Strategies for characterization of defect states and long-term stability of materials and devices including III-V and 2D materials

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III-V AND 2D MATERIALS WITH DEFECTS

Semiconductor materials other than Si, including III-V materials and 2-dimensional (2D) materials have been extensively investigated, especially graphene won the Nobel prize.[1-3] There are specialties of 2D materials which are regarded to be possible to potentially lead to a lot of applications. However, some severe problems as their main challenges must be addressed before their production and applications on integrated circuits (IC) which require high reliability, high yield and high performance. Among the problems, the poor stability, low carrier mobility and low conductivity, are all related to the defects, especially defect-related density of states below the bandgap , i.e., subgap density of states(DOS).[2,4] Therefore, the precise characterization of DOS is needed to improve the quality, performance and stability of III-V materials and 2D material devices.[2,4,5] DOS could enhance both the stability issue and the carrier mobility. Characterizing the density of states (DOS) to predict trade-off conditions is necessary before these 2D materials can be practical for deployment. In one word, a precise characterization of DOS is a prerequisite for the above study to improve materials.

2D materials refer to the films that basically consist of monolayer or few-layer materials with the nanometer scale length (1 nm) in the vertical direction.[2] Their special structures enable them to present special characteristics. As suggested in Figure 1A, the characteristics of 2D materials have stimulated their wide investigation and emergence. At first, the nanoscale thicknesses enable them to help extending the miniaturization restriction of optoelectronic and electronic devices. These attributes render them suitable for applications in field-effect transistors (FETs) and in the construction of sensors.[2] Besides, with 2D structures, the Coulomb screening could be reduced largely, which would enlarge many-body interactions including one order of magnitude stronger Coulomb interaction between holes and electrons in 2D materials than that in three-dimensional (3D) materials.[2] The lifetime of interlayer excitons would be increased, attributed to the stronger Coulomb binding. The observation of excitonic quantum behaviors long sought on quantum wells, including excitonic Bose-Einstein condensation, superfluidity, and electron-hole liquid, not only at room temperature, but also at high temperature. What's more, quasiparticles in 2D materials, such as spin, orbital, valley, layer and topology, have diverse degrees of freedom, which could interact with one another or with external fields to lead to different states and uses. The applications include valley-Hall transistors that employ valley-selective circular dichroism and spin-valley-coupled transport in transition metal dichalcogenides. Quantum devices with 2D quantum states have been proposed due to the interplay of symmetry and topology of 2D materials.[2]

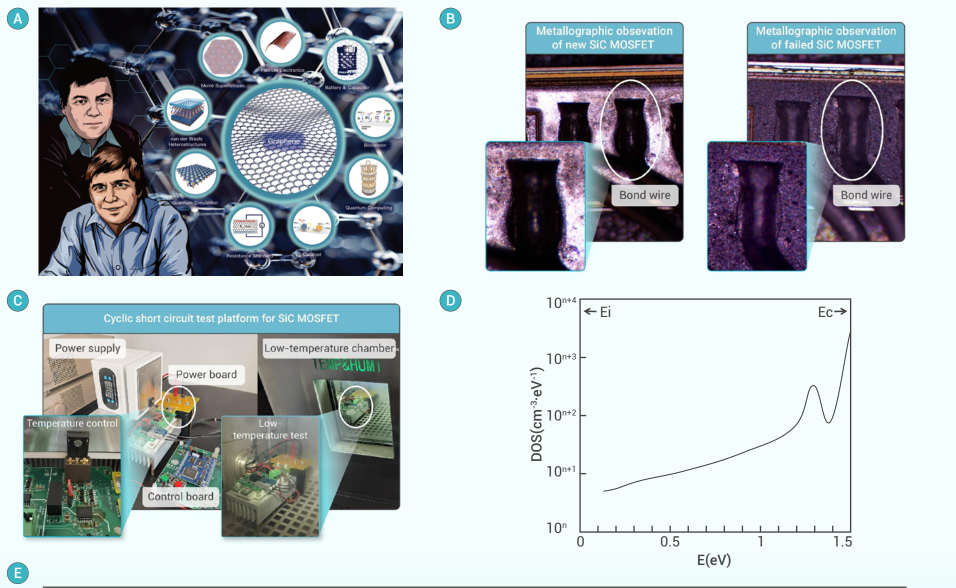
Mainly 4 great problems and challenges have to be solved, which persist at present. Initially, a lot of 2D materials have terrible stability properties, which limit their applications. In addition, single-layer 2D materials present low carrier mobilities and absorption rates, which restrict their optoelectronics/optics and electronics. Moreover, partly because of the localized orbitals, magnetic interaction and conductivities of 2D materials are low. Last but not least, extensive research efforts need to be performed because 2D materials processing with low contamination and cost but controllable integration and quality, as well as compatibility with the foundry process are needed. [2]

