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High Pressure Studies of MoS_2 and $MoSe_2$ Using Bridgeman Anvils

Dr. Bhupendra Mor[1], Dr. Kirti Korot[2]

[1]Department of Science and Humanities, Government Polytechnic, Palanpur, Gujarat, India
Email: *bhupendramor1980[at]gmail.com*
ORCID iD: 0009-0009-3320-9445

[2]Assistant Professor, Department of Science and Humanities, Government Engineering College, Palanpur, Gujarat, India
Email: *kirtiphysics[at]gmail.com*

Abstract: ***This study presents an in-depth analysis of the electrical transport behavior of MoS_2 and $MoSe_2$ single crystals under high-pressure conditions using the Bridgman anvil apparatus. Electrical resistivity was measured via a four-probe method up to a pressure of 6.5 GPa. The findings indicate a pronounced reduction in resistivity as pressure increases, suggesting a narrowing of the band gap and enhanced carrier mobility. The pressure-induced semiconductor-to-metal-like transition is attributed to modifications in the interlayer coupling and band structure, driven by orbital rearrangements. The study also explores the underlying density of states and interatomic interactions that evolve under compression. These results advance our understanding of pressure-tunable electronic transitions in layered TMDCs and highlight the potential of MoS_2 and $MoSe_2$ in future Nano electronic and high-pressure device applications.***

Keywords: Bridgman anvils, high pressure, MoS_2, $MoSe_2$, resistivity measurements, semiconductor-to-metal transition, transition metal dichalcogenides (TMDCs)

1. Introduction

The advent of two-dimensional (2D) materials has opened new frontiers in nanoscale electronics and optoelectronics. Although graphene initially attracted substantial attention due to its exceptional electronic properties, its gapless band structure limits its applicability in devices that require an on/off switching behavior or finite bandgap response. To address this limitation, a new class of 2D materials with intrinsic bandgaps—such as hexagonal boron nitride (h-BN), transition metal dichalcogenides (TMDCs), and certain transition metal oxides—has been extensively investigated [1–3].

TMDCs, typically represented by the formula MX_2 (where M = Mo, W and X = S, Se, Te), consist of hexagonally arranged layers in which a transition metal atom is covalently bonded to two chalcogen atoms. These materials exhibit strong in-plane ionic-covalent bonding and weak interlayer van der Waals interactions, allowing for easy exfoliation into monolayers [4]. Depending on their composition and structure, TMDCs display a rich diversity of physical behaviors, including metallic, semiconducting, superconducting, and charge density wave (CDW) states, as well as Mott-insulating phases [5–7]. Prominent TMDCs such as MoS_2, $MoSe_2$, $MoTe_2$, WS_2, and WSe_2 have emerged as candidates for applications in field-effect transistors, photodetectors, thermo electrics, and flexible electronics [8–10].

Modifying the electronic and optical properties of TMDCs through external stimuli is a promising route for device optimization. One effective and reversible approach involves the application of hydrostatic pressure, which can tune interatomic distances and thus alter the band structure and carrier mobility. Theoretical and experimental studies have demonstrated that pressure can induce semiconductor-to-metal transitions in layered TMDCs, particularly in bilayer configurations [11–13]. Measuring pressure-dependent changes in electrical resistivity provides valuable insight into such transitions.

High-pressure science has evolved into a powerful discipline over the past few decades, with relevance across materials science, geophysics, and condensed matter physics. It offers an avenue for probing the behavior of matter under extreme conditions, where interatomic interactions are significantly altered [14]. Structural phase transitions, electronic topological changes, and modifications in lattice dynamics can be induced and studied through techniques such as X-ray diffraction (XRD), electrical transport measurements, and optical spectroscopy under pressure [15–17]. The field is also instrumental in the development of superhard materials like diamond and cubic boron nitride, which are vital for industrial applications.

From a geophysical standpoint, high-pressure research is crucial for simulating conditions within the Earth's mantle, where materials exist under immense pressure and temperature. In materials research, it enables the design of adaptive electronic and mechanical properties without introducing chemical impurities. Lamellar solids such as TMDCs are especially suitable for high-pressure studies due to their layered structure, which facilitates shearing under load and enhances their performance as extreme pressure lubricants [18].

In this context, the present study investigates the pressure-dependent electrical resistivity of MoS_2 and $MoSe_2$ single crystals using a four-probe technique within a Bridgman anvil setup. The aim is to explore potential electronic phase transitions and structural responses by analyzing resistivity trends as a function of applied pressure.

2. Experimental Aspects

2.1 Generation of pressure

There has been an explosive growth in high pressure research in recent years. Without question, the great interest manifested in this field stalked from the diamond synthesis announcement of the General Electric Company in 1955. When considered in detail, there are perhaps as many high pressure devices as there are high pressure researchers, because each worker seems to develop certain aspects of the art to suit his own tastes [20, 31]. When considered in broad perspective, however, there are a limited number of basic apparatus that have been developed for simultaneous use at high pressure and high temperature. They are:

- Piston-cylinder device
- Bridgman anvil device
- Belt device
- Multiple anvil device
- Supported piston apparatus

2.2 Bridgman anvils

In 1950, P. W. Bridgman [22] reported the construction of an anvil apparatus utilizing two important principles: the principle of massive support and the principle of motion by means of a compressible gasket.

