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One-dimensional van der Waals materials–Advent of a new research field

Cite as: Appl. Phys. Lett. **121**, 040401 (2022); doi: 10.1063/5.0108414 Submitted: 8 July 2022 · Accepted: 9 July 2022 · Published Online: 25 July 2022

Alexander A. Balandin,^{1,a)} (D Roger K. Lake,¹ (D and Tina T. Salguero² (D

AFFILIATIONS

¹Department of Electrical and Computer Engineering, Materials Science and Engineering Program, University of California, Riverside, California 92521, USA

²Department of Chemistry, University of Georgia, Athens, Georgia 30602, USA

Note: This paper is part of the APL Special Collection on One-Dimensional van der Waals Materials. ^{a)}Author to whom correspondence should be addressed: balandin@ee.ucr.edu

https://doi.org/10.1063/5.0108414

Investigations of the unique electrical, thermal, and optical properties of graphene have generated tremendous progress in fundamental and applied sciences.¹⁻⁵ The advent of graphene stimulated the search for other two-dimensional (2D) van der Waals atomic crystals with properties distinct from their corresponding bulk forms. A large number of materials in the family of transition metal dichalcogenides (TMDs) have weak van der Waals bonding between 2D structural units, allowing for exfoliation to quasi-2D layers. Other, less wellresearched classes of van der Waals materials have one-dimensional (1D) or quasi-1D structural units.⁶⁻¹⁵ Some of these, like TaSe₃, are quasi-1D in the sense that they have strong covalent bonds in one direction along the atomic chains and weaker bonds in the perpendicular plane.⁸ Other materials, like ZrTe₃, can be considered intermediate 2D/1D-type based on structure and properties.^{11,16} Yet, others are best considered true-1D materials; these have covalent bonds only along the atomic chains and much weaker van der Waals interactions in perpendicular directions.¹⁶ We consider both quasi- and true-1D examples to be "1D materials," especially if they are exfoliated or grown into individual atomic chains or atomic threads comprising just a few chains. It is important to note that the true- and quasi-1D van der Waals materials are fundamentally different from "nanowires" or "quantum wires"-understood to be nanostructures of conventional covalent or ionic semiconductors or metals. Such nanowires have larger diameters and lack the atomically sharp interfaces of van der Waals materials. Furthermore, owing to their crystal structures, covalent nanowires cannot be downscaled to individual atomic chains.

Machine learning studies suggest the existence of hundreds of 1D van der Waals materials with bandgaps ranging from metallic to insulating.¹⁸ One prominent group is the transition metal trichalcogenides (TMTs) with the formula MX₃ (where M = Mo, W, etc.; X = S, Se, Te). In the monoclinic crystal structure of TaSe₃, for example, the

trigonal prismatic TaSe₃ units form continuous chains extending along the *b*-axis and creating needlelike crystals.^{8,17} The TMT crystals exfoliate into chain structures, unlike TMDs that exfoliate into atomic planes. It is feasible that van der Waals crystals can be exfoliated or grown into atomic chains with cross-sectional dimensions of $\sim 1 \times 1 \text{ nm}^{2.16,19,20}$ The first studies of the exfoliated metallic TMT bundles discovered exceptionally high breakdown current densities in such materials, exceeding those in Cu and other elemental metals by more than an order of magnitude.^{8,11,16} A key characteristic of 1D van der Waals bundles or chains is that they can be well-ordered, singlecrystalline, in one direction, and have few or no dangling bonds. Some of these materials have revealed unusual properties related to strongly correlated quantum phenomena, e.g., charge density waves and topological effects.¹⁶ Related work has demonstrated that composites with fillers comprised of 1D van der Waals materials have exceptional electromagnetic shielding efficiency.^{21,22} These recent developments suggest that continued reduction in dimensionality to individual atomic chains can bring exciting prospects at the ultimate limit of material downscaling. This perspective motivated this timely Special Topic Issue with contributions focused on developments related to onedimensional van der Waals materials.²

