ARTICLES

Journal of Semiconductors
(2021) 42, 082002
doi: 10.1088/1674-4926/42/8/082002

Extensive study of optical contrast between bulk and nanoscale transition metal dichalcogenide semiconductors

Ankush Parmar[1], Jashangeet Kaur[2, †], Manish Dev Sharma[1], and Navdeep Goyal[1]

[1]Centre of Applied Sciences, Department of Physics, Sector-14, Panjab University, Chandigarh, 160014, India
[2]Department of Physics, G.G.D.S.D College, Sector-32, Chandigarh, 160030, India

Abstract: A remarkable refinement in the optical behavior of two-dimensional transition metal dichalcogenides (TMDs) has been brought to light when cleaved from their respective bulks. These atomically thin direct bandgap semiconductors are highly responsive to optical energy which proposes the route for futuristic photonic devices. In this manuscript, we have substantially focused on the optical study of MoS_2 and WS_2 nanosheets and comparative analysis with their bulk counterparts. The synthesis of nanosheets has been accomplished with liquid exfoliation followed by fabrication of thin films with drop-casting technique. X-ray diffraction and field emission scanning electron microscopy affirmed the morphology, whereas, UV–visible spectroscopy served as the primary tool for optical analysis. It was observed that several parameters, like optical conductivity, optical band-gap energy etc. have enhanced statistics in the case of exfoliated nanosheets as compared to their respective bulks. Some researchers have touched upon this analysis for MoS_2, but it is completely novel for WS_2. We expect our work to clearly distinguish between the optical behaviors of nanoscale and bulk TMDs so as to intensify and strengthen the research related to 2D-layered materials for optoelectronic and photovoltaic applications.

Key words: transition metal dichalcogenides; 2D layered materials; optical properties; liquid phase exfoliation; thin films; drop-casting

Citation: A Parmar, J Kaur, M D Sharma, and N Goyal, Extensive study of optical contrast between bulk and nanoscale transition metal dichalcogenide semiconductors[J]. *J. Semicond.*, 2021, 42(8), 082002. http://doi.org/10.1088/1674-4926/42/8/082002

SUPPORTING INFORMATION

FESEM

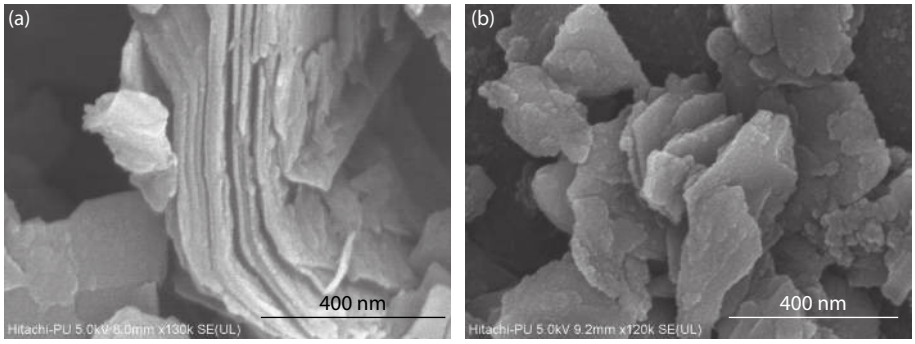

Fig. S1. FESEM images of (a) W_bulk and (b) W_exfoliated samples.

Optical conductivity

The optical conductivity (σ_{opt}) has been calculated using Eq. (11). In MoS_2 samples, σ_{opt} rises with increasing energy. In the visible region (lower energy), the spectra reveals maximas of conductivity which are blue shifted (shifted towards higher energy) for M_exfoliated samples as compared to M_bulk samples (see Fig. S2(a)). These peaks are at selective energies due to the fact that, at these energies, the incident photons have induced greater excitation of electrons in the sample. In the higher energy or ultraviolet region of incident spectrum, nanosheet thin films are more optically conducting than the bulk films. Moving to WS_2 samples, the bulk WS_2 doesn't show much variation in conductivity but in exfoliated WS_2 there are peaks in the spectrum just like M_exfoliated samples (Fig. S2(b)).

