Electronic Supplementary Material (ESI) for Nanoscale.

Supplementary Information: InSe: a two-dimensional semiconductor with superior flexibility

Qinghua Zhao,[a,b,c] Riccardo Frisenda,[*c] Tao Wang[*a,b] and Andres Castellanos-Gomez[*c]

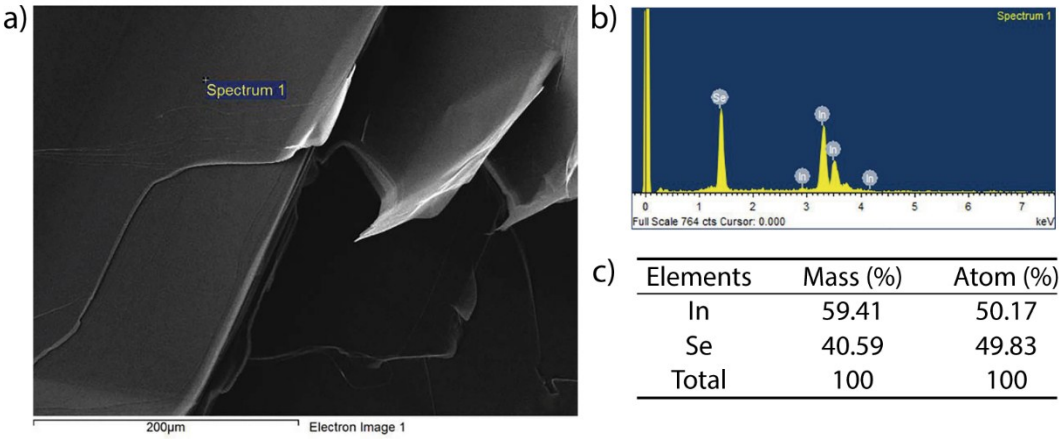
[a] State Key Laboratory of Solidification Processing, Northwestern Polytechnical University, Xi'an, 710072, P. R. China

[b] Key Laboratory of Radiation Detection Materials and Devices, Ministry of Industry and Information Technology, Xi'an, 710072, P. R. China

[c] Materials Science Factory. Instituto de Ciencia de Materiales de Madrid (ICMM-CSIC), Madrid, E-28049, Spain.

*E-mail: andres.castellanos@csic.es, riccardo.frisenda@csic.es, taowang@nwpu.edu.cn

Section 1: Characterization of Bulk InSe crystals



c)

Elements	Mass (%)	Atom (%)
In	59.41	50.17
Se	40.59	49.83
Total	100	100

Figure S1: The scanning electron microscopy (SEM) characterization of InSe bulks. a) The surface morphology of mechanical cleavage plane of InSe. b) The energy dispersive spectrum (EDS) of the position marked with Spectrum 1 in panel a. c) The composition of InSe bulks gotten from EDS result. The atomic ratio In:Se ≈ 1:1.

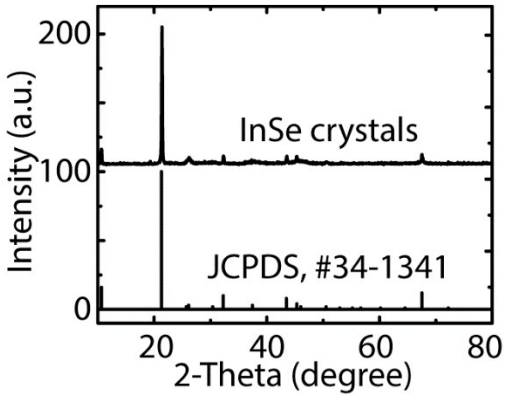


Figure S2: The X-ray diffraction (XRD) characterization of InSe crystals. The comparison between XRD spectrum of InSe crystals indicates a high agreement with the hexagonal InSe phase (JCPDS, card no. 34-1341).

