Bandgap Engineering in strained bulk and monolayer MoS_2

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Abstract

Strain in nanomaterials, especially light emitting 2D materials, is often an important parameter to examine due to its potential for bandgap modulation [1], as well as causing change in photoluminescence efficiency [2]. This study focuses specifically on MoS_2, a layered chalcogenide material with a bandgap which changes from indirect to direct in character when reduced to the monolayer form. Although many properties of MoS_2 are well studied, the effect of strain on band gap has not been investigated in a systematic way. In this study, we performed density functional theory (DFT) calculations using the HSE06 functional including Grimme's D3 corrections for Van der Waals interactions to investigate the effect of both biaxial and uniaxial strains on band gap within this material. calculations were performed for both the bulk and monolayer systems, with strain along several different crystal directions considered for uniaxially strained monolayers. Figure 1 shows the band structure varies more rapidly with biaxially applied strain than for uniaxially applied strain. Variation in band gap was found to be independent of the strain direction; this was characterised by the gradient of the strain-band gap graphs – for both direct and indirect band gaps, see Table 1. Thus crystal orientation with respect to strain direction is not necessary to be considered for strain induced bandgap engineering. These theoretical results provide inspiration for optoelectronic applications based on strain, for example, tunable and highly efficient MoS_2 light emitters.

References

[1] Amitesh Maiti, *Nature Materials* 2 (2003), 440–442

[2] H. J. Conley et al, *Nano Lett.* 13, 8 (2013), 3626–3630

Figures

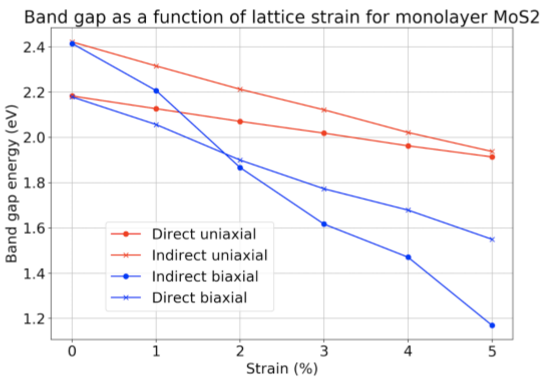

Figure 1: Band gap variation with applied strain for biaxial and uniaxial strain

Table 1: Gradients of the band gap-strain graph for various in plane uniaxial strain directions, with angle measured from one of the in plane lattice vectors

Strain angle (Degrees)	Direct gap Gradient (meV/% strain)	Indirect gap Gradient (meV/% strain)
0	-52.7±0.6	-95.3±0.2
15	-55.1±0.4	-98.9±0.2
60	-53.5±0.4	-96.2±0.1
90	-57.2±0.1	-100.0±0.2