Surface Science Reports 65 (2010) 111–127

Contents lists available at ScienceDirect

Surface Science Reports

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

Thermal conductance of the interfaces between the III-nitride materials and their substrates: Effects of intrinsic material properties and interface conditions

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ARTICLE INFO

Article history:
Accepted 29 January 2010
editor: L. Dobrzynski

To Joël, Alexandra Madeleine Marie,
Christian and Hayat

Keywords:
Interface thermal conductance
Phonon transmission
III-nitrides

ABSTRACT

This review is intended to provide a critical and up-to-date survey of the analytical approximation methods that are encountered in interface thermal conductance. Because of the importance of the III-nitride materials for novel technological applications, these methods are applied to the thermal conductance of the interfaces between the III-nitride thin films and their commonly used substrates. The phonon behavior and the probability that a phonon transmits from the III-nitride film to the substrate are described first within the context of two limiting models for the interface thermal conductance. The acoustic mismatch model, which assumes that all the phonons incident to the interface are specularly transmitted or specularly reflected, and the diffuse mismatch model, which assumes that all the phonons incident to the interface are diffusively transmitted or diffusively reflected. We show that these two limiting models give very different results for the thermal conductance of the interface between the III-nitride films and their substrates. Next, a statistical model which describes the reflection of plane waves from rough surface is employed to discriminate between the specularly transmitted phonons and the diffusively transmitted phonons. This model predicts that a reflected plane wave leads to a plane wave in the direction of specular reflection and to a contribution with a finite angular spread about that direction depending on the tangential correlation of the surface asperities. Based upon this result, a new model for the interface thermal conductance, that interpolates between the acoustic mismatch model and the diffuse mismatch model and takes into account, instead the Debye approximation, the detailed phonon spectra of the materials in contact, is developed and applied to the interfaces GaN/Si, GaN/SiC, AlN/Si, AlN/SiC, InN/Si, and InN/SiC. In addition to the phonon wavevector, or alternatively, the phonon energy and the angles of incidence, the probability of the specular transmission and the probability of the diffuse transmissions are taken to depend on the interface roughness and the tangential correlation of the interface asperities. Generally speaking, for the case of interface with zero tangential correlation the interface thermal conductance increases with increasing the interface roughness, whereas for an interface with infinite tangential correlation the interface thermal conductance depends on the mismatch between the phonon densities of states of the materials in contact.

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0167-5729/$ – see front matter © 2010 Elsevier B.V. All rights reserved.
doi:10.1016/j.surfrep.2010.02.001

1. Introduction

The III-nitride materials have long been viewed as promising systems for semiconductor device applications, particularly, optoelectronic [1,2] and thermoelectric devices [3]. However, with the continuous reduction in the size of the optoelectronic devices and their time scales, which requires fast removal of enormous heat, the maximization of the thermal conductivity of the III-nitride-based device becomes extremely important for an efficient thermal-management strategy and system failure prevention [4]. Conversely, for efficient III-nitride thermoelectric devices, the thermal conductivity of the nitride system should be minimized. Therefore, the thermal conductivities of the III-nitride materials have attracted much attention.

In an earlier work, Slack measured the effect of point defects (mainly oxygen impurity) on the thermal conductivity of aluminum nitride (AlN) and reported that the thermal conductivity of AlN can reach at room temperature 3.19 W/cm K [5]. This reported value for AlN thermal conductivity stimulated enormous research to optimize the growth conditions of single crystals and thin films of AlN with an eye toward developing efficient heat sink substrate or deep ultraviolet laser operating in harsh environments [6–15].

On the other hand, the thermal conductivity of gallium nitride (GaN), which is a promising semiconductor for technological application in ultraviolet wavelengths, has been investigated first by Sichel and Pankove. They found that at room temperature the thermal conductivity of GaN is 1.3 W/cm K [16]. Later, Asnin et al. performed high spatial resolution thermal conductivity measurements on different patterned sections of GaN/sapphire (0001) fabricated by lateral epitaxial overgrowth using a scanning thermal microscope. They reported for the GaN thermal conductivity at room temperature a value approximate to 1.7–1.8 W/cm K [17]. The GaN thermal conductivity measured by Asnin et al. agreed with that measured by Luo et al. [18]. However, by performing high spatial/depth resolution thermal conductivity measurements on both fully and partially coalesced GaN/sapphire (0001) samples fabricated by lateral epitaxial overgrowth, Florescu et al. found for the fully coalesced samples thermal conductivity values between 1.86 and 2.05 W/cm K and for the partially coalesced samples thermal conductivity values between 2.00 and 2.10 W/cm K [19]. These values were significantly higher than those reported previously and led to a correlation between low treading dislocation density and high thermal conductivity. Later, this correlation has been proven theoretically [20–22] and experimentally [23–27].