There are methods being proposed to face these above challenges for 2D materials with good qualities, controllability, conductivity and stability. For instance, atomic layer deposition (ALD) can be adopted to suppress material defects.[4] Different processing and measurement conditions could lead to different film profiles and properties, as demonstrated in Figures 1B-C. Additionally, benefiting from the recently established databases of two-dimensional materials, high-throughput calculations integrated with state-of-the-art machine learning methods greatly streamline the design of novel materials and the optimization of their functional properties toward practical applications.[2]

Taking into account the above four main problems mentioned, i.e., poor stability, low mobility, low conductivity and controllable quality film-making research,[2] defects are probably a key factor correlated with all these problems. DOS, a typical kind of defect density, has been regarded as an important parameter for many III-V and 2D materials.[4] On one hand, the channel carrier density is increased, attributed to DOS, which enhances the channel current of 2D materials.[4] On the other hand, defects relate to reliability and stability issues. DOS characterization is obviously important for better understanding and hence control of the performance and stability of III-V and 2D materials devices. A skematic of DOS distribution along the energy bandgap extracted by our proposed dual-gate pulse spectroscopy (GPS) method is demonstrated as Figure 1D.

METHODS FOR DOS MEASUREMENT

There are a lot of measurement methods for DOS extraction, as listed in Figure 1E, which are of importance for giving a precise model in predicting the transistor electrical properties and to give a guideline to design and process optimization.[5] In general, the models for DOS are proposed in two main types of equations, i.e., an exponential model on the band edge which refers to the types of tail states that were regarded to be originated from structure disorder with localized tail states and a Gaussian distribution model in the deep level energy bandgap which corresponds to the oxygen vacancies types. One primary and simple but indirect method is the extraction of DOS based on the proposed DOS model and measured DC IV curve. According to the DOS model including both the tail states model for the structure disordered defects and the midgap model for the oxygen vacancies defects, the key parameters of DOS model as well as the DOS values could be achieved by comparing and fitting the IV model including DOS models with the measurement results of IV characteristics, However, this method is not a direct method but an indirect method to extract DOS. One IV curve could have different DOS values and key parameters when fitting the DOS model and IV model with the measurement IV curve. Another method is the CV curve. By measuring CV curves, the measurement could give the result of low frequency DOS. However, it is regarded to be very complex. A general method is deep level transient spectroscopy (DLTS),[5] which is even used in commercial equipment. The general principle is to measure the transient capacitance and extract the different transient capacitance between a fixed interval of two measurement time in sequence. In this method, temperature changing is mainly involved. As illustrated in the Figures 1C, high temperature environment and equipment would lead to transistor properties change and thus DOS change. Another way is using photo spectroscopy, i.e., measurement involving light. However, adding light could lead to the photo persistent conductivity (PPC) effect. This means the photo involvement effect could lead



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Methods	Transient Dual Gate Pulse Spectroscopy(GPS)	C-V	DLTS	Photo Spectroscopy	DC I-V
Reference	Dai's group Scientific Reports 6, 24096 (2016)	Kimura's group Appl. Phys. Lett. 92, 133512 (2008)	Semetrol Co. J. Appl. Phys. 45, 3023-3032 (1974)	Shimadzu Co. Appl. Phys. Lett. 92, 202117 (2008)	Fung's group J. Appl. Phys. 106, 084511 (2009)
Frequency	Adjustable	<1 Hz	Single	/	/
Light	Unneeded	Unneeded	Unneeded	Needed	Unneeded
Temperature	Unneeded	Unneeded	77-500 K	Unneeded	Unneeded
Timing	Short	Long	Short	Long	Long
Precision	Better				