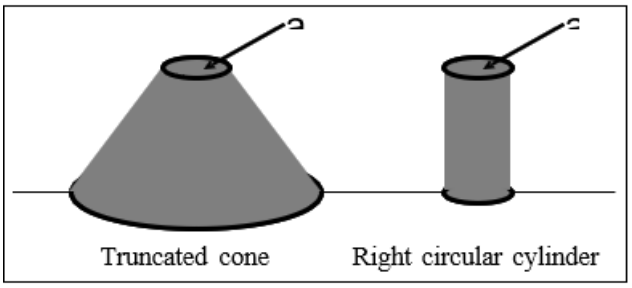

Figure 1: Principle of massive support.

The principle of massive support can be readily visualized from figure 1, where a broad truncated cone is depicted alongside of a right circular cylinder. The surface areas of the circular section marked (**a'**) and (**a**) are equal. If the cone and the cylinder are subjected to compressive load between flat plates, it will be observed that the pressure on (**a'**) will be much greater than the pressure on (**a**) at destructive failure of the cone and cylinder respectively. The reason for this lies in the fact that the circular tip near the apex of the cone has mechanical ties fanning out into a greater volume behind the tip than is the case in a right circular cylinder. The greater the included angle of the cone, the greater will be the pressure to which the tip can be subjected. Bridgman anvils, utilizing this principle, are shown in figure 2. Such anvils can be forced together until the force over area pressure existing on the two contact faces is as high as 200,000 atmospheres before failure of the carbide occurs. The maximum pressures above this limit are possible only when the carbide binding rings are surrounded by shrunk-on or interference fit steel binding rings. These provide lateral support to the carbide and absorb some of the tensile load that is fanned out from the truncated surface near the apex into the volume immediately behind.

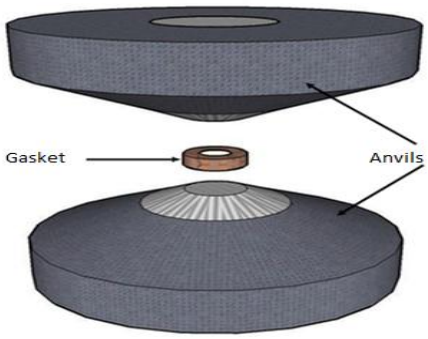

Figure 2: Gasket arrangements in Bridgman anvil apparatus.

There are limitations in the Bridgman anvil device that it would be desirable to overcome for some purposes. One limitation, of course, is the smallness of the sample. Another is the simple geometry (the sample is in fact, two dimensional). For many purposes it would be desirable to have a sample whose depth was of the same order of magnitude as its length and breadth. This would be particularly important in an apparatus design where in the specimen were to be heated internally by an electrical resistance furnace. Another limitation in this design is the fact that it is not possible to measure volume of the sample as a function of pressure. The principle of massive support was so effective in increasing the ultimate pressure obtainable in a single stage apparatus that several attempts have been made to utilize this principle in other ways in order to obtain an apparatus that was free from one or both of the afore mentioned limitations.

2.3 Gasket

Earliest experiments with Bridgman anvils were conducted by placing thin wafers of materials to be compressed between the anvil faces. As the anvils were forced together, material would extrude from between the faces until the lateral friction near the edges of the specimen was sufficient to balance the pressure towards the center of the specimen. In general, the higher the internal friction of a substance the thicker would be the resultant specimen when equilibrium between the frictional forces and the pressure would be attained. The type of experiment just described was not particularly useful. A device utilizing massive support was needed in which relative motion could be obtained and controlled. Bridgman solved this problem by surrounding a wafer like disc (now known as gasket) of the sample by a pipe stone ring as shown in figure 2. Pipe stone's frictional and compressive properties are such that the ring would form a seal around the wafer-like sample preventing its extrusion from between the anvils and, at the same time, it would compress with the anvil advance allowing motion to be obtained.

The first function performed by the gasket is that of "yielding" to the thrust placed on it by a moving anvil or similarly functioning apparatus component. Yielding can occur through simple compression of the gasket material by flow or by a combination of compression and flow. The amount of yielding should be relatively large in order that the anvils might move a sufficient amount to compress the contents of the high-pressure chamber. The second function of the gasket is that of "confining" (not yielding to the thrust