As an entirely new field, one-dimensional van der Waals materials encompass interdisciplinary work by physicists, chemists, materials scientists, and engineers. Therefore, the contributions in the Special Topic Issue span theoretical and computational developments pertinent to the prediction of the stable structures of such materials and their electronic and magnetic properties, as well as experimental studies that illustrate their preparation, properties, and prospects for practical applications.^{23–40} The 1D materials investigated include TMTs like TiS₃, ZrTe₃, and NbS₃;^{25,27,29–31,37} other metal chalcogenide compositions like Ta₂Se₃ and Ta₂Ni₃Se₈;^{33–35} emerging classes of 1D materials like metal halides, e.g., OsCl₄ and Bi₄Br₄, and chalcohalides, e.g., $(TaSe_4)_2I$ and BiSeI;^{23,24,28,32,36,40} and additional 1D systems ranging from elemental selenium to covalent organic framework-carbon nanotube heterostructures.^{26,38,39} Synthetic studies cover preparative techniques, such as alloying, doping, and exfoliation,^{29,33,35} as well as structural studies that demonstrate lattice engineering and clarify issues of polymorphism.^{29,33}

Specific contributions illustrate an ongoing research related to the properties of 1D van der Waals materials. The electronic and magnetic properties of 208 transition metal dihalide and trihalide nanowires are described in Ref. 23; a detailed account of the electronic and magnetic properties of OsCl₄ is provided in Ref. 24. Four papers focus on TiS₃ and its electronic, energy-storage, photonic, and piezoelectric properties.^{27,30,31,37} Its high-electric-field behavior and possible metal-insulator transition are experimentally analyzed in Ref. 37. The photoconductivity of TiS₃, measured over the temperature range of 5 to 300 K, is used to characterize the nature of possible phase transitions to the collective states in Ref. 30. The measured anisotropic piezoresistance of TiS₃ is found to have opposite signs when tensile strain is applied along the chains or perpendicular to the chains;²⁷ a high specific capacitance is measured for TiS3 used as a positive electrode in a supercapacitor device.³¹ Several contributions focus on optoelectronic properties. It was found that the photo-response of BiSeI is significantly enhanced in mechanically exfoliated thin wires compared to that of the bulk.²⁸ The predicted 1D topological insulator Bi_4Br_4 can be used as a saturable absorber integrated with a laser allowing modelocking at the near-infrared with sub-picosecond pulse duration.³⁶ Recently, there was considerable excitement over possible strong longitudinal magnetoresistance interpreted as evidence of axionic charge density waves in (TaSe₄)₂I. This issue is addressed in Ref. 40. Different physical mechanisms are discussed, and further experiments are proposed to probe the nature of the charge density wave state in (TaSe₄)₂I. This brief recount of the intriguing properties of 1D van der Waals materials should provide sufficient motivation for further browsing and perusal of this Special Topic Issue by interested readers.

In conclusion, this Special Topic Issue provides a glimpse of new, vibrant, and innovative research associated with 1D van der Waals materials. These contributions are defining this new field as it materializes from long-standing, broader interest in low-dimensional systems. Exciting progress is happening at a rapid pace, and we anticipate that this Issue will be relevant and interesting for many researchers.

We would like to thank all authors who contributed to this Special Topic issue of *Applied Physics Letters*. Special thanks go to Professor Lesley F. Cohen, Editor-in-Chief, for her attention to this Special Topic issue and her valuable suggestions and input. We also acknowledge Dr. Jenny Stein, Journal Manager, and Jaimee-Ian Rodriguez, Editorial Assistant, of *Applied Physics Letters* for their help in the preparation of this issue. A.A.B. acknowledges the support of the Vannevar Bush Faculty Fellowship from the Office of Secretary of Defense (OSD), under the Office of Naval Research (ONR) Contract No. N00014-21-1-2947, and the National Science Foundation (NSF) program Designing Materials to Revolutionize and Engineer our Future (DMREF) via Project No. DMR-1921958 entitled Collaborative Research: Data-Driven Discovery of Synthesis Pathways and Distinguishing Electronic Phenomena of 1D van der Waals Bonded Solids. The research work for these two projects inspired and motivated the proposal for the present Special Topic Issue.

AUTHOR DECLARATIONS

Author Contributions

Alexander A. Balandin: Conceptualization (equal). Roger K. Lake: Conceptualization (equal). Tina T. Salguero: Conceptualization (equal).

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