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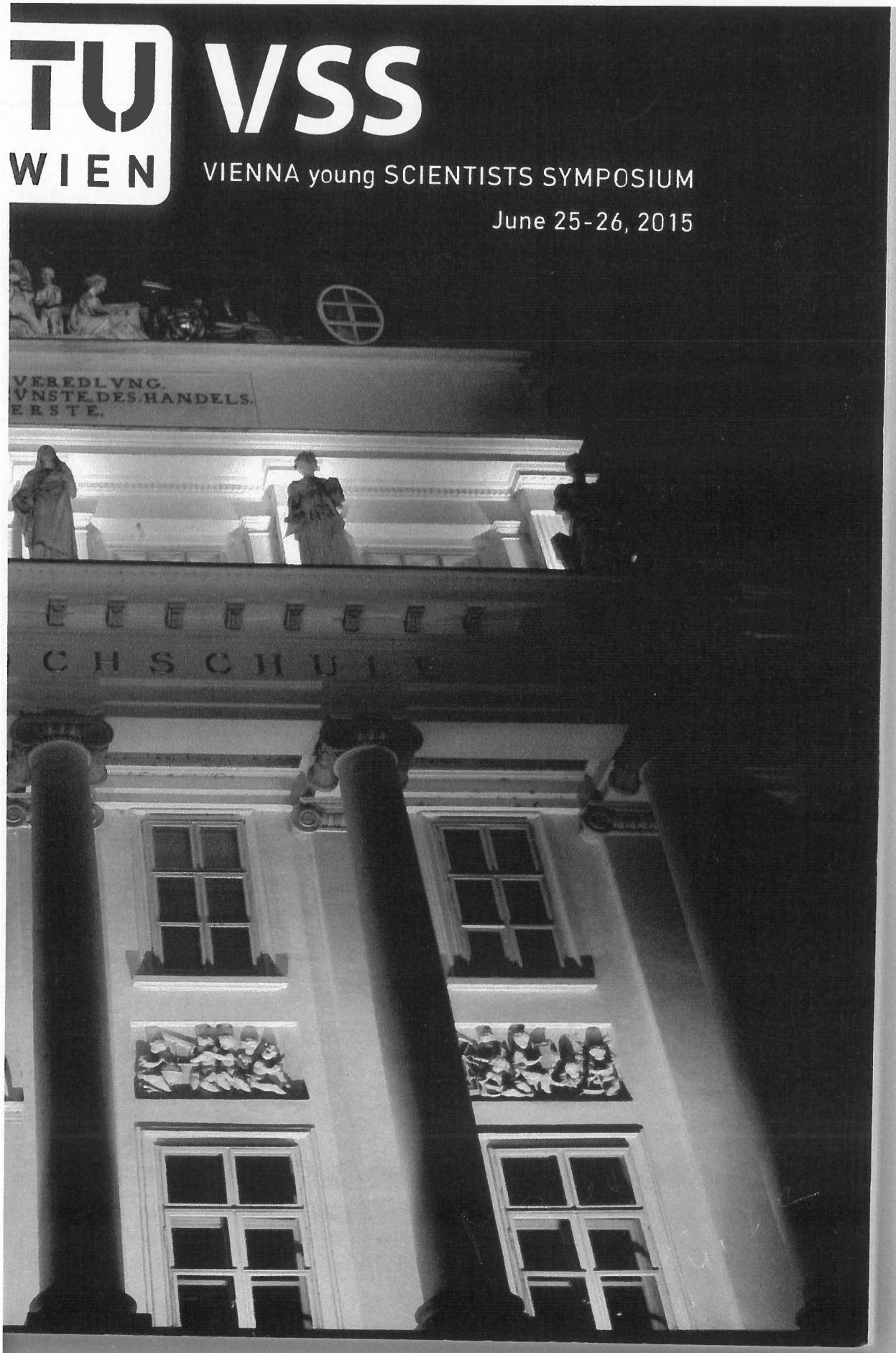

ATOMISTIC MODELING OF III-V SEMICONDUCTOR INTERFACES

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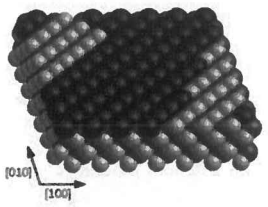
We investigate interfaces between III-V semiconductors using atomistic modeling, enabling us to determine the interface energy and the strain in each atomic layer.

INTRODUCTION

Quantum mechanical modeling of semiconductor superlattice-based devices, like quantum cascade lasers (QCLs), is a very challenging task. Simulations however are necessary to analyse and retrace the interface roughness, which were found to lead to additional scattering and therefore to a reduced device performance [1]. A very powerful tool are atomistic simulations, making it possible to study interface roughness or strain distributions. The insights found in these simulations allow more detailed models, which in return will lead to improved growth parameters and device designs.

METHOD & RESULTS

In the used model the lattice of single III-V semiconductor materials or even complete heterostructures is generated. Chemical bonds are modeled with simplified empirical potentials, which allow larger simulation cells compared to ab-initio methods, but preserve the crystal lattice [2], [3]. The generated structure is then relaxed using a Metropolis Monte Carlo solver. This model was shown to reproduce experimental data for elastic parameters and bond lengths in ternary III-V alloys with good accuracy [4], [5].
When observing e.g. the material system GaSb/InAs, the interface can either be formed by Ga-As or In-Sb type bonds and therefore build up a significant amount of strain, which limits the total layer thickness. Since the individual layers are only a few nanometers thick, their electronic properties are highly influenced by the strain at the interfaces. In our model we therefore analyse the strain distribution in such heterostructures with different bond configurations at the interfaces (see Fig. 1a).
Furthermore, we analyse different in-plane roughness patterns with respect to their total energy. Preliminary data show that structures with the lowest energy values have continuous lines of atoms in the [110] direction separated by trenches like the one shown in Fig. 1b. This clearly resembles reconstruction patterns during epitaxial growth.



(a) (b)

Fig. 1. Simulation Results: (a) strain in growth direction for an InAs/GaSb heterostructure, the first two traces show a differing share of As in the second interface plane i.e. 0 % (*0% As*) and 100 % (*100% As*), the last trace (*1 ML roughness*) shows an interface roughness of one ML at the second interface, data are offset for better clarity (a) GaSb/InAs interface showing continuous lines of atoms in the [110] direction (elements In-Sb-Ga from darkest to brightest)

Conclusion

Interfaces between III-V semiconductor layers are a very important, yet not fully understood part of superlattice structures. Our atomistic model allows detailed insight into different bond configurations as well as the strain distribution in heterostructures. Recent results indicate that the optimal interface structure consists of elongated features along the [110] direction, similar to reconstruction patterns during epitaxial growth. In future research we will extend this approach to other material combinations and more complex structures consisting of several layers and interfaces.

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