of) the material being compressed by the advancing anvil. The tasks of yielding and confining are, of course, contradictory and must somehow be reconciled. A third gasket function is that of "support." Just inside the inner edge of the gasket, the surfaces of the high-pressure apparatus components are subjected to the full pressure generated within the chamber. At the outer edge of the gasket, the apparatus components are subjected to only one atmosphere pressure. Ideally, the pressure exerted by the gasket against the components of the apparatus should gradually decrease from the full chamber pressure at the inner gasket edge to one atmosphere pressure at the outer edge. When this is the case, a sharp line of demarcation between chamber pressure and atmospheric pressure is avoided and consequently there will be no line of high stress concentration. If the gasket width and pressure gradient are judiciously chosen, the apparatus components will support each other and make it possible for the highly stressed portions of the components to with stand more load than would otherwise be possible. Pressure gradient patterns can be varied by choice of gasket materials and by changing the cross-sectional profile of the gasket from the inner to the outer edge. The gasket functions of yielding, confining, and supporting enumerated above, must, in any given design, be accomplished without having the gasket absorbs an in ordinate fraction of the ram thrust available for operating the device. In the belt and tetrahedral designs, the thrust absorbed by the gaskets and by the internal friction of the solid pressure transmitting medium has been kept rather low. It amounts to only 10 to 20 percent of the total applied thrust. These devices could probably be improved with respect to maximum pressure attainable and component lifetime by increasing the gasket-absorbed thrust to 50 percent of the total thrust. The additional thrust absorbed by the gaskets would be used to provide a more gradual pressure gradient from inner to outer edges of the gasket and to provide for additional component support. If yield to anvil advance were the only function to be performed by the gasket, the gasket material would, ideally, be extremely compressible and/or would flow very easily. The latter condition would be met by materials that have very low coefficients of internal friction. On the other hand, if confining the cell contents were the only function of the gasket, the gasket would ideally be composed of an extremely incompressible material that possessed great strength and a correspondingly high coefficient of internal friction. Selection of a material to meet these opposing requirements must be made from materials of intermediate compressibility and internal friction. Universal, optimum values of compressibility and internal friction probably do not exist. Optimum values of these quantities probably depend on geometrical parameters associated with each apparatus design. Some of the data collected are displayed in table 1 [22, 23]. Most ultrahigh-pressure gaskets in use today have coefficients of friction in the range of 0.25 to 0.50.

Table 1: Coefficient of Friction of Some Materials at ~2.4 GPa.

Material	Coefficient of friction
Ferric Oxide Powder	0.71
Aluminum Hydroxide Powder	0.39
Zinc Oxide Powder	0.58
Pumice Stone Powder	0.52
Chromic Oxide Powder	0.50
Pyrophyllite Powder	0.25
Pyrophyllite Natural Block	0.47
"Attasol" Clay Powder	0.47
Lead Dioxide Powder	0.46
Manganese Dioxide Powder	0.45
Titanium Dioxide Powder	0.45
Molybdenum Trioxide Powder	0.42
Tin Oxide Powder	0.41
Indium Sheet	0.01
Boron Carbide Powder	0.40
"Micro-Cell" Earth Powder	0.37
Calcium Hydroxide Powder	0.27
"Permagel" Clay Powder	0.18
Boric Acid Powder	0.14
KCl Powder	0.12
NaCl Powder	0.12
Mica Sheet	0.07
Boron Nitride Powder	0.07
Graphite Powder	0.04
Molybdenum disulfide Powder	0.04
Silver Chloride Powder	0.03

In order for the gasket to confine the material within the chamber, it must inherently possess great strength or else it must transmit the expulsion force imposed upon it by the chamber contents to the anvils or other apparatus components. Apparently, thin sheets of many substances subjected to heavy loads perpendicular to the sheet develop high strengths in directions parallel to the sheet. In spite of this, the gasket may be expelled or extruded by the expulsion force. This may be due to too low coefficient of internal friction of the gasket material or to too low coefficient of sliding friction between the gasket material and the apparatus components or both. The coefficient of sliding friction can be increased by roughening the anvils, by using a gasket material with a higher coefficient of internal friction, or by inter posing a thin layer of very high friction material between the gasket and the anvil. The latter procedure is used in the tetrahedral anvil device. In this instance a thin layer of rouge is applied to the surface of the pyrophyllite tetrahedron. In order for the gasket to successfully confine the chamber contents, it has been necessary to use the gasket material in relatively thin sections. This, of course, limits the relative motion of apparatus components and imposes limits on the chamber size for a given pressure. Additional relative motion was obtained in the belt design by using a sandwich gasket in which a thin sheet of steel was interposed between two sections of pyrophyllite. Appropriate geometrical considerations in the apparatus design, in this case, also increase the relative motion of the pressure generating components. There may be more elaborate composition-type gaskets constructed of multiple layers of materials with widely differing strength and frictional properties that would perform the tasks required of the gasket more effectively than does the sandwich gasket currently used in the belt.

2.4 Pressure Transmitting Medium

An effective way to subject a substance to high pressure for electrical measurements in anvil devices is to enclose the substance in a gasket to which pressure is transmitted by a solid medium. Ideally, this solid pressure transmitting medium must meet the requirements enumerated below.
It must:

- Transmit pressure hydrostatically.
- Have very low compressibility.
- Have very low thermal conductivity.
- Should be electrically insulator.
- Be chemically inert.

These requirements must be met at both ordinary and high pressures. In some instances additional special requirements must be met as would be the case where x-ray transparency is necessary for diffraction work at high pressure. Of course, it is impossible to find a solid pressure transmitting medium wherein all these requirements are fully and simultaneously met. Consequently, a compromise must be made. At the present time, pyrophyllite, talc, and hexagonal boron nitride are being widely used as pressure transmitting materials in high-pressure work. Each of these materials has its virtues and drawbacks. None of them transmits pressure as hydrostatically as would be desirable. It seems certain that no one has up to the present time, conducted a systematic investigation to discover materials that better meet the requirements enumerated above than do the materials now commonly used. Such research would indeed be important to the advancement of the high-pressure art. It seems reasonable that hydrostatic solids would possess low coefficients of friction as measured in Bridgman's shear apparatus. Some semi-quantitative information on this point has been obtained, but a great deal of additional work would be desirable.

