Mechanics of Materials 91 (2015) 382–398

Contents lists available at ScienceDirect

Mechanics of Materials

journal homepage: www.elsevier.com/locate/mechmat

Strain effects on thermoelectric properties of two-dimensional materials

Gang Zhang *, Yong-Wei Zhang *

*Institute of High Performance Computing, A*STAR, Singapore*

ARTICLE INFO

Article history:
Received 29 December 2014
Received in revised form 9 March 2015
Available online 2 April 2015

Keywords:
Strain effects
Thermoelectric
Two-dimensional materials

ABSTRACT

Two-dimensional (2D) materials, such as graphene, hexagonal boron nitride (hBN), phosphorene, transition metal dichalcogenides (e.g., MoS_2, WS_2, etc.), metal oxides (e.g., MoO_3) have attracted much attention recently due to their extraordinary structural, mechanical and physical properties. In particular, 2D materials have shown great potential for thermal management and thermoelectric energy generation due to their fascinating electrical and thermal transport properties, which can lead to a significantly large figure-of-merit. Also due to their large stretchability, 2D materials are promising for using strain engineering to tune and modulate their electronic and thermal properties, which can further enhance their figure-of-merit. In this article, we give a review on the recent advances in the study of strain-engineering on the thermoelectric properties of 2D materials. We first review some important aspects in thermoelectric effects, such as Peltier effect, Seebeck effect, the coefficient of performance and figure-of-merit (ZT) and discuss why 2D materials are ideal candidates for thermal management and thermoelectric applications. We then briefly discuss the strain (stress) generation in 2D materials and their structure integrity under strain (stress). Next, we discuss how strain affects the electronic properties of 2D materials, followed by the discussion on the effects of strain on the thermal properties of 2D materials. Subsequently, we discuss the strain effects on two important thermoelectric properties, Seebeck coefficient and figure-of-merit ZT. Finally, we present our conclusions and future perspective.

1. Introduction

Energy shortage is likely to be a great challenge in the near future to our society. The world's energy demands are expected to rise 60% by 2030. Today, approximately 80% of the world's energy is generated by heat engines that use fossil fuel as source, which is responsible for a large fraction of carbon dioxide (CO_2) emission worldwide. These heat engines typically operate at a 30–40% efficiency (Yazawa and Shakouri, 2011). This means that roughly 10 TW of heat is lost to the environment. Hence, by enhancing the utilization efficiency of heat engines and/or converting the waste heat back to useful energy, it is possible that we can solve the global energy shortage crisis. Thermoelectric modules are able to convert heat directly into electricity, which can lead to an increase in the utilization efficiency and a reduction in the usage of fossil fuels and also carbon emission.

The rapid growth in high-performance integrated circuits (ICs) demands a faster switching speed, larger number of transistors and higher integration density (Moore, 1998). This in turn leads to a dramatic increase in power dissipation and heat generation, which causes a large number of heat concentrated zones (called hotspots).

---

* Corresponding author.

E-mail addresses: zhangg@ihpc.a-star.edu.sg (G. Zhang), zhangyw@ihpc.a-star.edu.sg (Y.-W. Zhang).

http://dx.doi.org/10.1016/j.mechmat.2015.03.009
0167-6636/

It is known that the majority of the thermal power dissipated in ICs arises from signal switching. As the clock frequency continues to climb, the power consumption in the chips is rapidly becoming unmanageable. The heat dissipation issue is becoming crucial for ICs, which can cause degradation in device performance, increase junction leakage, and accelerate electromigration and other failure modes. In fact, power dissipation issue has recently become one of the greatest challenges for modern integrated electronics, which limits the performance of electronics from handheld devices to massive data centers (Goodson and Ju, 1999). For instance, the energy use for information technology infrastructure in the United States is currently in excess of 20 GW, or 5–10% of the total annual national capacity (ITRS, 2001). Currently, for every kilowatt-hour of energy consumed by a computer in a data centre, another kWh is used for cooling (Pop, 2010). With the application of advanced thermoelectric energy conversion technologies, huge energy saving is expected.

