as the origin of CDW and the determination of the properties of topological excitation. Future research on CDW materials can focus on the following aspects:

1. Although CDW materials have been widely studied, there are still disputes over the formation mechanism of different systems, so exploring the origin of CDW is an important topic.
2. CDW material systems tend to have strong electric-phonon coupling interactions and their relevance to superconductivity remains an interesting topic.
3. How can we combine CDW physical properties with practical applications.

However, it is believed that with the advancement of science and technology. In the future, more studies will reveal common patterns of CDW origin mechanisms and expand the applications of CDW in various systems.

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