2.5 Pressure measurement

Pressure is directly related to the applied force F and cross sectional area of piston A as

$$P = F/A \quad (1)$$

In this way it seems very easy to determine the pressure generated in the piston-cylinder type high pressure devices, but in fact it is quite difficult due to the spending of a large amount of applied force in compressing the gasket and in opposing the friction between piston and cylinder. In order to determine the generated pressure with accuracy as much as possible, different techniques are available today [24]. Each of them is having their own merits and demerits according to the type of measurements to be performed. These techniques are listed below;

- Primary scale
- Thermodynamic absolute pressure scale
- Ruby scale
- X-ray gauges
- Equation of state
- Fixed pressure points (Secondary pressure scale)

The fixed pressure point scale has been replaced in many experiments now days by ruby and X-ray gauges but still it is effectively used in large anvil systems. It also serves for calibration of some other gauges. In this technique reproducible phase transitions of some materials are used for scaling the pressure. General requirements for such calibrants are as under;

- The measured effect (electrical resistance, volume etc.) should be large.
- Hysteresis of the phase transition should be small.
- Temperature effect on transition pressure should be small.

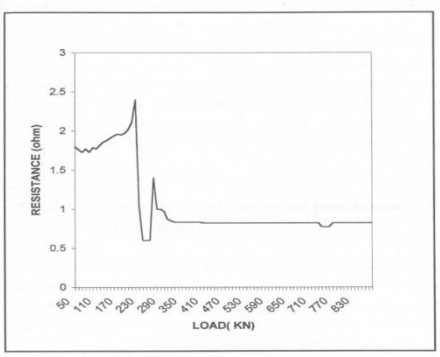

Figure 3: Resistance changes associated with Bi I-II and Bi II-III transitions at 30 0C.

Above figure 3 shows the Bi I-II and Bi II-III transitions at 30 0C at fixed point pressure for the calibration of pressure gauge.

Table 2: Recommended phase transitions for fixed pressure points.

Transition	Pressure (GPa)	Remarks
BiI-II	2.55±0.006	Midpoint of Hysteresis
BiII-III	5.5±0.010	Midpoint of Hysteresis
BiIII-IV	7.7±0.300	Change in the value of Resistance in its high pressure phase
BaI-II	5.5±0.200	Midpoint of Hysteresis
TlI-II	3.67±0.030	Midpoint of Hysteresis
Si	12.5±0.500	Confirmed by NaCl scale
ZnSe	13.7±0.300	Confirmed by NaCl scale
ZnS	15.0±0.500	Confirmed by NaCl scale
GaP	22.0±1.000	Confirmed by NaCl scale
NaCl	29.2±1.000	Confirmed by Ruby scale

Some widely accepted phase transitions recommended by various researchers are summarized in table 2. These values are widely accepted and used for calibration of several other pressure gauges.

3. Measurement of Electrical Resistance with Pressure

3.1 Experimental arrangement

The measurements of in–plane resistivity of MoS_2 and $MoSe_2$ single crystals were performed using Bridgman anvils pressed against each other by piston cylinder type hydraulic press. A photograph of the high-pressure hydraulic set-up is shown in figure 4. The Bridgman anvils consist of a tungsten carbide cylindrical piece, one face of which is ground in a tapered form ending with a flat anvil surface (culet). In a typical anvil, the anvil has a diameter of 100 mm, the WC cylinder is of 25 mm diameter with the culet surface of 11.2 mm diameter and the taper angle about 10^0. The anvil face experiences a high pressure but the material is heavily supported to prevent a failure of the material. Thus the anvil faces can support pressures in excess of 10 GPa. Typical anvil dimensions are depicted in figure 5.

Figure 4: Hydraulic press used to generate high pressure.

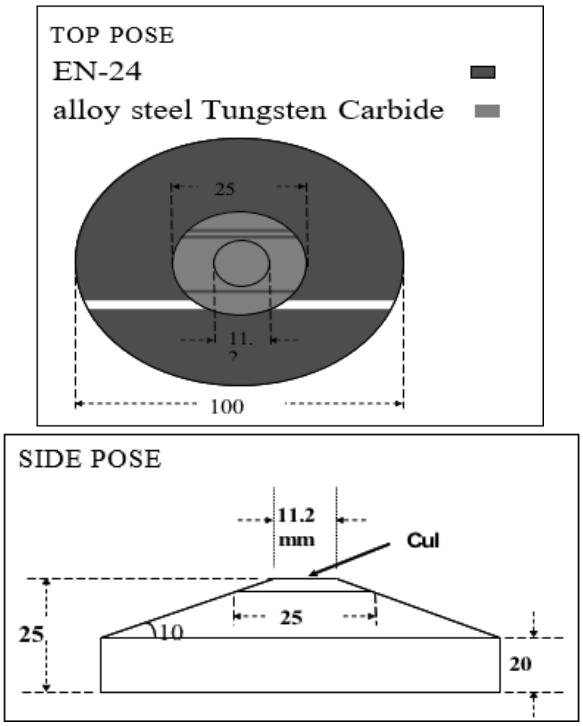

Figure 5: Typical anvil dimensions

Initially a pyrophellite gasket of ~150 µm thickness is fixed on the culet of anvil with epoxy. After that the crater inside the gasket is filled by putting a disc of pressure transmitting medium (talc). The sample is directly placed on this disc and four wires are drawn above it as shown in figure 6. Then another such gasketed anvil is placed on it. Whole assembly is pressed in a hydraulic press to generate high pressure. Generated pressure is measured by fixed pressure point scale utilizing pressure dependent electrical resistance of bismuth.