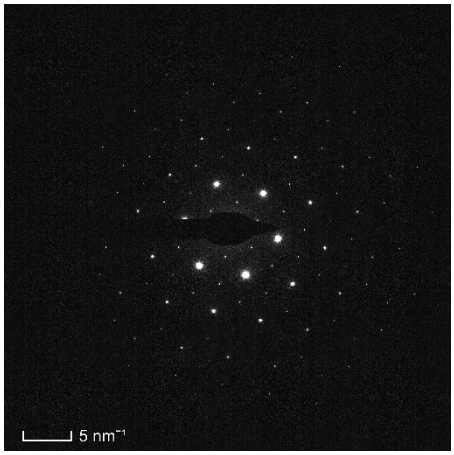


Figure S3: The electron diffraction pattern of InSe crystals by transmission electron microscopy (TEM).

Section 2: Atomic force microscopy (AFM) thickness measurements of few layer InSe

In order to estimate the thickness of InSe we used the AFM in dynamic mode to record the topography of the various InSe flakes deposited onto SiO_2/Si. It is known from literature that dynamic mode AFM may induce an offset in the absolute thickness of 2D materials, because of the different tip interaction the 2D flake and the substrate and the eventual presence of adsorbate layers. This effect has been observed in previously in graphene and few-layer graphite.[1, 2] In order to estimate the offset present in our AFM measurements we combine the information from optical absorption (defined as 1-transmission) of InSe and the wavelength of the wrinkle in this material. Both these quantities are expected to depend linearly on the thickness (for the absorption this is only valid in the small thickness regime) and to go to zero in the case of zero thickness. Figure S4 shows the wrinkle wavelength (left) and the absorption (right) of all the InSe flakes studied in this work plotted as a function of the flake height measured by the AFM. In both cases a linear relation is present between the data points and the height as can be seen from the good quality of the linear fit. From these two plots one can extract the offset by extrapolating the intercept between the fitted curve and the x-axis. We find an offset of 4.9 ± 0.5 nm.

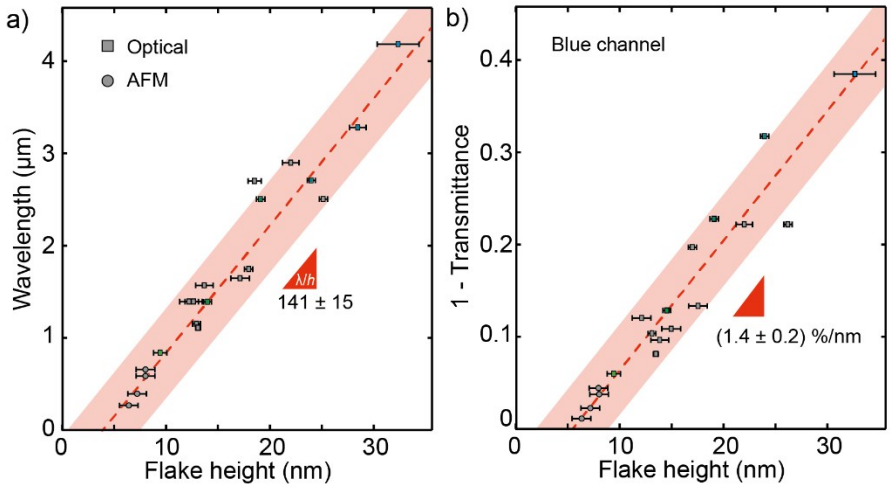


Figure S4. a-b) Wavelength of the wrinkles (a) and optical absorption in the blue channel (b) as a function of the flake height obtained by AFM. The dashed red line is a linear fit to the data and the shaded region represents the 95% confidence bands.

Figure S5 shows an example of a few-layer thin InSe flake. The top left panel shows an optical picture of a wrinkled InSe flake deposited onto PDMS recorded in reflection illumination mode. The top right panel shows the transmission microscope image, one can appreciate how in this case the thin part of the InSe flake is highly transparent. In the bottom left panel we show the intensity of the blue channel of the transmission image mentioned above. The arrows indicate the position of the shown blue channel transmission line profiles. The step height in blue channel transmission is ~1.4% (for MoS_2 this value is 7% and for graphene 2.3%). In the bottom right panel there is reported the AFM phase topology, from which we extract the wavelength of the ripples in the ultra-thin regions. Notice that the wrinkles (with wavelength < 800 nm) in the thinnest regions, which are visible in the AFM image, could not be observed optically.