Figure 1. Schematic illustrations of semiconductor materials with DOS characteristics and DOS extraction methods (A) 2D Materials.[1] (B) The comparison of the new SiC MOSFET with the failed SiC MOSFET with metallographic MOSFET.[3] (C) Cyclic short circuit test platform for SiC.[3] (D) Schematic and illustrated diagram of DOS distribution along the energy bandgap. (E) Comparison of present representative methods for the DOS extraction.

to a redistribution of DOS and thus a different conductivity. Charge pumping method is regarded to be less susceptible to gate leakage. However, it could only be used to measure a value of the interface trap density, whereas other characteristics could not be gained.

Some recent methods proposed to extract DOS are the pulse method, especially our proposed GPS shown in Figure 1E.[5] By comparing CV method and the pulse method, the latter could be more suitable for characterizing a transistor sample working under high frequency conditions. Taking the frequency dependence of DOS values, a transient measurement is required. Given the transient measurement conditions, the noise arising during the transient measurement environment should be taken into account. By comparing DC IV method and the pulse method, the latter could be used to measure the transistor in an AC working condition more precisely than that with DC IV methods, because DOS has a frequency dependence which means DOS measured in a high frequency way is different from DOS measured in a DC way. Pulse methods are also superior to CV in simplicity, to DLTS in overcoming the temperature involvement and to photo spectroscopy without light involvement. Therefore, compared with other methods, pulse methods considering transient noise reduction are preferred. In a pulse method, DOS in 2D materials transistors could be extracted properly and hence understood and modeled for the prediction of electrical characteristics more precisely. As a consequence, the 2D materials transistors could be more likely to find a tradeoff of DOS, neither too high for the device to show a poorer stability, nor too low for the channel to have enough carrier density.

As shown in the Figure 1E, a comparative analysis of five primary methods for characterizing DOS in 2D materials is presented, highlighting their key operational parameters and requirements.

Here, the fundamental working principle of method GPS could be found in our previous paper as shown in Figure 1E. The GPS could overcome the temperature-dependent limit of present commercial DLTS method, and the light-dependent PPC effect or DC limit of other methods.

CONCLUSION

The characterization results obtained from GPS and other methods provide a solid foundation for developing practical stability enhancement strategies. The frequency-dependent DOS extracted by GPS can guide the selection of optimal passivation materials and annealing temperatures: traps with short response times (high frequency) require different treatments than slow traps. Thus, DOS characterization is not merely an evaluation tool but a core enabler for achieving the necessary trade-off between device performance and long-term reliability.

REFERENCES

1. Yang W. and Dong F. (2025). Degradation breakthrough of stabilized compounds with C-F bonds. *Innova. Mater.* **3**:100142. DOI:10.59717/j.xinn-mater.2025.100142
2. Zou X., Yong Xu, Wenhui Duan, et al. (2021). 2D materials: Rising star for future applications. *The Innovation* **2**:100115. DOI:10.1016/j.xinn.2021.100115
3. Zhang P., Yang Y. (2024). The operating life of a wide-bandgap power device over a wide temperature range. *The Innovation Energy* **1**(2):100017. DOI:10.59717/j.xinn-energy.2024.100017
4. Cao W., Bu H., Vinet M., et al. (2023). The future transistors. *Nature* **620**:501–515. DOI:10.1038/s41586-023-06145-x
5. Zou X., Yang J., Qiao Q., et al. (2023). Trap characterization techniques for GaN-based HEMTs: A critical review. *Micromachines,* **14**:2044. DOI:10.3390/mi14112044

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AUTHOR CONTRIBUTIONS

All authors contributed to the manuscript and approved the final version.

DECLARATION OF INTERESTS

The authors declare no competing interests.