3.2 Anvils

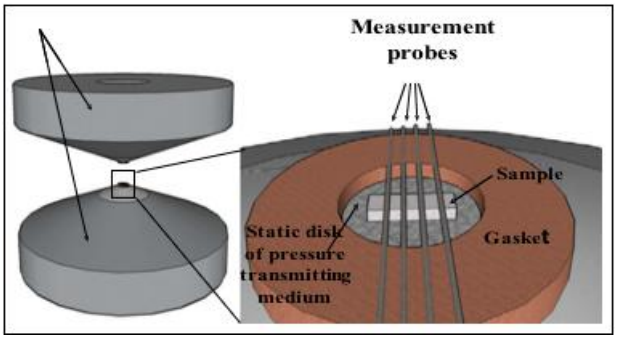

Figure 6: Arrangement of sample and probes in the pressure dependent electrical resistivity measurement system

Using described experimental arrangement four-probe resistivity measurements (As shown in Fig 7) were performed on single crystals grown by chemical vapor transport technique. All the measurements were performed at room temperature. Obtained results are plotted in figures 8 -9.

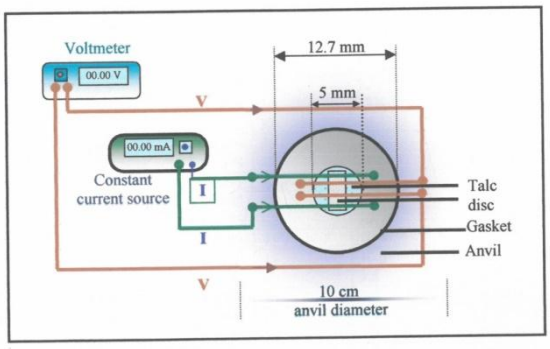

Figure 7: Schematic diagram of the four probe arrangement for the measurement of resistance as the function of pressure.

Table 3: Results of Resistance measurement of MoS_2 single crystal

Pressure 1 (kbar)	Resistance 1 (kΩ)	Log R1	Pressure 2 (kbar)	Resistance 2 (kΩ)	Log R2
0.0	29.3	1.4668	33.0	13.4	1.1271
1.0	28.6	1.4563	34.0	13.0	1.1139
2.0	28.3	1.4517	35.0	12.9	1.1105
3.0	27.6	1.4409	36.0	12.4	1.0934
4.0	26.5	1.4232	37.0	12.1	1.0827
5.0	26.0	1.4149	38.0	11.9	1.0755
6.0	25.7	1.4099	39.0	11.6	1.0644
7.0	24.5	1.3891	40.0	11.1	1.0453
8.0	24.0	1.3802	41.0	10.9	1.0374
9.0	23.9	1.3783	42.0	10.7	1.0293
10.0	22.6	1.3541	43.0	10.4	1.0171
11.0	22.3	1.3483	44.0	10.1	1.0043
12.0	22.0	1.3424	45.0	9.8	0.9912
13.0	19.9	1.2988	46.0	9.6	0.9822
14.0	19.5	1.29	47.0	9.4	0.9731
15.0	19.3	1.2855	48.0	9.2	0.9637
16.0	18.7	1.2718	49.0	9.0	0.9542
17.0	18.6	1.2695	50.0	8.9	0.9493
18.0	18.3	1.2624	51.0	8.7	0.9395
19.0	18.0	1.2552	52.0	8.3	0.919
20.0	17.9	1.2528	53.0	8.2	0.9138
21.0	17.1	1.2329	54.0	8.0	0.903
22.0	16.8	1.2253	55.0	7.7	0.8864
23.0	16.2	1.2095	56.0	7.5	0.875
24.0	15.8	1.1986	57.0	7.1	0.8512
25.0	15.5	1.1903	58.0	6.8	0.8325
26.0	15.0	1.176	59.0	6.5	0.8129
27.0	14.8	1.1643	60.0	6.2	0.7923
28.0	14.6	1.1553	61.0	6.0	0.7781
29.0	14.3	1.1492	62.0	5.7	0.7558
30.0	14.1	1.1461	63.0	5.4	0.7323
31.0	14.0	1.1367	64.0	5.1	0.7075
32.0	13.7	1.1367	65.0	5.0	0.6989

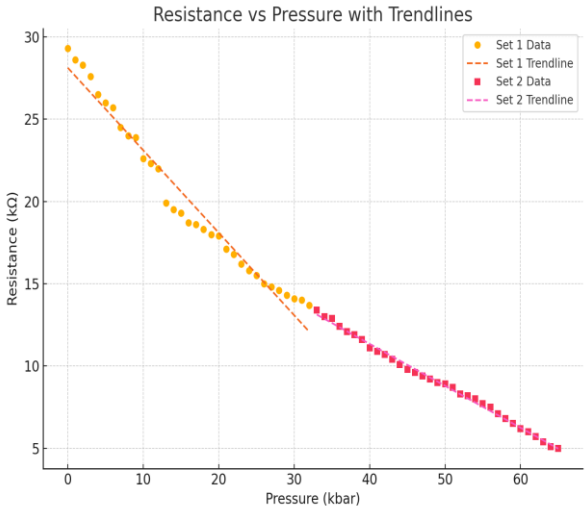

Figure 8: Resistance vs Pressure with trend lines for both data sets of MoS_2 single crystals.

