Single Layer MoS_2 under Direct Compression: Low Pressure Band-gap Engineering

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Abstract
Recently, the unique electronic properties of few layered transition metal dichalcogenides, such as MoS_2, have been revealed. Monolayer MoS_2 present a direct gap which evolves into an indirect one, as the number of layers increases [1]. Moreover, it has been observed that monolayer MoS_2 may turn into an indirect gap semiconductor itself by applying stress, and even transform into a semimetal if the strain is increased [2,3,4]. The regime of the deformation (uniaxial, biaxial, hydrostatic…) and its sign (tensile or compressive) governs the possibility of achieving such electronic transformations, as well as the level of strain required for achieving the changes. In this work, we subject monolayer MoS_2 samples to uniaxial compression along the *c* axis (up to 5 GPa), using a high pressure anvil cell, while monitoring the evolution of the samples with both Raman spectroscopy and photoluminescence measurements. From the evolution of the Raman frequencies of the normal modes with pressure we can distinguish three different electronic states: the direct and indirect gap semiconductor and the semimetal. But interestingly, and in contrast with previous works, the pressure levels required for observing these electronic changes are quite low and they are easily accessible under our experimental configuration: MoS_2 samples directly compressed between two hard materials. The change to indirect gap semiconductor is observed just by closing the gem anvil cell, at around 0.5 GPa, and the transition to semimetal is achieved when pressure is increased above 2 GPa. Such results were confirmed by means of theoretical calculations and photoluminescence measurements. The later also provided information about the reversibility of the electronic changes observed under pressure. The transition from direct to indirect semiconductor is a reversible process; however, once the semimetal state is reached the sample does not recover its semiconductor character after the pressure release. These results open new avenues for the application and development of optoelectronic devices based on these new materials of the family of molybdenum disulphide.
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References

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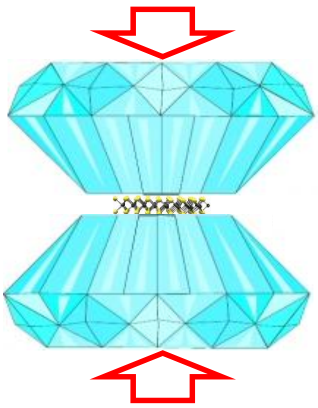
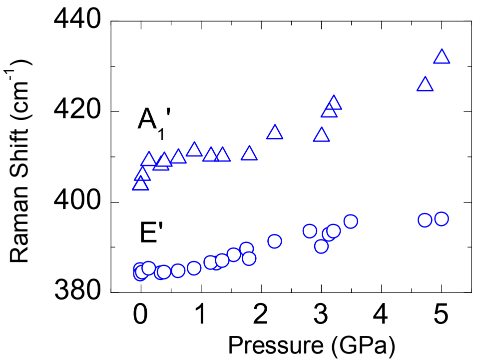
Figure





Schematic lateral view of a single layer MoS_2 directly compressed in a gem anvil cell.
Raman frequencies of the active normal modes of MoS_2 as a function of loading pressure.