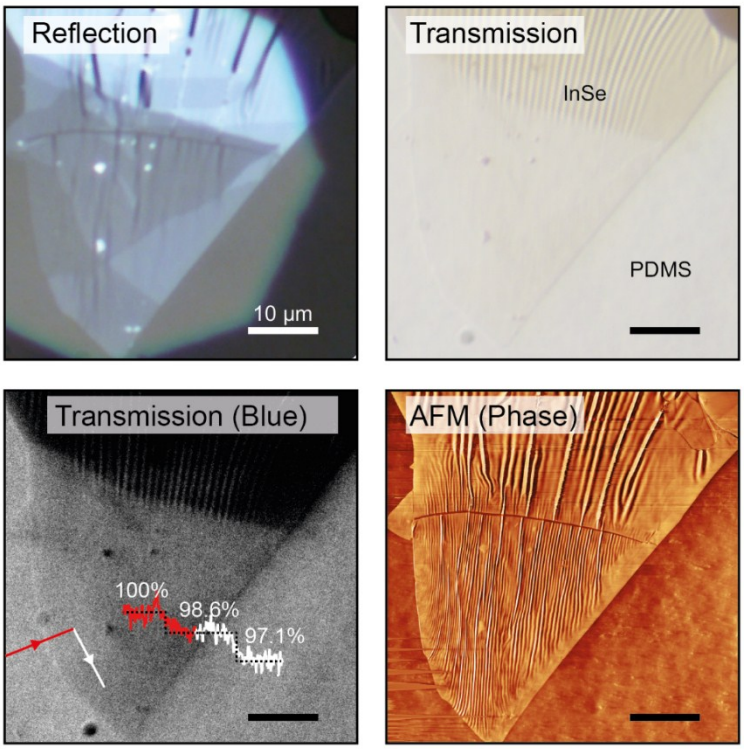


Figure S5. Optical pictures of a wrinkled InSe flake deposited onto PDMS in reflection illumination mode (top left) and transmission (top right). Bottom left: intensity of the blue channel of the transmission image. The line with arrows indicate the position of the shown line profiles. Bottom right: AFM phase topology. Notice that the wrinkles (with wavelength < 800 nm) in the thinnest regions, which are visible in the AFM image, could not be observed optically.

Section 3: Strain **transfer simulation by finite element analysis (FEA)**

The simulation of the strain transfer between a substrate and a 2D flake deposited on top has been carried out in COMSOL. The solver that was used in COMSOL is MUMPS (MUltifrontal Massively Parallel Sparse direct Solver). To model the system composed of a three-dimensional substrate and an atomically thin flake, we use in our simulation a geometry with a very large aspect-ratio. We model the system in a axisymmetric representation, the substrate is modelled with a cylinder (height 1000 µm, diameter 10000 µm) and the flake by a cylinder (height 10 nm, diameter 20 µm) located in the centre of the substrate. The complete mesh consists of 72214 elements (Minimum quality: 0.335, average quality: 0.9758). Figure S6 shows some cross sections of the model with superimposed the mesh elements and Figure S7 shows the three dimensional visualization of the model.