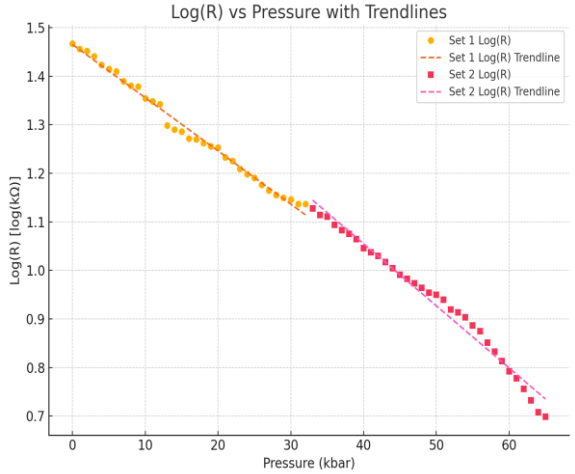

Figure 9: Log(R) vs Pressure with trend lines for both data sets of MoS_2 single crystals.

This graph presents the logarithmic scale of resistance (Log R) against applied pressure. Linear trend lines show how the resistance decreases logarithmically with increasing pressure.

Table 4: Results of Resistance measurement of $MoSe_2$ single crystal

Pressure (k bar)	Resistance (k ohm)	Log R	Pressure (k bar)	Resistance (k ohm)	Log R
0	62.85	1.4668	33	6.9	0.8388
1	60.01	1.4563	34	6.54	0.8155
2	58.6	1.4517	35	6.02	0.7795
3	54.5	1.4409	36	5.95	0.7745
4	51.2	1.4232	37	5.55	0.7442
5	49.3	1.4149	38	5.2	0.7160
6	47.2	1.4099	39	5.0	0.6989
7	45.4	1.3891	40	4.79	0.6803
8	41	1.3802	41	4.52	0.6551
9	38.57	1.3783	42	4.21	0.6242
10	34.56	1.3541	43	4.0	0.6020
11	28.54	1.3483	44	3.97	0.5987
12	25.6	1.4082	45	3.82	0.5879
13	23.8	1.3765	46	3.65	0.5820
14	20.7	1.3159	47	3.42	0.5622
15	18.95	1.2776	48	3.24	0.5340
16	15.06	1.1778	49	3.1	0.4913
17	13.3	1.2385	50	2.98	0.4742
18	12.56	1.0989	51	2.75	0.4393
19	12.01	1.0795	52	2.64	0.4216
20	11.85	1.0737	53	2.55	0.4065
21	11.02	1.0421	54	2.46	0.3909
22	10.08	1.0334	55	2.32	0.3654
23	10.02	1.0008	56	2.11	0.3242
24	9.87	0.9943	57	2.1	0.3222
25	9.5	0.9777	58	2.02	0.3053
26	8.95	0.9518	59	2.0	0.3010
27	8.54	0.9314	60	1.97	0.2944
28	8.03	0.9047	61	1.95	0.2900
29	7.08	0.8500	62	1.76	0.2455
30	7.04	0.8475	63	1.64	0.2148
31	7.01	0.8457	64	1.52	0.1818
32	6.98	0.8438	65	1.35	0.1303

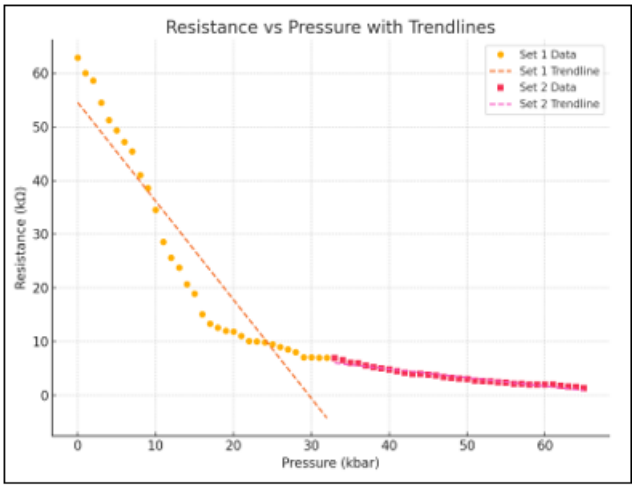

Figure 10: Resistance vs Pressure with trend lines for both data sets of $MoSe_2$ single crystals.

