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Robust T_c in element molybdenum up to 160 GPa

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Element superconductors with the single atoms provide clean and fundamental platforms for studying superconductivity. Although elements with d electrons are usually not favored by conventional BCS, the record superconducting critical temperature (T_c) in element scandium (Sc) has further ignited the intensive attention on transition metals. The element molybdenum (Mo) with a half-full d-orbital is studied in our work, which fills the gap in the study of Mo under high pressure and investigates the pressure dependence of superconductivity. In this work, we exhibit a robust superconductivity of Mo in the pressure range of 5 GPa to 160 GPa via high-pressure electrical transport measurements, the T_c varies at a rate of 0.013 K/GPa to 8.56 K at 160 GPa. Moreover, the superconductivity is evidenced by the T_c shifting to lower temperature under applied magnetic fields, and the upper critical magnetic fields are extrapolated by the WHH equation and GL equation; the results indicate that the maximum upper critical magnetic field is estimated to be 8.24 T at 137 GPa. We further investigate the superconducting mechanism of Mo, the theoretical calculations indicate that the superconductivity can be attributed to the strong coupling between the electrons from the partially filled d band and the phonons from the frequency zone of 200–400 cm^{-1}.

Keywords: molybdenum, element superconductor, high pressure, superconductivity

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1. Introduction

The research of superconductivity is of great significance to the social development, and room temperature superconductivity is regarded as the "holy grail" of condensed matter physics. As the most straightforward material systems, elemental materials provide the best platforms for studying superconductivity. The superconductivity of 29 elements[1,2] was observed at ambient pressure, such as beryllium (Be),[3] technetium (Tc),[4] and hafnium (Hf),[5] with the transition metal niobium exhibiting the highest superconducting critical temperature of 9.2 K.[6,7] As a powerful means of altering material properties, high pressure can change the microscopic structure of materials and significantly increase the T_c of certain elements.[8–10] With the introduction of pressure, the superconducting transition temperatures of some elements are significantly increased, such as lithium (Li),[11] zirconium (Zr),[12] and lanthanum (La).[13] Furthermore, a number of non-superconducting materials can transform into the superconducting phases under high-pressure conditions, for instance, phosphorus (P),[14] boron (B),[15] and sulfur (S).[16] In particular, the non-metallic element hydrogen can be converted into a metal at high pressure, which is proposed to be a room-temperature superconductor.[17–20] Superconductivity has been observed in more than 50 elements at ambient pressure and high pressure.

Among elemental superconductors, the high T_c and superconducting mechanism of calcium (Ca) have attracted research interest. Previous works reported that the T_c of Ca increases with compression to a maximum of 29 K at 216 GPa.[21,22] The high T_c is attributed to the phenomenon of s–d electrons transfer under high pressure.[23] As for transition metals with d-electron occupancy at ambient pressure, yttrium (Y) and vanadium (V) also exhibit superconductivity with high T_c under high pressure. The T_c of Y is 19.5 K at 115 GPa[24,25] and that of V is 17.2 K at 120 GPa.[26] In particular, the metals Sc and titanium (Ti) have recently been reported as high T_c elemental superconductors, the T_c of Ti increases to 26 K at 240 GPa,[27–29] and Sc has a critical temperature up to 36 K at 250 GPa, which is the highest recorded T_c in superconducting elements.[30–32]

Transition metals are characterized by a partially filled d-band, and the d-occupation number greatly impacts the metal crystal structure[33–35] and superconductivity.[23] Most transition metals are superconducting at ambient pressure due to their specific d-occupation. Under high pressure, tran-

