Lattice dynamics in bulk tungsten diselenide (WSe_2)

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Tungsten diselenide (WSe_2) belongs to a large group of layered transition metal dichalcogenides (LTMDs). Such materials, which exhibit unique and fascinating physical properties that result from the 3D to 2D transition, have recently attracted a great deal of attention. WSe_2 is an inorganic compound with hexagonal crystalline structure similar to molybdenum disulfide. As other LTMDs, it shows a weak interlayer van der Waals bonding and strong intralayer ionic-covalent bonding. A single layer of this material consists of one plane of tungsten atoms sandwiched between two planes of selenium atoms and is a direct-gap semiconductor with a band gap of around 1.4 eV [1]. WSe_2 has found numerous practical applications, such as photoelectrodes in electrochemical solar cells [2] or as transparent photovoltaic devices and ultra-thin LEDs [3].

In this communication, we report our research on the optical properties of bulk synthesized WSe_2 crystals, thinned down by exfoliation with a high-quality backgrinding tape and transferred onto a Si/SiO_2 substrate with the aid of an all-dry, non-deterministic, polydimethylsiloxan-based stamping technique [4]. We found such an approach to be especially well suited for cleaving LTMDs, which as compared to graphite are much more brittle, and thus turning them into a form of thin flakes with an area that is sufficient to be probed with a laser beam, represents a challenging task. The optical properties of samples prepared in this way were next studied by micro-Raman spectroscopy.

The Raman scattering measurements have been carried out in two excitation modes: a resonant (λ=632.8 nm) and an off-resonant (λ=532 nm). Both in the off-resonance and in-resonance spectra (see Fig. 1) the peaks due to the first- and second-order Raman scattering processes can be seen. The most intensive ones centred at ~249 and ~256 cm^{-1} are assigned to the first-order A_{1g} and the second-order 2LA(M) mode. Detailed analysis of the latter peak's line shape suggests its bimodal character. The possible attribution of an additional component of this peak is discussed. The peaks at ~373 cm^{-1} and ~395 cm^{-1} can be assigned to the second-order processes: $E_{2g}^{1}(M)$+LA(M) and $A_{1g}(M)$+LA(M), respectively. Moreover, in the non-resonantly excited spectrum we observe two more peaks denoted by arrows, which identification is also the subject of discussion.

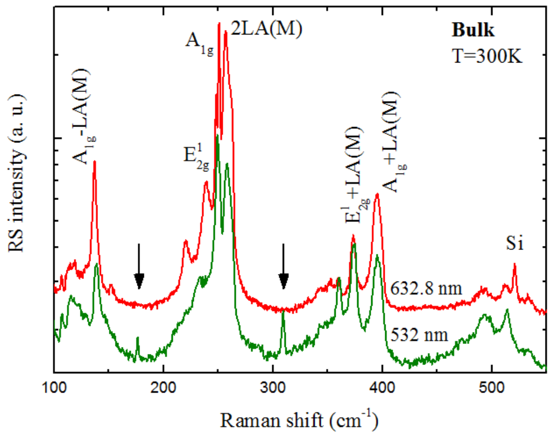

Figure 1. Raman spectra of bulk WSe_2 in two excitation modes: a resonant (top curve) and an off-resonant (bottom curve).

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