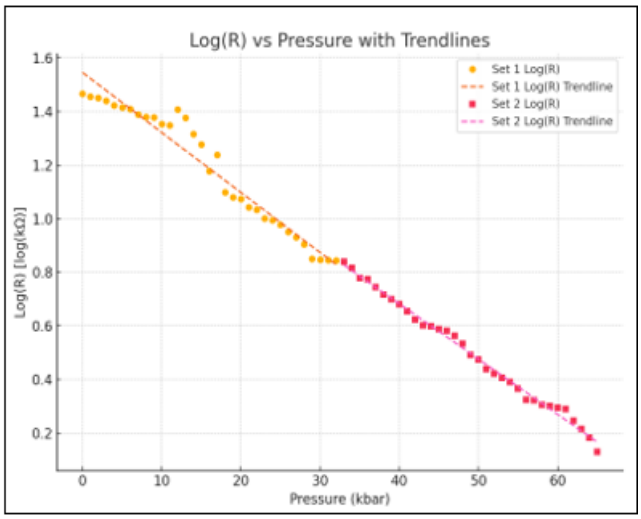

Figure 11: Log(R) vs Pressure with trend lines for both data sets of $MoSe_2$ single crystals.

From the graphical analysis, it is observed that both the resistance and its logarithmic transformation decrease monotonically with increasing pressure. This suggests a pressure-driven band gap narrowing or an increase in charge carrier mobility within the crystal structure. Such behavior is commonly observed in layered materials like MoS_2 or $MoSe_2$ under external compression. The linear trend lines further support a predictable modulation of electronic properties with pressure.

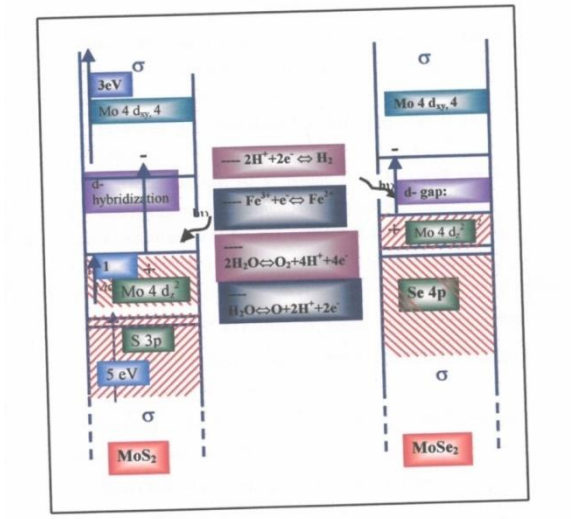

Figure 12: Energy Schemes & approximate energetic positions of MoS_2 and $MoSe_2$ Single Crystal.

4. Results and discussion

Analysis of the experimental data (Figures 8–12) reveals a consistent pressure-dependent trend in the electrical resistivity of MoS_2 and $MoSe_2$ single crystals. In the low-pressure regime, resistivity drops rapidly, while at higher pressures, this decrease becomes more gradual and follows a near-linear trend. This behavior suggests a pressure-induced transition in electronic structure, where the initial rapid decline corresponds to significant compression of the interlayer van der Waals gaps, enhancing charge carrier mobility.

The observed reduction in resistance with increasing pressure can be explained by considering the underlying band structure of these materials. In both MoS_2 and $MoSe_2$, the conduction and valence bands are separated by a relatively narrow bandgap—approximately 1.75 eV for MoS_2 and 1.4 eV for $MoSe_2$. Under hydrostatic pressure, this bandgap narrows due to increased orbital overlap, particularly between the chalcogen p-orbitals (S 3p and Se 4p) in the valence band and the molybdenum 4d orbitals in the conduction band. As a result, electrons from the valence band are more readily excited into the conduction band, thereby increasing conductivity.

Pressure affects both interlayer and intralayer interactions in layered TMDCs. The interlayer spacing, governed by weak van der Waals forces, compresses more readily than the covalently bonded intralayer structure. This reduction in spacing at lower pressures contributes significantly to the initial sharp decrease in resistance. At higher pressures, further compression leads to structural reorganization that enhances carrier delocalization and flattens the resistance-pressure curve.

The increase in carrier mobility can also be attributed to a transition from a predominantly two-dimensional transport mechanism to a more three-dimensional character under compression. This dimensional crossover enhances interlayer coupling and facilitates more efficient carrier transport. Moreover, density of states (DOS) calculations indicate that pressure shifts both the conduction band minimum (CBM) and valence band maximum (VBM) closer to the Fermi level. This shift reduces the energy barrier for electronic transitions and increases the availability of states near the Fermi level, further enhancing conductivity.

Orbital contributions to the CBM and VBM evolve with pressure. Specifically, the contribution of Mo-d and S/Se-p orbitals to the CBM decreases, while the involvement of S/Se-d orbitals increases. This orbital hybridization under pressure plays a crucial role in modifying the band structure and transport characteristics of these materials.

Furthermore, the experimental data suggest that continued application of pressure may eventually drive the system toward a metallic state. The trend of decreasing resistivity indicates enhanced metallic behavior, particularly in $MoSe_2$, which shows a more pronounced drop due to selenium's lower electronegativity and larger atomic radius compared to sulfur. This leads to stronger pressure-induced orbital overlap and more significant bandgap narrowing.