Correspondence to: J Kaur, jashan2191@yahoo.com
Received 10 MARCH 2021; Revised 26 MARCH 2021.

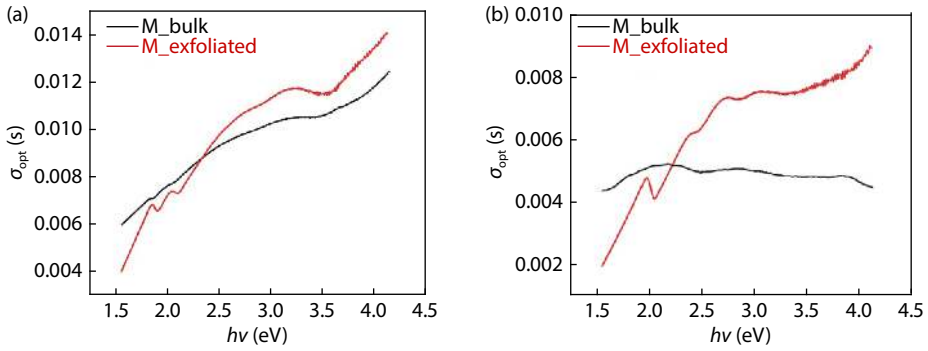

Fig. S2. Plot of optical conductivity (σ_{opt}) with incident energy (hv) for (a) M_bulk, M_exfoliated and (b) W_bulk, W_exfoliated.

Optical density & skin depth

As optical density is directly proportional to α(see Eq. 10), maximum density is achieved at energies of inter-band optical transitions as shown in Fig. S3. Skin depth is basically a measure of penetration of radiation into the thin film. Mathematically, it is just the reciprocal of absorption coefficient (Eq. 9). Looking at the variation of skin depth with wavelength for our samples in Fig. S4, the penetration minimizes at the wavelengths corresponding to inter-band transitions or excitonic peaks. This is because at these points, the absorption coefficient maximizes and the electromagnetic radiation gets absorbed and therefore, the skin depth drops.

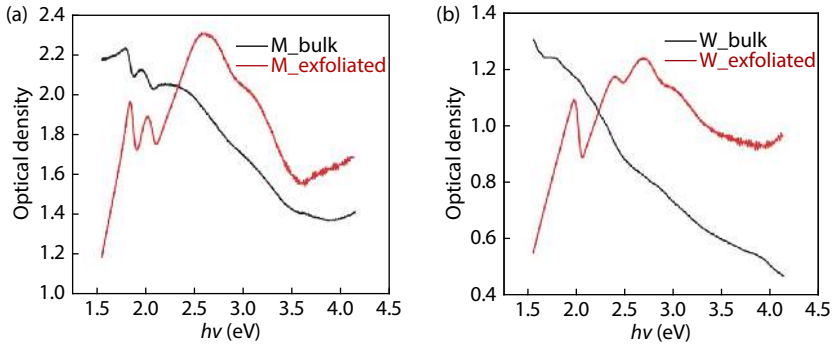

Fig. S3. Variation of optical density with incident energy (hv) for (a) M_bulk, M_exfoliated and (b) W_bulk, W_exfoliated.

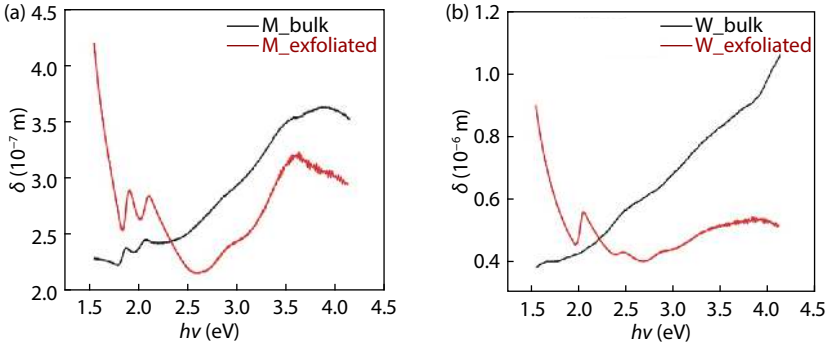

Fig. S4. Plot of skin depth (δ) vs incident energy (*hv*) for (a) M_bulk, M_exfoliated and (b) W_bulk, W_exfoliated.