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sition metals have shown the effects of Fermi level and crystal structural changes on T_c,[36] and exhibit considerable superconductivity.[26,28,31] Mo, an element with a half-full d-orbital, exhibits typical properties of transition metals, and the T_c is 0.98 K at ambient pressure.[37] Besides, under high pressure, Mo exhibits excellent phase stability, the bcc-Mo phase (space group $Im\bar{3}m$) was found to be stable up to 600 GPa.[38,39] A recent work reported a T_c up to 32 K in MoB_2 under high pressure, which is the highest T_c in transition-metal borides.[40] It is worth noting that the theoretical results indicate the positive effect of pressures on superconductivity in element Mo.[41]

In our work, to further investigate the effect of d-electrons on superconductivity, we compressed the Mo sample up to 160 GPa to research its superconductivity via electrical resistance measurement. The experiments show that the T_c varies at a rate of 0.013 K/GPa to 8.56 K at 160 GPa, which indicates the robust superconductivity of Mo. And theoretical calculations reveal that the superconductivity can be attributed to the strong coupling between the electrons from the partially filled d band and the phonons from the frequency zone of 200–400 cm^{-1}.

2. Experimental and theoretical methods

We used the target Mo sample, which was scraped off the target material with a purity of 99.95%. The piston-cylinder diamond anvil cell (DAC) made of NiCrAl alloy was loaded for performing the electrical resistance measurements, and an anvil with a beveled culet size of 100 μm was adopted to generate ultra-high pressure in the experiments. The pressure was determined by the shift of the first-order Raman edge frequency from the diamond anvil.[42] The sample chamber consisted of an insulating layer (cubic boron nitride, aluminum oxide powder mixed with epoxy resin adhesive), pressure-transmitting media (PTM) (ammonia borane, NH_3BH_3), and sample (Mo), which was loaded into the sample chamber in air. The electrical resistance measurements were performed by using the four-probe van der Pauw method, four Pt foils with a thickness of approximately 4 μm were selected as the electrodes. The diamond anvil cell was put into a MagLab system that provided extreme environments with temperatures from 300 K to 1.5 K and magnetic fields up to 7 T for the electrical transport measurements.

The structural relaxations and electronic property calculations were performed within the density functional theory[43–45] using generalized gradient approximation with the Perdew–Burke–Ernzerhof functional and the projector augmented wave potentials as implemented in the VASP code.[46,47] Plane-wave kinetic energy cutoff was set to 800 eV and Monkhorst–Pack k-meshes with grid spacing of $2\pi \times 0.03$ $Å^{-1}$ were adopted. The electron–phonon coupling (EPC) calculations were performed using density functional perturbation theory[48] as implemented in the Quantum Espresso package.[49] The relativistic norm-conserving kind of pseudopotential was used with a kinetic energy cutoff of 80 Ry and $6 \times 6 \times 6$ q-mesh and $24 \times 24 \times 24$ k-mesh were utilized. The T_cs were estimated with the Eliashberg equation.[50]

3. Results and discussion

To investigate the superconducting properties of the metal Mo under high pressure, we achieved high pressure conditions by using the DAC, and performed high-pressure resistance measurements. The schematic of the DAC used for electrical transport measurements is shown in Fig. 1(a). We chose NH_3BH_3 as the PTM, and applied the high pressure up to 160 GPa to explore the superconductivity of Mo. A microphotograph of the sample chamber is shown in Fig. 1(b), the sample with a size of ~ 30 μm$\times 15$ μm is surrounded by NH_3BH_3, which reduces the influence of non-hydrostatic pressure on the experiment.