In conclusion, the pressure-dependent decrease in electrical resistivity observed in MoS_2 and $MoSe_2$ is a consequence of band structure modifications induced by enhanced interlayer coupling, orbital hybridization, and a reduction in bandgap. As pressure increases, the materials exhibit a transition from semiconducting to more metallic behavior. The sharper response in $MoSe_2$ compared to MoS_2 is consistent with differences in their electronic configurations and atomic properties. These findings highlight the tunability of electronic transport in TMDCs under hydrostatic pressure and their potential for pressure-sensitive electronic applications.

5. Comparison with Literature

The pressure-induced decrease in electrical resistivity observed in this study for MoS_2 and $MoSe_2$ is consistent with previously reported trends for layered transition metal dichalcogenides (TMDCs). Earlier work by Nayak et al. demonstrated a semiconductor-to-metal-like transition in multilayer MoS_2 under hydrostatic pressure, with a significant drop in resistance as the interlayer spacing decreased and the bandgap narrowed [11]. Similar behavior was also reported by Chi et al., where high-pressure X-ray diffraction and electrical measurements confirmed metallization in MoS_2 beyond 20 GPa due to structural and electronic changes in the crystal lattice [12].

For $MoSe_2$, pressure-dependent studies have shown a comparable trend, albeit with a more pronounced transition. The larger atomic radius and lower electronegativity of selenium compared to sulfur result in stronger pressure-induced orbital hybridization and bandgap narrowing. This observation is in agreement with findings by Gao et al., who reported that $MoSe_2$ undergoes a rapid change in conductivity under pressure, attributed to the closure of the indirect bandgap and evolution of electronic states near the Fermi level [26].

Theoretical calculations support these experimental results. Aksoy et al. reported that under increasing pressure, the conduction and valence bands of MoS_2 shift closer to the Fermi level, leading to enhanced electronic transport properties and eventual band overlap, signaling the onset of

metallicity [13]. First-principles density functional theory (DFT) calculations also predict significant reductions in the bandgap of TMDCs under compression, which corroborates the experimental resistivity trends observed in our study [27, 28].

In terms of magnitude, our measurements indicate a resistivity drop of nearly 80% in MoS_2 and over 95% in $MoSe_2$ up to 65 kbar, which falls within the range reported in prior high-pressure electrical transport studies. The sharp decline in resistivity at lower pressures, followed by a more gradual slope, aligns with the two-stage conductivity enhancement reported in both experimental and theoretical literature [29, 30].

Additionally, the increase in carrier mobility and transition to quasi-metallic behavior under high pressure parallels earlier interpretations by Livneh and Sterer, who highlighted the role of pressure-induced changes in electron-phonon coupling and lattice symmetry breaking in TMDCs [31].

Furthermore, high-pressure Raman and optical spectroscopy studies conducted by Livneh et al. and Nayak et al. provide evidence for the band structure evolution under compression, supporting our interpretation of the pressure-driven enhancement in conductivity [32, 33].

Therefore, the results obtained in this work not only validate existing high-pressure studies on MoS_2 and $MoSe_2$ but also extend the understanding of their resistive behavior up to higher pressure ranges using the Bridgman anvil technique. This comparison reinforces the applicability of hydrostatic pressure as a reversible and precise tuning parameter for tailoring the electronic transport properties of TMDC-based devices.

6. Conclusion

This study provides a comprehensive understanding of the electrical transport behavior of MoS_2 and $MoSe_2$ single crystals under hydrostatic pressure using the Bridgman anvil technique. The pressure-induced decline in resistivity indicates a clear transition from semiconducting to a quasi-metallic state, which is attributed to bandgap narrowing and increased orbital overlap. The enhanced interlayer interactions and orbital hybridization under compression significantly contribute to the observed conductivity enhancement.

$MoSe_2$ exhibits a more pronounced resistivity reduction than MoS_2, attributed to its larger atomic radius and lower electronegativity, which promote stronger orbital coupling under pressure. These results align with recent experimental and theoretical findings that highlight the tunable electronic properties of TMDCs via external stimuli such as strain and pressure [34–36]. The successful application of the Bridgman anvil device in this work underscores its utility in probing material behavior under extreme conditions. Overall, the findings affirm that pressure is a powerful tool for modulating the electronic structure and transport characteristics of layered semiconductors.

7. Applications

- The pressure-responsive behavior of MoS_2 and $MoSe_2$ opens up several promising applications:
- Pressure-Sensitive Electronics: The reversible tuning of resistivity under compression positions these TMDCs as strong candidates for high-performance pressure sensors and tunable resistors in next-generation electronics [37, 38].
- Flexible Nanoelectronics: Their mechanical flexibility and response to strain make them suitable for adaptive and wearable devices that require mechanical-to-electrical conversion functionalities [39].
- High-Pressure Optoelectronics: The observed bandgap tunability under pressure can be harnessed in photodetectors and modulators that function in variable environmental conditions [40].
- Earth and Planetary Simulation Studies: Due to their robustness under extreme conditions, these materials serve as analogs for simulating geophysical phenomena and exploring planetary materials science [41].
- Quantum and Memory Devices: Pressure-induced changes in electronic phases may enable development of memory elements and quantum switches based on phase-change characteristics in TMDCs [42].
- These applications underline the technological relevance of TMDCs in pressure-tunable and adaptive systems for electronics, sensing, and quantum technologies.

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