Urbach Energy (E_u)

To derive the structural order in the samples, Urbach Energy (E_u) plays an important role as described in theory. The obtained values for all the samples are listed in Table 1. From the table, E_u is higher for the bulk samples as compared to their respective nanosheets. This implies that the nanosheets obtained after liquid exfoliation are more ordered. This reconfirms the XRD results in which we observed that the M_exfoliated and W_exfioliated samples are oriented in a single crystalline phase (002), whereas, the XRD patterns of M_bulk and W_bulk consisted of various phases. Therefore, there is more order in the obtained nanosheets of MoS_2 and WS_2.

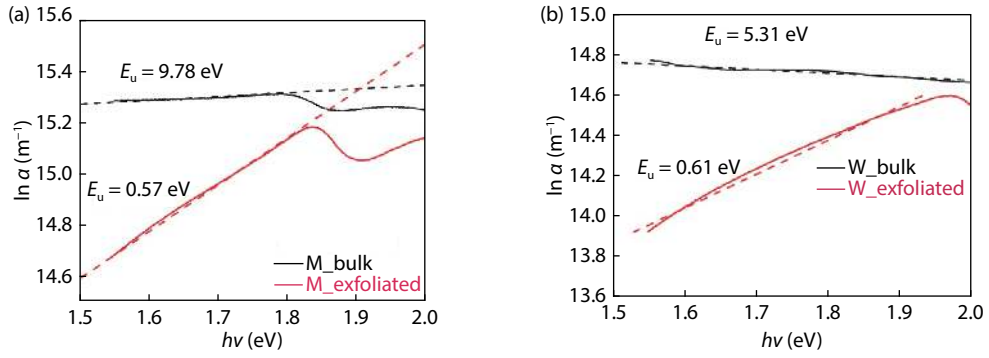

Fig. S5. Plot of urbach energy (E_u) with incident energy ($h\nu$) for (a) M_bulk, M_exfoliated and (b) W_bulk, W_exfoliated.

Single Sellmeier Model (SSM)

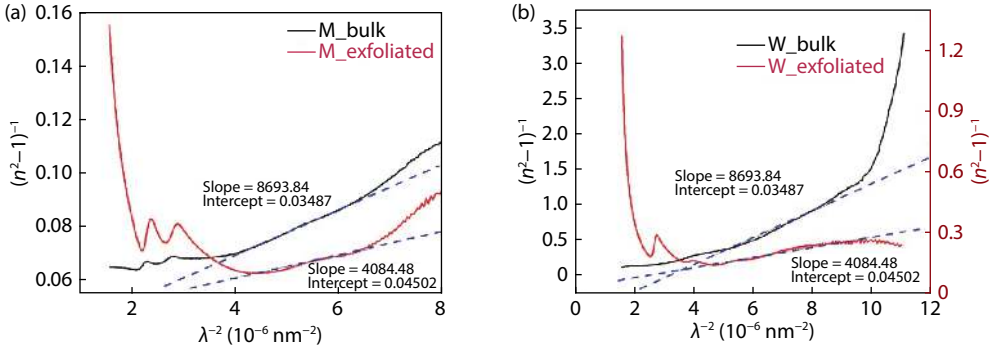

Fig. S6. Plot of $(n^2-1)^{-1}$ v/s λ^{-2} for (a) M_bulk, M_exfoliated and (b) W_bulk, W_exfoliated.