We performed high-pressure electrical resistance measurements to explore pressure dependence T_c of metal Mo. During the cooling from 300 K to 1.5 K, the temperature dependences of the resistance of Mo at various pressures are shown in Fig. 1(c). The resistance of the sample first exhibits apparent metal-like behavior, then drops sharply to zero near the transition temperature. The superconducting transition temperature T_c is determined by the temperature where the resistance begins to drop. Above 56 GPa, the resistance shows an upward trend before dropping sharply, and a narrow resistance peak in the superconducting state appears near T_c. A similar phenomenon was previously observed in disordered superconductors, such as La,[13] Y,[24] stannum (Sn) and indium (In),[51] which can be attributed to the generation of superconducting states being surrounded by normal states near T_c. In the pressure range of 5–160 GPa, the superconducting transition is sharp, with a width less than 1 K (from 10% to 90% of the normal state resistance at T_c^{onset}), indicating the superconducting phase with good homogeneity.[13] And during the compression, the T_c of Mo is up to 8.56 K at 160 GPa with a rate of about 0.0134 K/GPa, as shown in Fig. 1(d). Compared with the T_c of Sc and Ti, the T_c of Mo is almost constant for pressures ranging from 5 GPa to 160 GPa, which exhibits robust superconductivity to external pressure.

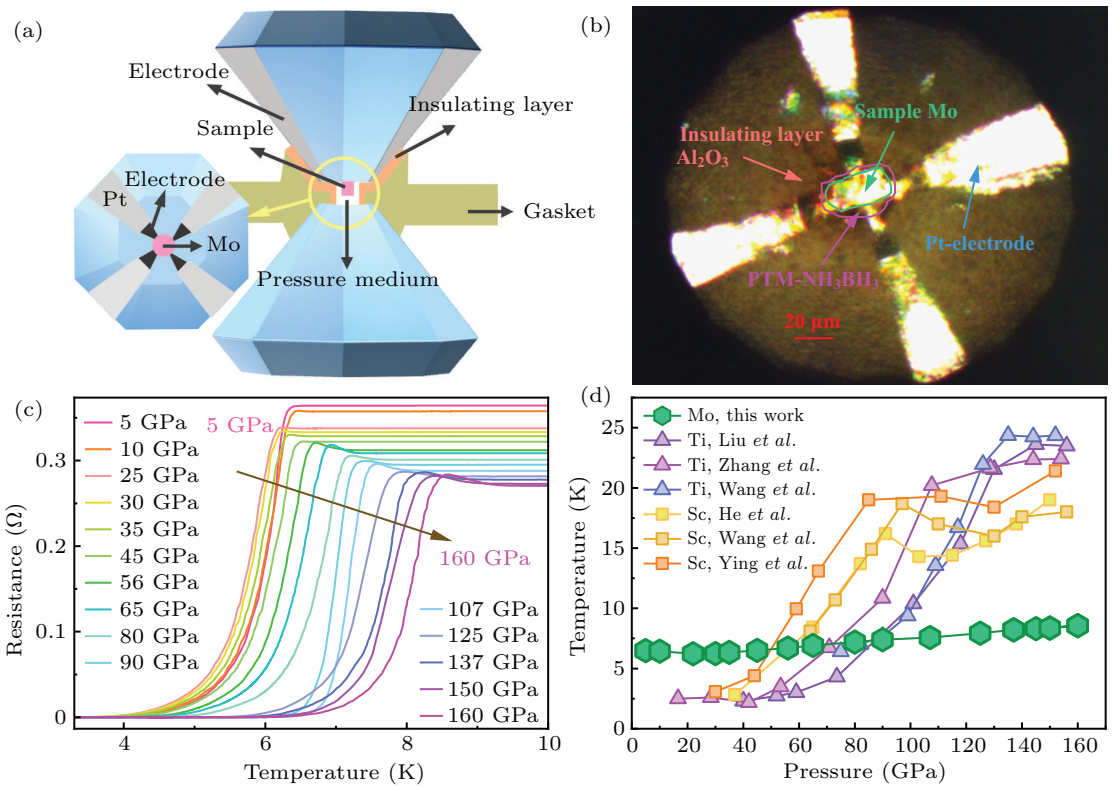


Fig. 1. DAC diagram of the setup for the van der Pauw method and transport properties of metallic Mo at various pressures. (a) Schematic of the DAC used for electrical transport measurements. The sample chamber is consisted of a gasket (W) with an insulating layer (Al_2O_3 mixed with epoxy). (b) A microphotograph of the sample chamber at 160 GPa illuminated from the top. (c) Resistance of the Mo sample as a function of temperature at various pressures from 5 GPa to 160 GPa during cooling. (d) Pressure dependence of the critical temperature. The hexagon symbols indicate data from Mo (this work), square symbols indicate data from Sc (from Refs. [30–32]), and triangle symbols indicate data from Ti (from Refs. [27–29]).