Two-dimensional (2D) materials, including graphene, hexagonal boron nitride (hBN), phosphorene, transition metal dichalcogenides (e.g., MoS_2, WS_2, etc.), metal oxides (e.g., MoO_3) have attracted much attention recently due to their extraordinary structural, mechanical and physical properties, with great interest in both fundamental science and engineering applications (Fiori et al., 2014). The value of bandgap in 2D materials ranges from zero (graphene, silicene), to about 0.5–1.0 eV in phosphorene, to about 1.0–2.0 eV in transition metallic dichalcogenides, and to about 3.0–6.0 eV in some metal oxides and hBN. This wide range of bandgap energy available in 2D materials is extremely conducive for developing different types of electronic devices (Blase et al., 1995; Watanabe et al., 2004; Akinwande et al., 2014; Churchill and Jarillo-Herrero, 2014). Recently, 2D heterostructures, for example, graphene/h-BN, graphene/MoS_2, MoS_2/$MoSe_2$, and MoS_2/h-BN, etc., have emerged as a fascinating research topic. Importantly, the possibility of making 2D heterostructures has been demonstrated experimentally (Ponomarenko et al., 2011; Britnell et al., 2012; Haigh et al., 2012; Georgiou et al., 2013; Geim and Grigorieva, 2013; Yu et al., 2013). The basic principle of 2D heterostructures is to stack different monolayers, such as graphene, h-BN, phosphorene, MoS_2 on top of one another in a desirable sequence. The resulting stack represents an artificial material, which may possess unusual physical and chemical properties. Due to their large stretchability, bendability and foldability, these materials are promising for applications in ubiquitous electronics, flexible displays, smart health diagnostics and wearable computing. The applications of 2D materials and 2D heterostructures in thermal management and thermoelectric energy generation are also promising due to their fascinating electrical and thermal transport properties. In addition, the large stretchability of 2D materials enables the direct tuning and modulation of their electronic and thermal properties by applying strain, which provides a viable route to enhance their thermoelectric properties. To construct 2D materials-based thermoelectric devices, the ability to modulate their electronic and thermal properties is highly desired. Strain engineering has been successfully employed to improve the thermoelectric (electronic and thermal) properties of 2D materials (Fiori et al., 2014). To fully realize the potential of 2D materials for applications in thermal management and heat-to-electricity conversion, a comprehensive understanding of strain effect on the electronic, thermal and thermoelectric properties of 2D materials is indispensable.

In this article, we would like to give a review on the recent advances in the study of strain engineering on the electronic, thermal and thermoelectric properties of 2D materials, from both the experimental and theoretical points of view. The rest of this article is organized as follows: Section 2 introduces the basic theory in thermoelectric effects. Section 3 discusses the strain generation and structure stability under strain in 2D materials. Section 4 discusses the effect of strain on the electronic property of 2D materials. Section 5 is devoted to the discussion of strain effects on the thermal property of 2D materials. In Section 6, we address the strain effect on two important thermoelectric properties, Seebeck coefficient and figure-of-merit ZT. Finally, in Section 7, we present the conclusions and brief outlook.

We also note that there exist a number of articles and studies on different aspects of thermal and electronic properties of low-dimensional systems. For comprehensive reviews on thermal properties of nanomaterials, please refer to references (Balandin, 2011; Sadeghi et al., 2012; Cahill et al., 2014; Zhang and Li, 2010; Yang et al., 2012; Zhang and Zhang, 2013). There are also several reviews on anomalous heat transport in low-dimensional systems from the viewpoint of fundamental statistical physics, such as references (Li et al., 2012; Dubi and Di Ventra, 2011; Liu et al., 2012). For reviews on the structure and mechanical properties of 2D materials, please refer to reference (Kostarelos and Novoselov, 2014) for graphene, reference (Sorkin et al., 2014) for MoS_2, and reference (Balendhran et al., 2013) for other 2D materials. Due to the limit of length, we mainly address one of the most fundamental issues here, i.e., the strain effect on the thermoelectric properties of 2D materials.

2. Thermoelectric effects

The thermoelectric effects which underlie heat-to-electricity conversion can be conveniently discussed with reference to the schematic of a thermocouple as shown in Fig. 1a. In a typical thermoelectric device, a junction is formed between two different types of conducting materials, with one being p-type containing positive charge carriers (holes) while the other being n-type containing negative charge carriers (electrons). When an electric current I is passing through the junction, both electrons and holes move away from the junction and carry heat energy Q away, thus cooling the junction, which is called Peltier effect. The ratio of Q to I is defined as the Peltier coefficient, which is in volts. On the other hand, as shown in Fig. 1b, a temperature difference ΔT at the junction causes the carriers to flow away from the junction, leading to an open circuit electromotive force V and thus forming an electrical generator. This is called as Seebeck effect,