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Investigation of cyclotron-phonon resonance in monolayer molybdenum disulfide

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ABSTRACT

Transition-metal dichalcogenide monolayers recently have attracted much attention motivated by their exotic physical properties. In this paper, we theoretically investigate the optical absorption in the monolayer MoS_2 which is subjected to a uniform static magnetic field and an electromagnetic wave. The magneto-optical absorption power (MOAP) is calculated using the projection operator technique in the linear response scheme, taking account of the electron–optical phonon interaction at high temperature. Both phonon emission and phonon absorption processes are included. The cyclotron–phonon resonance (CPR) is observed in the photon energy dependence of the MOAP. Numerical analyses show that the photon energy satisfying CPR condition depends linearly on the strength of magnetic field, which is similar to that in conventional low-dimensional semiconductors but different from that in graphene. The increase of the full width at half maximum (FWHM) of CPR peaks with increasing magnetic field shows a similar behaviour to that in graphene. In addition, FWHM increases slightly with temperature, which is different from that in graphene where the FWHM is temperature independent. Our investigation provides basic information about the magneto-optical properties of the monolayer MoS_2 that are useful for further experiments and applications.

1. Introduction

The discovery of graphene about a decade ago marked the beginning of the era of atomic monolayers and their heterostructures. These novel two-dimensional (2D) materials possess numerous exotic physical properties not found in conventional low-dimensional structures, making them potential candidates for future nano-electronic devices. For example, the carriers in a single-layer graphene are massless Dirac fermions moving at very high speed, about 1/300 of the speed of light [1–3]. This results in a very high carrier mobility in graphene, about 2.10^5 cm^2/V.s at room temperature [3]. However, graphene can not be implemented in optoelectronic devices as it is because of the lack of its band gap. Therefore, in parallel with studying and developing graphene-based applications, researchers have been investigating novel layered materials and their heterostructures [4–17], each structure having its own physical characteristics, suitable for specific applications. A typical example of graphene-like 2D family is transition-metal dichalcogenide (TMD) monolayers having formula MX_2 with M and X being, respectively, a transition metal (Mo, W) and a dichalcogenide (S, Se, Te) element. In general, TMD monolayers have a specified band gap, overcoming the disadvantage of the single-layer graphene whose band gap is zero. One of the first TMD monolayers to be successfully created and widely studied was molybdenum disulfide (MoS_2) monolayers. The monolayer MoS_2 has a high on/off current ratio () [18] and high carrier mobility of ~ 200 cm^2/V.s at room temperature [19,20] allowing it a potential material for novel field-effect transistors (FETs) and

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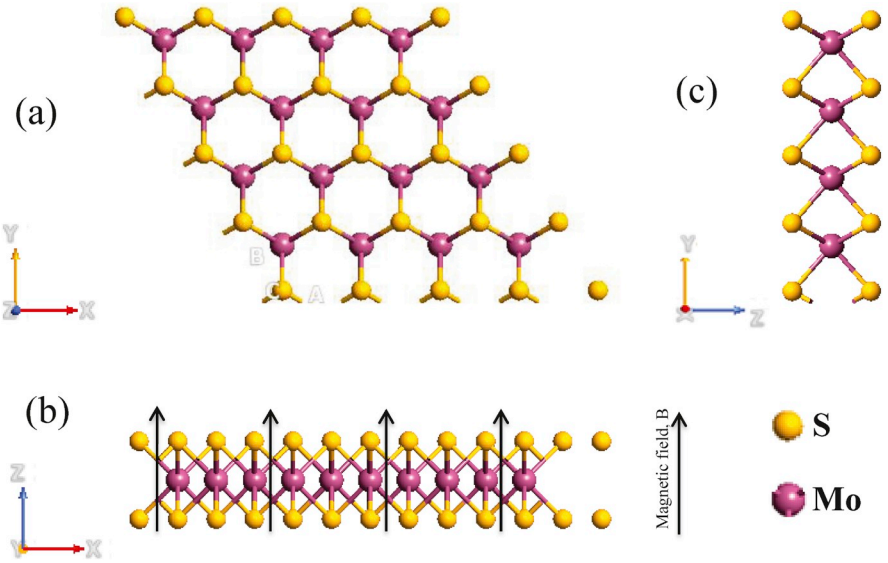

Fig. 1. The atomic structure of MoS_2 monolayer with the top view (a) and side views (b, c). Mo and S atoms are modeled, respectively, by the violet and yellow balls. Fig. 1(b) shows the MoS_2 monolayer in a uniform static magnetic field which is considered in the present calculation.

photodetectors. In addition, the MoS_2 monolayer is a buckling structure in which Mo atoms and S atoms do not locate in the same plane as shown in Fig. 1. This asymmetric arrangement opens a finite energy band gap of ~ 1.8 eV in the material at the equilibrium state [21]. Moreover, this band gap can be adjusted by changing some parameters such as strain, applied electric field, layer thickness, and so on. The asymmetry over its plane also leads to the strong spin-orbit interaction in MoS_2 which opens possible applications to spintronics.