In order to further confirm that the observed phenomenon is indeed superconducting transition of Mo at various pressures, we measured the transport properties under different external magnetic fields from 0 to 7 T, as shown in Fig. 2. Figures 2(a), 2(b), and 2(c) illustrate the cooling curves of the resistance at 90 GPa, 107 GPa and 137 GPa with applied magnetic fields H, respectively. The T_c decreases with the increase of the magnetic field, and the transition width expands observably, confirming that the observed phenomenon is indeed a superconducting transition. The experimental data shows that the superconductivity with transition temperature above 1.5 K is completely suppressed when the applied magnetic field is 7 T. To estimate the upper critical magnetic field $\mu_0 H_{c2}(0)$, we use the Werthamer–Helfand–Hohenberg (WHH) model[52] simplified by Baumgartner[53]

$$\mu_0 H_{c2}(T) = \frac{\mu_0 H_{c2}(0)}{0.693}\left[\left(1-\frac{T}{T_c}\right) - 0.153\times\left(1-\frac{T}{T_c}\right)^2 - 0.152\times\left(1-\frac{T}{T_c}\right)^4\right], \quad (1)$$

and the Ginzburg-Landau (GL) equation[54]

$$\mu_0 H_{c2}(T) = \mu_0 H_{c2}(0)\left(1-\frac{T^2}{T_c^2}\right) \quad (2)$$

to extrapolate the $\mu_0 H_{c2}(0)$. Figures 2(d) and 2(e) show the fitting of $\mu_0 H_{c2}(0)$ at various pressures by the two models, the balls of orange, cyan, and purple represent our experimental data at 90 GPa, 107 GPa, and 137 GPa, respectively. The maximum of $\mu_0 H_{c2}(0)$ estimated is 8.24 T at 137 GPa by the equation of WHH model. The values of $\mu_0 H_{c2}(0)$ do not exhibit anomalies with the compression, and the fitting results are consistent with our experimental data.

We fit the normal state resistances by the equation of $R(T) = R(0) + AT^n$[55] from 10 K to 70 K, where $R(0)$, A and n are defined as the residual resistance, coefficient related to the behavior of Fermi liquid, and temperature exponent, respectively. The fitting results at various pressures are plotted in Fig. S1, they are in good consistency with the temperature dependences of the resistance measured in our experiments. The main parameters vary with pressure from 5 GPa to 160 GPa as shown in Fig. S2.

As the pressure increases, the normal state resistance decreases regularly without any abnormal change. This indicates that the stability of the crystal structure and electronic structure in the metal Mo within the pressure range studied in this work. The coefficient A gradually increases, and the exponent n gradually decreases as the pressure increases to 73 GPa, then both coefficient A and exponent n become stable at higher pressures. Significantly, the value of n is close to 3, indicating that the electron transport is dominated by inter-band scattering of s–d orbitals.[56]