In the case of indium nitride (InN), the values for the thermal conductivity reported in the literature disagreed significantly with each other, probably due to different amounts of crystal defects in the samples investigated. In fact, the phonon lifetime, which is the only determinant of the thermal conductivity of a semiconductor, is due to the combined effects of anharmonic decay, which determines the intrinsic decay, together with defect scattering. As such, Krukowski reported a measured InN thermal conductivity of 0.45 W/cm K which is much below 1.76 W/cm K, the ideal value estimated based on phonon–phonon inelastic scattering calculation [28]. Yamamoto and Yamaguchi performed laser flash measurements on bulk InN. They obtained for the InN thermal conductivity a value of 0.17 W/cm K [29]. So far, unlike the cases of AlN and GaN, the intrinsic thermal conductivity of InN could not be systematically measured.

Indeed, the analysis of the III-nitride materials thermal conductivities contributed significantly to the thermal management of various III-nitride-based devices. However, for the use in technologies, AlN, GaN, and InN are currently heteroepitaxially grown in the form of thin films on several substrates. In the presence of a heat flux across the interface between an III-nitride film and a substrate (case of III-nitride-based active device), there will be a finite thermal boundary resistance which will cause a thermal discontinuity at the interface. The thermal boundary resistance is defined as the ratio of this temperature discontinuity at the interface to the power per unit area flowing across the interface, and will certainly limit the heat dissipation in the device. Therefore, the knowledge of the interface thermal resistance, or alternatively, thermal conductance is of utmost importance for technological applications.

The first developed experiment for measuring the thermal conductance of an interface between two solids is that used by Neeper and Dillinger in 1964; Wolfmeyer, Fox, and Dillinger in 1970; Schmidt and Umlauf in 1976 to measure the thermal conductance of the interface between Indium and sapphire [30–32]. In these experiments, the indium was vapor deposited or ultrasonically soldered onto sapphire rods, the two rods were pressed together with additional indium in between, and the "sandwich" was annealed. Then, the thermal conductance of the interface between the indium and the sapphire was deduced from the measurement of the temperature difference between the two sapphire rods by using thermometers placed very close to the indium film. However, in this measurement technique, the positioning of the thermometers usually is critical. At both sides of the interface, the thermometers must be placed within a phonon mean-free-path length of the interface. This can be easily accomplished at very low temperatures (few tens of Kelvins), where the phonon mean-free-path is relatively large, but not at higher temperatures, where the anharmonic processes decrease the phonon mean-free-path dramatically. Furthermore, if the thermometers scatter phonons so strongly, that they significantly influence the phonon mean-free-path, there may be no reasonable place to put the thermometers. Thus, a contactless measurement technique was extremely needed.

A contactless time-domain thermoreflectance technique was used by Stoner and Maris in 1993; Taketoshi, Baba and Ono in 1999; Stevens in 2005; Lyeo and Cahill in 2006 to measure the thermal conductance of the interfaces between two solids [33–35]. The principle of the time-domain thermoreflectance measurement is that a modulated pump beam is sent to heat up the sample, and changes in the temperature of the thin film are monitored by changes in the intensity of a probe beam which is reflected from the surface. The small changes in the intensity of the reflected probe that are created by the pump beam can be measured by using a lock-in detection as a function of the delay time t between the pump and probe pulses. To a good approximation, the in-phase signal of the reference lock-in amplifier is proportional to the time evolution of the temperature of the film. In Ref. [33–35], only the in-phase signal is analyzed to extract the thermal properties of the sample. However, Lyeo and Cahill [36] noticed that this approach works well when the relaxation rate of the surface temperature is relatively fast, but not when it is slow. In the case of slow relaxation rate of the surface temperature, the authors reasonably argued that a special care is needed to minimize systematic errors created by

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