Studying of resonant effects related to interaction of carriers, such as electron–phonon, electron–impurity interaction leads to structural information of the materials including the carrier effective mass, the distance between energy subbands, the phonon energy, and so on. Therefore, resonant effects such as magnetophonon resonance, cyclotron resonance in bulk materials in general, and in low-dimensional structures in particular, have been numerously investigated for the past decades [22–35]. Theoretically, up to date there has been no formula determining the full width at half maximum (FWHM) or half width at half maximum (HWHM) of a resonant peak. It has been shown by T. C. Phong and co-workers that the FWHM/HWHM can be extracted from the graph describing the dependence of absorption power (AP) or absorption coefficient (AC) on the photon energy. In their works, the authors proposed the so-called profile method to determine the FWHM/HWHM by computational program. The obtained results are consistent with previous theoretical predictions and available measurements [36]– [40]. Recently, some theoretical studies on the transport properties in MoS_2 monolayers in external electromagnetic fields have been carried out [18,41–43]. By using a direct relation between the absorption coefficient and transition probability of 2D electrons, Bhargavi et al. [18] calculated the optical AC in an *n*-type monolayer MoS_2 and other TMDs, taking account of the piezoelectric (PE) and deformation potential (DP) electron–acoustic phonon coupling regime. The results show that for both unscreened PE and DP coupling regime, the absorption coefficient is independent on the carrier effective mass. This behaviour is different from that in bulk semiconductors. In the work by Wang and Lei [41], the authors studied the linear magnetotransport in a monolayer MoS_2 by calculating the magnetoresistance for electron–phonon and electron–impurity interactions at high and low temperatures, respectively. The spin-orbit interaction was also included. The Shubnikov de Haas (SdH) oscillations were observed at low temperature. At high temperature, both optical phonons and acoustic phonons contribute to the magnetophonon resonances which emerge for a suspended system with high mobility. Moreover, for the electron–optical phonon (OP) interaction, a beating pattern of magnetophonon resonance was observed. In another work [42] Tahir et al. used linear response formulae to calculate the longitudinal and Hall conductivity/resistivity in a MoS_2 monolayer subjected to a perpendicular magnetic field (B). The spin and valley Zeeman effects were taken into account. The authors showed that these effects lead to new quantum Hall plateaux and new peaks in the dependence of the longitudinal resistivity on magnetic field. The presence of magnetic field results in a significant enhancement of the spin splitting as well as in a beating of the SdH oscillations at low B. The spin and valley polarisations were also investigated for the magnetic field up to 30 T. At low fields, the spin and valley polarisation show a similar behaviour whereas they are strongly separated in high-field regime. Very recently, Chuong et al. [43] have studied theoretically transport properties of a monolayer MoS_2 laid on some polar substrates in a perpendicular B and a light wave. The authors calculated the magneto-optical AC by including interaction of carriers with intrinsic acoustic and optical phonons, and surface optical phonons induced by the polar substrates. The FWHM was shown to increase with increasing magnetic field. Also, the effects of different substrates on the AC and the FWHM were compared and discussed in details. However, to our knowledge, experimental measurements of the cyclotron resonance line-width in MoS_2 monolayers have not yet been carried out. Therefore, systematic studies on the optical absorption and FWHM in this structure using different methods are currently necessary for future experiments and applications.

In this work, we investigate the magneto-optical absorption in MoS2 monolayers stimulated simultaneously by a perpendicular static magnetic field and an electromagnetic wave (EMW). By using projection operator technique, we calculate the AP taking account of the electron–OP interaction at high temperature. Both phonon emission and phonon absorption processes are considered. The AP is numerically evaluated and plotted to clarify resonant effects from absorption spectra. The paper is organised as follows. In Sec. 2, we introduce the theoretical model and basic formulae for the calculation. The brief derivation of the AP for electron–OP interaction is introduced in Sec. 3. Sec. 4 presents the numerical results and discussion. Finally, the main conclusions are shown in Sec. 5.

2. Basic formulation

In this calculation, we deal with a monolayer MoS_2 crystal with its