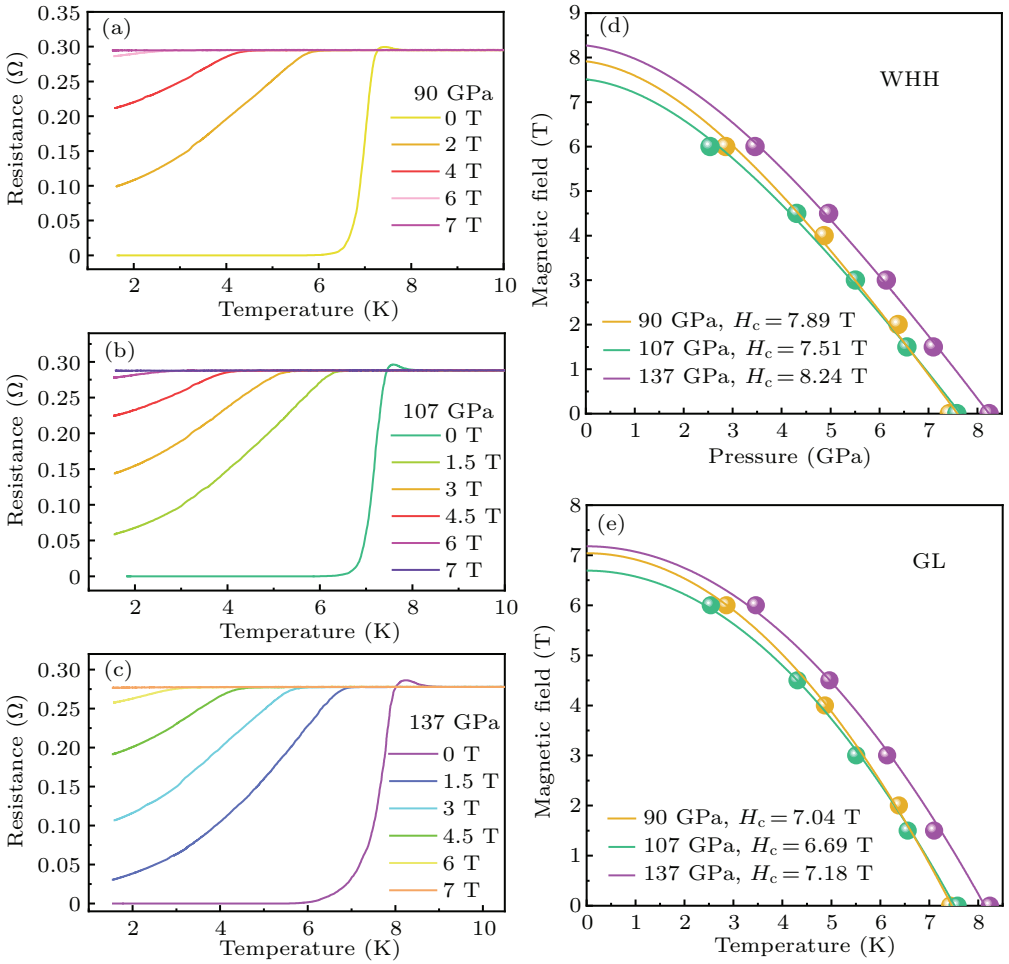


Fig. 2. Transport properties of the Mo sample with applied magnetic fields. (a)–(c) Superconducting transition of the Mo sample with applied magnetic fields up to 7 T at 90 GPa, 107 GPa and 137 GPa, respectively. (d), (e) Upper critical fields $\mu_0 H_{c2}(0)$ extrapolated to the zero temperature at various pressures by the equations of WHH model (from Refs. [52,53]) and GL model (from Ref. [54]), respectively, and the balls represent our experimental data.

