Molecular dynamics calculations of the cross-plane thermal conductivity of GaAs/AlAs superlattices with rough interfaces.

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A molecular dynamics investigation of the thermal conductivity of superlattices is presented. The interface roughness is modeled using rectangular islands, as in the case of realistic interfaces. Our results confirm the findings of previous studies. When interfaces with heights of two monolayers are considered, the thermal conductivity is higher than that in the case of perfect interfaces.

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I. INTRODUCTION

Superlattices (SLs) are periodic composite structures made of alternating material layers; the periodicities of SLs can reach several atomic layers. Semiconductor superlattices are interesting candidates for efficient thermoelectric energy conversion devices, where low thermal conductance is needed, while the use for lasers requires high thermal conductivity. The control of TC is crucial in several device applications. The GaAs/AlAs SLs are of interest mainly because of their optical properties, and they are used in several devices such as electro-optical modulators [1], optical switching devices [2], and pressure sensors [3].

In general, the TC of SLs is significantly smaller than their bulk constituent values. Simulated cross-plane TC curves of SLs show a minimum for SL periods of 8 to 10 monolayers (MLs), which is in contrast to experimental results [4–10]. This discrepancy between experiment and theory may be because of the quality of the interfaces [4]. The theoretical results are based on a comparison of simulations of smooth-interface SLs in which the TC curve displays a minimum due to miniband formation [8]; this minimum is not observed in the case of rough interfaces. This can explain the absence of a minimum in the TC curve obtained in experiments. Other important parameters that affect this minimum are the ratio between the phonon mean free path and the SL period and the ratio of the lattice constants of the two materials. When the lattice mismatch value is greater than 4%, the minimum in the TC curve disappears [8].

The TC is determined by several parameters such as the periodicity of SLs; the quality

of the interface, which includes factors such as the height and shape of the interfaces; and the coverage of species. Theoretical studies [4, 9] of GaAs/AlAs SLs with smooth interfaces show that the TC decreases and after increases in increasing the SL period reaching a minimum. The TC in the case of SLs with rough interfaces is less than that in the case of SLs with smooth interfaces; further, the minimum in the TC curve is not observed in the former. All previous theoretical investigations have dealt with interfaces with a height of one atomic layer formed by a stochastic distribution of atoms of type A or B. The current study is focused on parameters of SL interfaces that have not been studied, such as interfaces with a height of 2 MLs and the exact shape of interfaces (rectangular). In dielectric or semiconductor materials (in the case of GaAs and AlAs, the electronic contribution to heat transfer is negligible compared to the contribution of phonons to heat transfer), phonons are the main carriers responsible for heat transfer. Thus, a molecular dynamics method may be used to simulate heat transfer.

II. MOLECULAR DYNAMICS METHOD

The nonequilibrium molecular dynamics (NEMD) method is used to investigate the influence of SL periodicity and surface roughness on the TC. Details of the NEMD method can be found in a plethora of articles [11–15]. Using the NEMD or direct method, a temperature gradient is imposed across the structure, and the heat flux is then measured. We use the methodology proposed by Shelling et al. [15], who suggested a method for extrapolating the TC curves for an infinite system size; we plot the inverse of the TC as a function of the inverse of the system size. Periodic boundary conditions are considered in all directions.

Unlike previous studies, we consider that two interfaces do not have same shape (fig. 1). Large islands are formed when an AlAs layer grows on a GaAs layer, whereas small islands are formed when a GaAs layer grows on an AlAs layer [16, 17]. The quality of interfaces is influenced by the atomic mobility of atoms and the exchange mechanisms [18]. A coverage of 50% is considered in this study. Calculations of the TC function the height of interfaces of one and two monolayers have been performed. The interatomic potential model used by us is a simplified model in which two atoms of a unit cell of GaAs or AlAs are represented by a single atom in an fcc lattice [4, 9]. The interactions between the atoms of the two materials are described by the Lennard-Jones (LJ) potential and differ only in their mass (mass ratio is 1.5). The above mass ratio is analogous to the acoustic impedance ratio of AlAs and GaAs.

III. RESULTS AND DISCUSSION

The TC for a LJ system with mass equal to 1 (LJ), $\sigma = \varepsilon = 1$ (LJ) is $\lambda_{m1} = 73.9 \pm 1.5$ (LJ) and for $m_2 = 1.5$ is $\lambda_{m1} = 60.3 \pm 1.5$ (LJ) for average temperature of the system equal to 0.15 (LJ). The TC of SLs with smooth interfaces is reduced to 39.1 (LJ) for an

