Investigation of thermal transport and dislocations in lattice-matched InGaAs/InAlAs superlattices by nonequlibrium molecular dynamics simulations

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InGaAs/InAlAs superlattices are widely used in optoelectronic and thermoelectric devices, such as quantum cascade lasers (QCLs). High thermal conductivity is desired in the active region of QCLs to prevent the accumulation of heat which eventually leads to dislocation formation and catastrophic optical damage [1]. Many factors lower thermal conductivity, among them the slow anharmonic decay of optical phonons, mass-difference scattering, interface roughness, etc.

Mei and Knezevic investigated the thermal conductivity in the binary compounds InAs, GaAs and AlAs and their ternary alloys, $In_xGa_{1-x}As$ and $In_yAl_{1-y}As$ by equilibrium molecular dynamics (EMD) simulations [2]. However, in practice, QCLs often experience significant temperature fluctuations under nonequilibrium conditions owing to thermal runaway mechanisms. These fluctuations can cause certain regions to reach critical temperatures and stresses, leading to the formation of dislocations [3]. Hence, it is worthwhile to investigate this phenomenon using nonequilibrium molecular dynamics (NEMD). We have primarily accurately calculated the thermal conductivity of the InAs, GaAs, AlAs, $In_{0.53}Ga_{0.47}As$ and $In_{0.52}Al_{0.48}As$ at room temperature using the NEMD method and the values were very close to [2]. We were also able to successfully generate dislocations by applying compressive uniaxial strain to $In_{0.53}Ga_{0.47}As/In_{0.52}Al_{0.48}As$ superlattices, as shown in Fig. 1. Zinc blende semiconductors are known to show perfect dislocations with $1/2< 110 >$ burgers vectors which glide on $\{111\}$ planes. These perfect dislocations often dissociate into partial dislocations of type $1/6< 112 >$ creating stalking faults in the structure. Both types were observed in the simulation.

Thermal conductivities (TC) of InAs, GaAs, and AlAs, $In_{0.53}Ga_{0.47}As$ and $In_{0.52}Al_{0.48}As$ at room temperature were calculated by NEMD simulations in LAMMPS. The system, with periodic boundaries, was first equilibrated using NVT and NVE ensembles and then Langevin thermostats were applied to impose heat flux. TC for each simulation cell was determined using Fourier's Law, and bulk TC was calculated by extrapolating $1/\kappa$ vs $1/L$ graph as shown in Fig. 2b. Separately, compressive strain at a high strain rate was applied on superlattices made of random alloys of $In_{0.53}Ga_{0.47}As$ and $In_{0.52}Al_{0.48}As$ and dislocations were observed. Tensile strain was also applied to investigate the fracture mechanism.

In conclusion, the goal of this work is to do atomistic modeling of nucleation of dislocations because of nonequilibrium conditions and thermal stress in InGaAs/InAlAs superlattices. From primary simulations, it is clear that the binary potentials produce accurate results for thermal conductivity at nonequilibrium conditions and the superlattices also show the right type of dislocations under strain.

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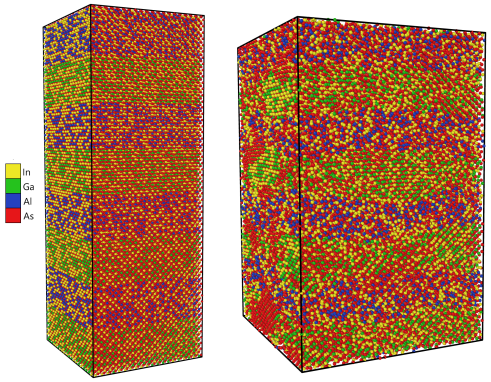

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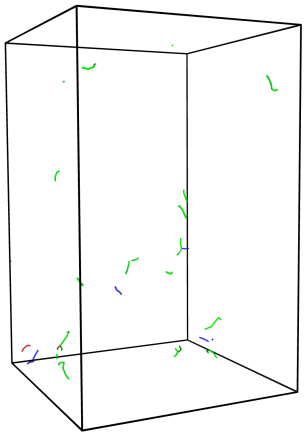
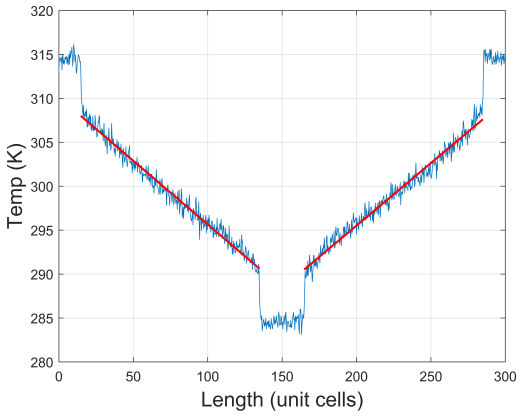


(b)

Fig. 1: Nucleation of dislocations in $In_{0.53}Ga_{0.47}As/In_{0.52}Al_{0.48}As$ superlattice by compressive strain at 800K. (a) A sample of $In_{0.53}Ga_{0.47}As/In_{0.52}Al_{0.48}As$ superlattice (left) and its strained picture (right) rendered in Ovito. (b) 1/2$<$ 110 $>$ (blue) 1/6$<$ 112 $>$ (green) type dislocations shown by dislcoation analysis (DXA) in Ovito.



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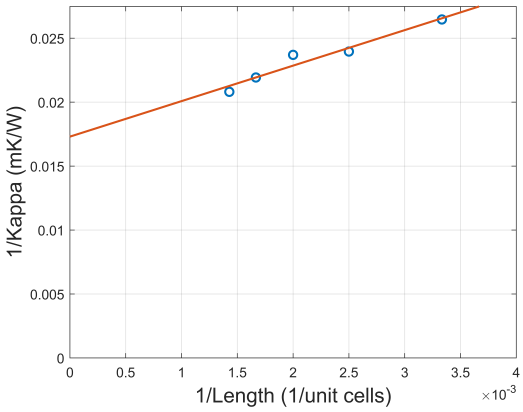

(b)

Fig. 2: Thermal conductivity calculation at room temperature by NEMD. (a) Sample steady-state thermal profile for a GaAs sample. (b) Variation of $1/\kappa$ with $1/L$ for GaAs at room temperature.