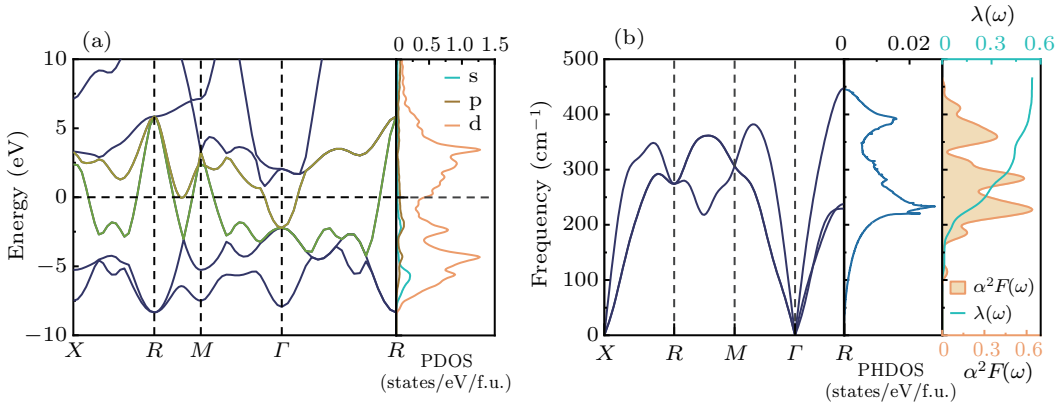


Fig. 3. Electronic and lattice properties of Mo at 150 GPa. (a) Projected band structure and density of states. Cyan, brown and orange lines represent the contributions of electrons from s, p, and d orbitals, respectively. (b) Phonon spectrum, projected phonon density of states (PHDOS), Eliashberg phonon function $\alpha^2F(\omega)$ and its integral electron–phonon coupling strength $\lambda(\omega)$.

To further confirm the superconducting mechanism of Mo, we calculated the band structures and superconducting parameters of Mo at 150 GPa, as illustrated in Fig. 3. The estimated T_c is 7.2 K at Coulomb pseudopotential $\mu^* = 0.1$ with electron–phonon coupling constant $\lambda = 0.55$ and logarithmic average phonon frequency $\omega_{log} = 372.792$ K, which is close to the experimental value of 8.4 K. So, we believe that our theoretical calculation results are reliable. As shown in Fig. 3(a), flat and steep bands overlap at the Fermi level, indicating the potential for superconductivity in Mo. There are two energy bands across the Fermi level, most of which come from the contribution of electrons that unfilled d-orbitals, and the total density of states at the Fermi level is mainly from these d electrons. Figure 3(b) shows the phonon spectrum, the pro-

jected phonon density of states, Eliashberg phonon function $\alpha^2F(\omega)$ and its integral electron–phonon coupling strength $\lambda(\omega)$. The absence of imaginary frequencies indicates the dynamic stability of bcc-Mo phase at 150 GPa. The strong coupling mainly comes from the phonons in the frequency zone of 200–400 cm^{-1}, which contributes about 85.77% of the electron–phonon coupling strength λ. Thus, the T_c of Mo can be attributed to the strong coupling between the electrons from the unfilled d-orbitals and the phonons from the frequency zone of 200–400 cm^{-1}.

Different from Sc and Ti with high T_c, the T_c of Mo does not exhibit a significant increase under high pressure. As for Sc with one d-electron and Ti with two d-electrons in the valence band, the phenomenon of s–d electrons transfer occurs with increasing pressure, and the increase of the d-occupation number has a positive effect on the superconductivity.[30,57] In addition, phonon softening under high pressure was observed in both Sc[32] and Ti,[27] which promotes electron–phonon coupling. We believe that the similar phenomenon may have occurred in Mo, but the inhibition of superconductivity by compression and the promotion by phonon softening offset each other, making Mo be a robust superconductor under high pressure.

4. Conclusions

In conclusion, we have studied the superconductivity of the metallic Mo at pressures up to 160 GPa. The superconducting transition temperature of bcc-Mo was determined to increase at a rate of 0.013 K/GPa to 8.56 K at 160 GPa by performing transport measurements, and the result indicated the robust superconductivity of Mo. We investigated the influence of applied magnetic fields on T_c by WHH and GL equations, and the maximum upper critical magnetic field was estimated to be 8.24 T at 137 GPa by WHH equation. The results of our first principles calculations are consistent with the experimental results. Theoretical calculations show that Mo is a traditional phonon-mediated superconductor, and the T_c can be attributed to the strong coupling between the electrons from the partially filled d band and the phonons from the frequency zone of 200–400 cm^{-1}.

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