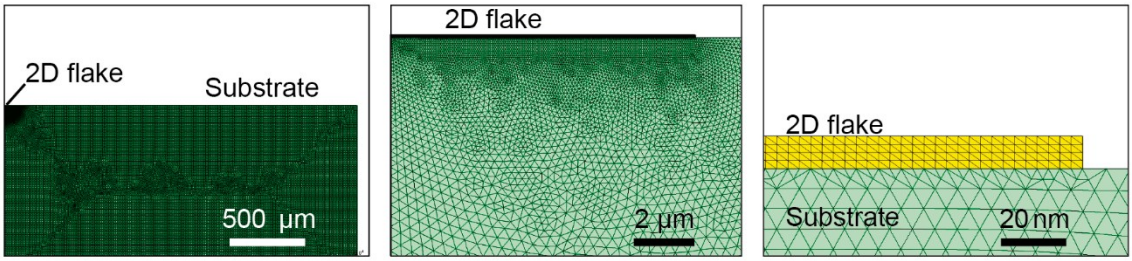


Figure S6. Pictures of the axisymmetric geometry used in COMSOL to simulate the strain transfer from a substrate (green) to a flake deposited on top (yellow) taken at different magnifications.

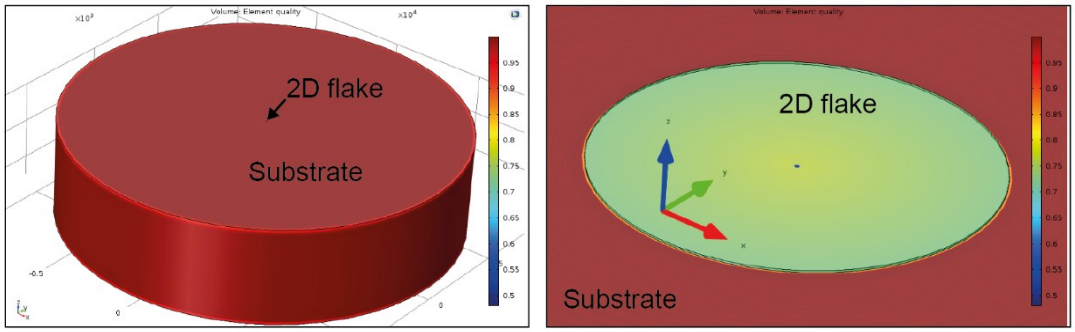


Figure S7. Pictures of the final 3D geometry used in COMSOL to simulate the strain transfer from a substrate to a flake deposited on top taken at two different magnifications.

In the calculation reported in the main text we used a substrate thickness of 1000 µm. To check that this thickness does not influence the results obtained, we performed various simulations varying the thickness (from 10 µm to 10000 µm) of the substrate and we extracted the amount of strain transferred to the deposited flake. Figure S8 shows the strain transferred to the flake as a function of the thickness of the substrate (for different values of the substrate Young's modulus).

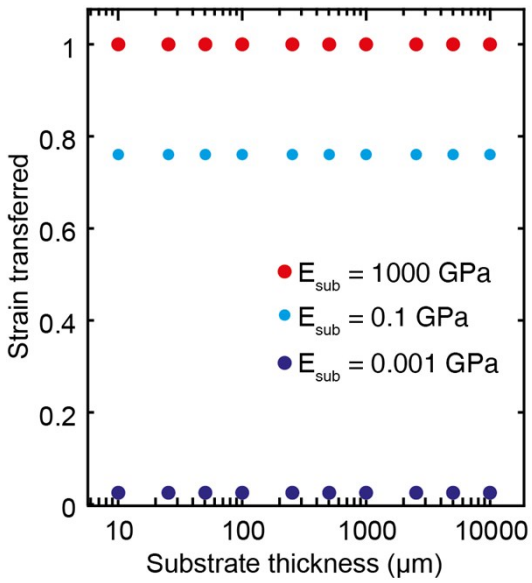


Figure S8. Finite element analysis simulation of the strain transferred to a 10 nm thick InSe flake as a function of the thickness of the substrate for different values of the substrate Young's modulus.

References

1. C. J. Shearer, A. D. Slattery, A. J. Stapleton, J. G. Shapter and C. T. Gibson, *Nanotechnology*, 2016, **27**, 125704.
2. P. Nemes-Incze, Z. Osváth, K. Kamarás and L. Biró, *Carbon*, 2008, **46**, 1435-1442.