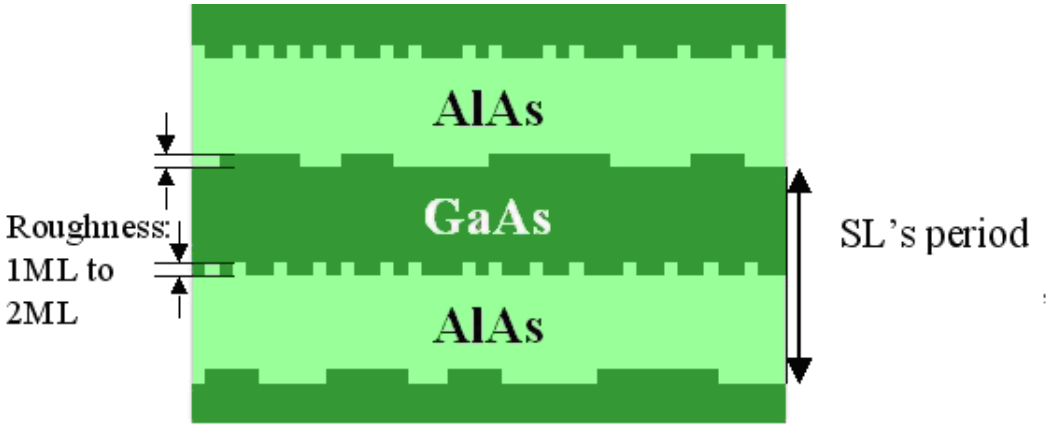

FIG. 1: Schematic representation of GaAs/AlAs SLs with different types of interfaces between GaAs/AlAs and AlAs/GaAs interfaces. The periodicity of interfaces varies between 1 and 20 lattice constants, and the height of the interfaces is considered to be 1 or 2 monolayers (MLs).

SL period of $20a_0$ and to 25.2 (LJ) for an SL period of $2a_0$. The behavior of TC versus the SL periodicity is the same as predicted in previous theoretical studies [4, 9]; the minimum of the TC curve corresponds to an SL period of 4 MLs. After reaching a minimum, the TC increases monotonically with increasing SL period (Fig.2). SLs with rough interfaces with a roughness height of 1 ML and coverage of 50% exhibit a monotonic increase in their TC with an increase in the SL period. This result confirms previous theoretical results [4, 9] and shows that the shape/form of interfaces is not a crucial parameter that affects the behavior of phonons on the interfaces.

In the case of rough interfaces with a height of 2 MLs, unexpected results were obtained for SL periodicities smaller than six lattice constants. The TC curves of these SLs show a maximum for a period of four atomic constants and minimum for a period of six atomic constants; this was an unexpected result. In addition, it was not expected that the TC value of the interface would almost reach the TC values of the constituent materials. In general, defects at the interfaces are considered to cause phonon scattering and therefore to lead to a reduction in thermal conduction. This is in agreement with the simulation results corresponding to a roughness height of 1 ML. However, some studies have stressed that inelastic scattering could enhance energy transport through interfaces [19]. This mechanism could be active in the case of our present simulations and could explain the unexpected behavior of the TC curve for an interface height of 2 MLs. Note that the TC is almost independent of the interface quality for SL periods greater than six or eight lattice constants.

The TC of GaAs/AlAs SLs with smooth and rough interfaces has been studied by the NEMD method. Realistic types of roughness that are in agreement with experimental data have been considered; interfaces with 1-ML- and 2-ML-thick islands have been considered. In the case of the 1-ML-thick islands, previously obtained results were confirmed [4, 9]. Unexpected TC behavior was observed in the case of the 2-ML-thick islands. In SLs with

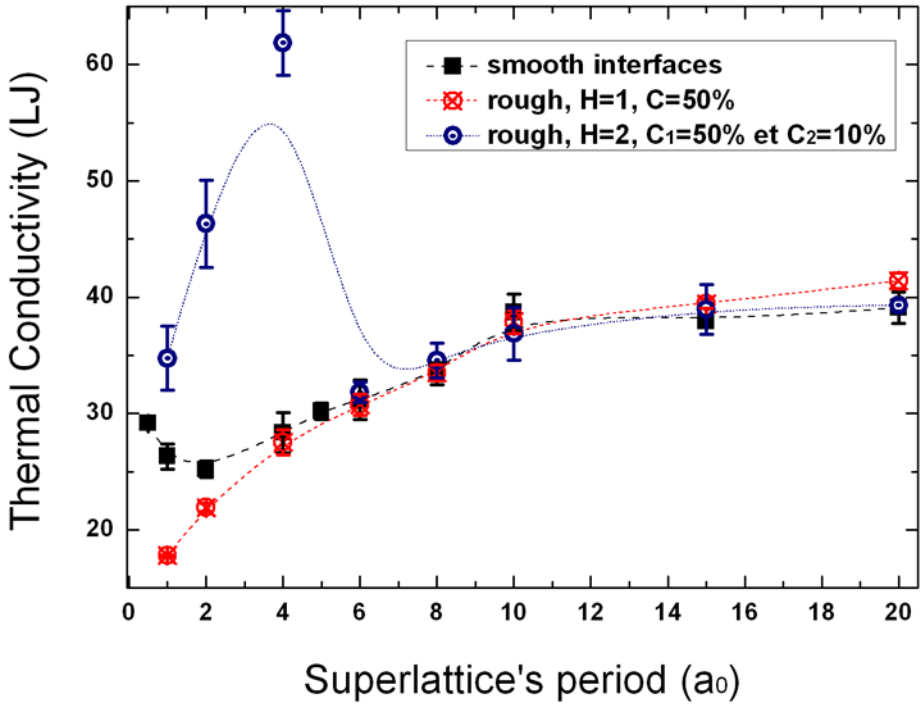

FIG. 2: Thermal conductivity as a function of GaAs/AlAs superlattice period for smooth interfaces (full squares) and for rough interfaces with heights of 1 monolayer (ML) (open red squares) and 2 MLs (open circles).

2-ML-thick islands, the TC versus SL periodicity curve shows a maximum. Competition between different tendencies, arising from different types of roughness, could explain the low sensitivity of TC against interface quality [20]. In future, we plan to explore the influence of the coverage on the cross-plane TC of GaAs/AlAs SLs and phenomena related to the interdiffusion of atoms along the interfaces.

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